Grating Diffraction Calculator (GD-Calc®) – Coupled-Wave Theory for Biperiodic Diffraction Gratings

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1. Introduction

GD-Calc computes diffraction efficiencies of a biperiodic grating structure comprising linear, isotropic, and non-magnetic optical media. Part 1 of this document defines the class of optical geometries that can be modeled with GD-Calc, describes the electromagnetic field characteristics, and provides a conceptual framework for the software user interface. Part 2 describes the numerical algorithms used in the software.

The grating diffraction theory developed in Part 2 is based on a generalization of the rigorous coupled-wave (RCW) method reviewed in Ref. 1. The general biperiodic grating theory has some commonality with the coupled-mode method described in Ref. 2 (e.g., the use of S-matrices [Ref. 3] and Fast Fourier Factorization [Ref. 4]), but the grating is described relative to a rectangular coordinate system in which only one of the grating period vectors need be aligned to the coordinate axes.

Part 1: User's Reference

2. Notation:

(…)	grouping parentheses, matrices
[…]	function arguments, superscript indices and annotation
{…}	set
$\hat{e}_1$, $\hat{e}_2$, $\hat{e}_3$	unit basis vectors
$\vec{x} = \hat{e}_1 x_1 + \hat{e}_2 x_2 + \hat{e}_3 x_3$	position vector
$\vec{f} = \hat{e}_1 f_1 + \hat{e}_2 f_2 + \hat{e}_3 f_3$	spatial frequency vector
$\vec{E} = \hat{e}_1 E_1 + \hat{e}_2 E_2 + \hat{e}_3 E_3$	electric field vector
$\vec{H} = \hat{e}_1 H_1 + \hat{e}_2 H_2 + \hat{e}_3 H_3$	magnetic field vector
ε	complex permittivity
I	identity matrix
0	zero matrix or vector

3. Grating geometry

The biperiodic grating structure shown in Figure 1 will be used to illustrate the types of geometries that can be modeled with GD-Calc. The grating comprises square-section bars that are stacked to form an array of "#" structures. Only four such structures are shown, but the pattern extends periodically in two dimensions.

Position vectors are denoted $\vec{x} = \hat{e}_1\, x_1 + \hat{e}_2\, x_2 + \hat{e}_3\, x_3$, where $\hat{e}_1$, $\hat{e}_2$, and $\hat{e}_3$ are orthonormal unit basis vectors. The grating structure is represented as a stack of grating strata bounded by planes of constant x_1, with boundaries at $x_1 = b_1^{[0]}, b_1^{[1]}, \ldots$:

$$b_1^{[l_1-1]} < x_1 < b_1^{[l_1]} \text{ in stratum } l_1;\; l_1 = 1 \ldots L_1 \tag{3.1}$$

L_1 is the number of strata. (The "l_1" index is generally used as a stratum identifier.) The strata do not necessarily represent physically distinct layers with different material compositions. Typically, the grating is partitioned into strata in order to approximate sloped-wall layers by "staircase" profiles[1]. The grating is sandwiched between a substrate medium below the grating and a superstrate medium (e.g., vacuum) above the grating. In accordance with Eq. 3.1, the substrate and superstrate are considered to be semi-infinite strata defined by

$$-\infty = b_1^{[-1]} < x_1 < b_1^{[0]} \text{ in the substrate} \tag{3.2}$$

$$b_1^{[L_1]} < x_1 < b_1^{[L_1+1]} = +\infty \text{ in the superstrate} \tag{3.3}$$

Note that the x_1 coordinate increases toward the superstrate side of the grating and the strata are numbered from bottom (substrate) to top (superstrate). Incident illumination enters from the superstrate side and is downward-directed.

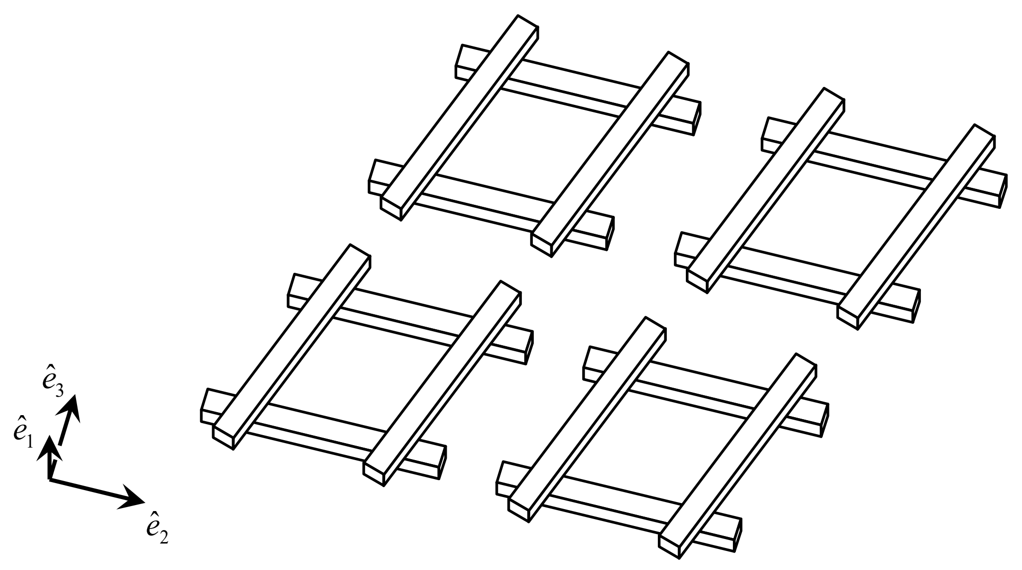

Figure 1. Biperiodic grating structure.

[1] Stratification of sloped-wall profiles should be used with caution. Increasing the number of strata might not improve (and could actually degrade) calculation accuracy unless the number of diffraction orders is also significantly increased. This limitation of coupled-wave theory is discussed in Ref. 1, Sect. VI.5.

The grating comprises isotropic, non-magnetic optical media, so its optical properties are fully characterized by its scalar, complex permittivity ε as a function of $\vec{x}$. This is the relative permittivity, equal to the square of the complex refractive index. ε is 1 in vacuum, and according to the assumed sign conventions the imaginary part of ε is non-negative,

$$\mathrm{Im}[\varepsilon] \ge 0 \tag{3.4}$$

The grating is characterized by two fundamental vector periods, $\vec{d}_1^{[g]}$ and $\vec{d}_2^{[g]}$, which describe the permittivity function's translational symmetry characteristics. These vectors are parallel to the substrate and have the following coordinate representations,

$$\vec{d}_1^{[g]} = \hat{e}_2\, d_{2,1}^{[g]} + \hat{e}_3\, d_{3,1}^{[g]} \tag{3.5}$$

$$\vec{d}_2^{[g]} = \hat{e}_2\, d_{2,2}^{[g]} + \hat{e}_3\, d_{3,2}^{[g]} \tag{3.6}$$

The vectors are linearly independent,

$$d_{2,1}^{[g]}\, d_{3,2}^{[g]} \ne d_{3,1}^{[g]}\, d_{2,2}^{[g]} \tag{3.7}$$

The permittivity is invariant with respect to translational displacement by either vector $\vec{d}_1^{[g]}$ or $\vec{d}_2^{[g]}$,

$$\varepsilon[\vec{x} + \vec{d}_1^{[g]}] = \varepsilon[\vec{x}] \tag{3.8}$$

$$\varepsilon[\vec{x} + \vec{d}_2^{[g]}] = \varepsilon[\vec{x}] \tag{3.9}$$

For example, Figure 2 illustrates a plan view of the Figure 1 structure, showing the fundamental periods $\vec{d}_1^{[g]}$ and $\vec{d}_2^{[g]}$.

$\varepsilon[\vec{x}]$ is constant outside of the grating structure, with a value $\varepsilon^{[\mathrm{sub}]}$ in the substrate and $\varepsilon^{[\mathrm{sup}]}$ in the superstrate, and it is independent of x_1 within each stratum. The top boundary coordinate for stratum l_1 (or for the substrate, if $l_1 = 0$) is denoted as $b_1^{[l_1]}$ (cf. Eq's. 3.1-3.3),

$$\varepsilon[\vec{x}] = \varepsilon 1^{[l_1]}[x_2, x_3] \quad \text{for } b_1^{[l_1-1]} < x_1 < b_1^{[l_1]} \tag{3.10}$$

$$\varepsilon 1^{[0]}[x_2, x_3] = \varepsilon^{[\mathrm{sub}]} \tag{3.11}$$

$$\varepsilon 1^{[L_1+1]}[x_2, x_3] = \varepsilon^{[\mathrm{sup}]} \tag{3.12}$$

(The x_1 independence of $\varepsilon 1$ implies that the grating walls are perpendicular to the substrate within each stratum – hence the "staircase" approximation.) Based on Eq's. 3.8 and 3.9, $\varepsilon 1$ satisfies the periodicity conditions

$$\varepsilon 1^{[l_1]}[x_2 + d_{2,1}^{[\mathrm{g}]}, x_3 + d_{3,1}^{[\mathrm{g}]}] = \varepsilon 1^{[l_1]}[x_2, x_3] \tag{3.13}$$

$$\varepsilon 1^{[l_1]}[x_2 + d_{2,2}^{[\mathrm{g}]}, x_3 + d_{3,2}^{[\mathrm{g}]}] = \varepsilon 1^{[l_1]}[x_2, x_3] \tag{3.14}$$

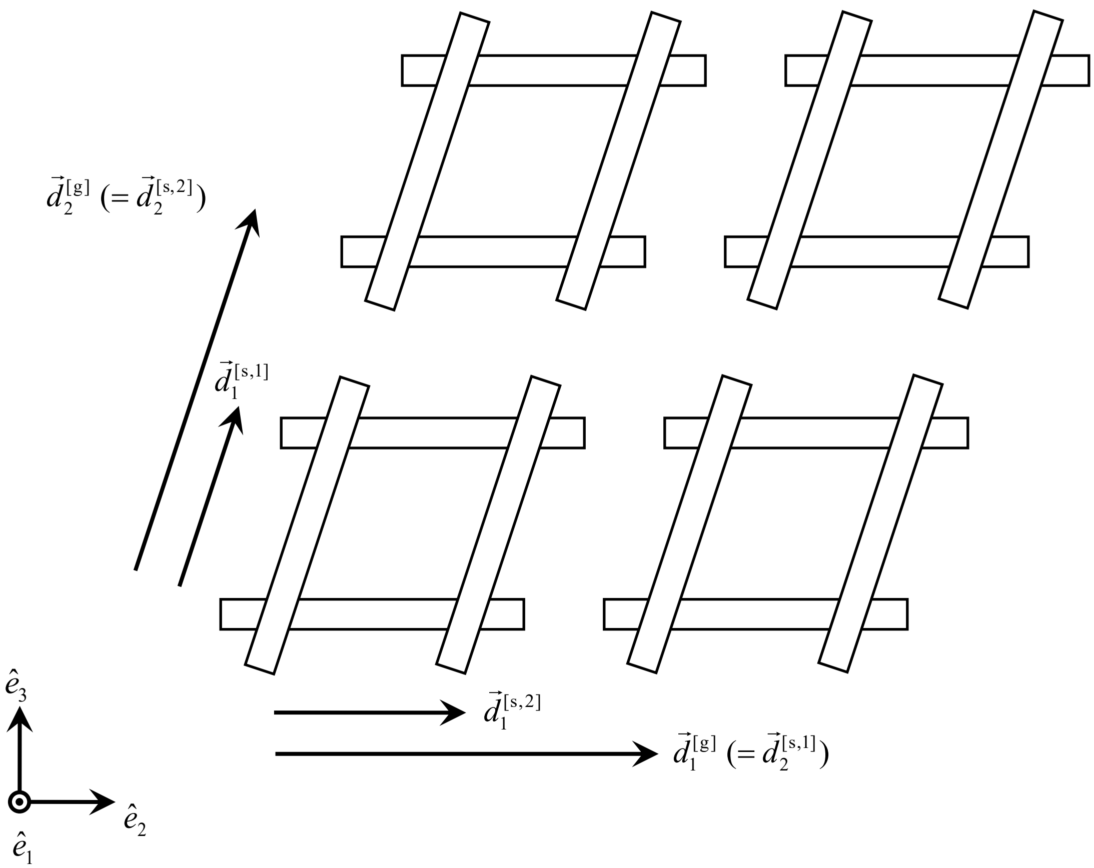

Figure 2. Grating and stratum periods.

Stratum l_1 is characterized by at most two stratum-specific vector periods, $\vec{d}_1^{[\mathrm{s},l_1]}$ and $\vec{d}_2^{[\mathrm{s},l_1]}$ (not necessarily identical to $\vec{d}_1^{[\mathrm{g}]}$ and $\vec{d}_2^{[\mathrm{g}]}$), which are parallel to the substrate and have coordinate representations similar to Eq's. 3.5 and 3.6,

$$\vec{d}_1^{[\mathrm{s},l_1]} = \hat{e}_2\, d_{2,1}^{[\mathrm{s},l_1]} + \hat{e}_3\, d_{3,1}^{[\mathrm{s},l_1]} \tag{3.15}$$

$$\vec{d}_2^{[\mathrm{s},l_1]} = \hat{e}_2\, d_{2,2}^{[\mathrm{s},l_1]} + \hat{e}_3\, d_{3,2}^{[\mathrm{s},l_1]} \tag{3.16}$$

The “ s ” superscript connotes “stratum”. The permittivity in stratum l_1 is invariant with respect to translational displacement by either of these vectors,

$$\varepsilon 1^{[l_1]}[x_2 + d_{2,1}^{[\mathrm{s},l_1]}, x_3 + d_{3,1}^{[\mathrm{s},l_1]}] = \varepsilon 1^{[l_1]}[x_2, x_3] \tag{3.17}$$

$$\varepsilon 1^{[l_1]}[x_2 + d_{2,2}^{[\mathrm{s},l_1]}, x_3 + d_{3,2}^{[\mathrm{s},l_1]}] = \varepsilon 1^{[l_1]}[x_2, x_3] \tag{3.18}$$

These periodicity conditions are stronger than Eq’s. 3.13 and 3.14, which apply to all strata. For example, Figure 2 illustrates periods $\vec{d}_1^{[\mathrm{s},1]}$ and $\vec{d}_2^{[\mathrm{s},1]}$ for stratum 1, and $\vec{d}_1^{[\mathrm{s},2]}$ and $\vec{d}_2^{[\mathrm{s},2]}$ for stratum 2. $\vec{d}_1^{[\mathrm{s},l_1]}$ and $\vec{d}_2^{[\mathrm{s},l_1]}$ could be defined to be respectively equal to $\vec{d}_1^{[\mathrm{g}]}$ and $\vec{d}_2^{[\mathrm{g}]}$ for all strata, but the geometry description is simplified and the electromagnetic simulations are more efficient if $\vec{d}_1^{[\mathrm{s},l_1]}$ and $\vec{d}_2^{[\mathrm{s},l_1]}$ are chosen so that their cross product, $\vec{d}_1^{[\mathrm{s},l_1]} \times \vec{d}_2^{[\mathrm{s},l_1]}$, has the smallest possible magnitude (i.e., the stratum “unit cell” defined by $\vec{d}_1^{[\mathrm{s},l_1]}$ and $\vec{d}_2^{[\mathrm{s},l_1]}$ should preferably have minimal area).

The above description applies to the general case of a “biperiodic stratum” comprising a biperiodic grating structure. There are two special cases of strata that are treated differently than the biperiodic case.

First, a “uniperiodic stratum” comprises a lamellar line grating structure. This type of stratum is characterized by a single period $\vec{d}_1^{[\mathrm{s},l_1]}$, which is (by convention) chosen to be perpendicular to the grating lines. (In this case, $\vec{d}_2^{[\mathrm{s},l_1]}$ is implicitly perpendicular to $\vec{d}_1^{[\mathrm{s},l_1]}$ and is of infinite length.)

Second, a “homogeneous stratum” comprises a homogeneous film, which is not characterized by periods. ($\vec{d}_1^{[\mathrm{s},l_1]}$ and $\vec{d}_2^{[\mathrm{s},l_1]}$ are both implicitly of infinite length.)

Each stratum’s type (biperiodic, uniperiodic, or homogeneous) and associated periods (if any) are defined in terms of the fundamental grating periods, $\vec{d}_1^{[\mathrm{g}]}$ and $\vec{d}_2^{[\mathrm{g}]}$, and four stratum-specific “harmonic indices” $h_{1,1}^{[l_1]}$, $h_{1,2}^{[l_1]}$, $h_{2,1}^{[l_1]}$, and $h_{2,2}^{[l_1]}$ (for stratum l_1). The harmonic indices are integers, which define the stratum’s periods as follows:

For a biperiodic stratum, the matrix of harmonic indices is non-singular,

$$h_{1,1}^{[l_1]}\, h_{2,2}^{[l_1]} \neq h_{1,2}^{[l_1]}\, h_{2,1}^{[l_1]} \quad \text{(biperiodic stratum)} \tag{3.19}$$

and the stratum’s periods are defined by

$$\begin{pmatrix} d_{2,1}^{[\mathrm{g}]} & d_{2,2}^{[\mathrm{g}]} \\ d_{3,1}^{[\mathrm{g}]} & d_{3,2}^{[\mathrm{g}]} \end{pmatrix} = \begin{pmatrix} d_{2,1}^{[\mathrm{s},l_1]} & d_{2,2}^{[\mathrm{s},l_1]} \\ d_{3,1}^{[\mathrm{s},l_1]} & d_{3,2}^{[\mathrm{s},l_1]} \end{pmatrix} \begin{pmatrix} h_{1,1}^{[l_1]} & h_{1,2}^{[l_1]} \\ h_{2,1}^{[l_1]} & h_{2,2}^{[l_1]} \end{pmatrix} \tag{3.20}$$

For example, in Figure 2 the following relations hold: $\vec{d}_1^{[\mathrm{g}]} = \vec{d}_2^{[\mathrm{s},1]} = 2\,\vec{d}_1^{[\mathrm{s},2]}$, $\vec{d}_2^{[\mathrm{g}]} = 2\,\vec{d}_1^{[\mathrm{s},1]} = \vec{d}_2^{[\mathrm{s},2]}$; or equivalently,

$$\begin{pmatrix} d_{2,1}^{[\mathrm{g}]} & d_{2,2}^{[\mathrm{g}]} \\ d_{3,1}^{[\mathrm{g}]} & d_{3,2}^{[\mathrm{g}]} \end{pmatrix} = \begin{pmatrix} d_{2,1}^{[\mathrm{s},1]} & d_{2,2}^{[\mathrm{s},1]} \\ d_{3,1}^{[\mathrm{s}.1]} & d_{3,2}^{[\mathrm{s},1]} \end{pmatrix} \begin{pmatrix} 0 & 2 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} d_{2,1}^{[\mathrm{s},2]} & d_{2,2}^{[\mathrm{s},2]} \\ d_{3,1}^{[\mathrm{s},2]} & d_{3,2}^{[\mathrm{s},2]} \end{pmatrix} \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix} \tag{3.21}$$

Hence, the harmonic coefficients for the two strata are

$$\begin{pmatrix} h_{1,1}^{[1]} & h_{1,2}^{[1]} \\ h_{2,1}^{[1]} & h_{2,2}^{[1]} \end{pmatrix} = \begin{pmatrix} 0 & 2 \\ 1 & 0 \end{pmatrix}, \quad \begin{pmatrix} h_{1,1}^{[2]} & h_{1,2}^{[2]} \\ h_{2,1}^{[2]} & h_{2,2}^{[2]} \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix} \tag{3.22}$$

For a uniperiodic stratum the harmonic indices satisfy the following conditions,

$$h_{1,1}^{[l_1]} \neq 0 \text{ or } h_{1,2}^{[l_1]} \neq 0; \quad h_{2,1}^{[l_1]} = 0 \text{ and } h_{2,2}^{[l_1]} = 0 \quad \text{(uniperiodic stratum)} \tag{3.23}$$

and the period $\vec{d}_1^{[\mathrm{s},l_1]}$ is defined as follows: First compute the spatial frequency quantities

$$\begin{pmatrix} f_{2,1}^{[\mathrm{s},l_1]} & f_{3,1}^{[\mathrm{s},l_1]} \end{pmatrix} = \begin{pmatrix} h_{1,1}^{[l_1]} & h_{1,2}^{[l_1]} \end{pmatrix} \begin{pmatrix} d_{2,1}^{[\mathrm{g}]} & d_{2,2}^{[\mathrm{g}]} \\ d_{3,1}^{[\mathrm{g}]} & d_{3,2}^{[\mathrm{g}]} \end{pmatrix}^{-1} \tag{3.24}$$

and then define

$$\begin{pmatrix} d_{2,1}^{[\mathrm{s},l_1]} & d_{3,1}^{[\mathrm{s},l_1]} \end{pmatrix} = \frac{\begin{pmatrix} f_{2,1}^{[\mathrm{s},l_1]} & f_{3,1}^{[\mathrm{s}.l_1]} \end{pmatrix}}{(f_{2,1}^{[\mathrm{s},l_1]})^2 + (f_{3,1}^{[\mathrm{s}.l_1]})^2} \tag{3.25}$$

For a homogeneous stratum the harmonic indices are all zero,

$$h_{1,1}^{[l_1]} = h_{1,2}^{[l_1]} = h_{2,1}^{[l_1]} = h_{2,2}^{[l_1]} = 0 \quad \text{(homogeneous stratum)} \tag{3.26}$$

The above relations are conceptually simpler when expressed in terms of the grating's spatial frequencies. The grating has two fundamental spatial-frequency vectors $\vec{f}_1^{[\mathrm{g}]}$ and $\vec{f}_2^{[\mathrm{g}]}$, which have the coordinate representations

$$\vec{f}_1^{[\mathrm{g}]} = \hat{e}_2\, f_{2,1}^{[\mathrm{g}]} + \hat{e}_3\, f_{3,1}^{[\mathrm{g}]} \tag{3.27}$$

$$\vec{f}_2^{[\mathrm{g}]} = \hat{e}_2\, f_{2,2}^{[\mathrm{g}]} + \hat{e}_3\, f_{3,2}^{[\mathrm{g}]} \tag{3.28}$$

and which have the following reciprocal relationship to $\vec{d}_1^{[\mathrm{g}]}$ and $\vec{d}_2^{[\mathrm{g}]}$,

$$\begin{pmatrix} f_{2,1}^{[g]} & f_{3,1}^{[g]} \\ f_{2,2}^{[g]} & f_{3,2}^{[g]} \end{pmatrix} \begin{pmatrix} d_{2,1}^{[g]} & d_{2,2}^{[g]} \\ d_{3,1}^{[g]} & d_{3,2}^{[g]} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{3.29}$$

Similarly, each stratum is characterized by its own spatial-frequency basis vectors $\vec{f}_1^{[s,l_1]}$ and $\vec{f}_2^{[s,l_1]}$ (for stratum l_1), which have the same reciprocal relationship to $\vec{d}_1^{[s,l_1]}$ and $\vec{d}_2^{[s,l_1]}$,

$$\vec{f}_1^{[s,l_1]} = \hat{e}_2\, f_{2,1}^{[s,l_1]} + \hat{e}_3\, f_{3,1}^{[s,l_1]} \tag{3.30}$$

$$\vec{f}_2^{[s,l_1]} = \hat{e}_2\, f_{2,2}^{[s,l_1]} + \hat{e}_3\, f_{3,2}^{[s,l_1]} \tag{3.31}$$

$$\begin{pmatrix} f_{2,1}^{[s,l_1]} & f_{3,1}^{[s,l_1]} \\ f_{2,2}^{[s,l_1]} & f_{3,2}^{[s,l_1]} \end{pmatrix} \begin{pmatrix} d_{2,1}^{[s,l_1]} & d_{2,2}^{[s,l_1]} \\ d_{3,1}^{[s,l_1]} & d_{3,2}^{[s,l_1]} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{3.32}$$

For all three stratum types – biperiodic, uniperiodic, and homogeneous – a stratum's basis frequencies are a linear combination (i.e., "harmonics") of the grating's fundamental basis frequencies,

$$\begin{pmatrix} f_{2,1}^{[s,l_1]} & f_{3,1}^{[s,l_1]} \\ f_{2,2}^{[s,l_1]} & f_{3,2}^{[s,l_1]} \end{pmatrix} = \begin{pmatrix} h_{1,1}^{[l_1]} & h_{1,2}^{[l_1]} \\ h_{2,1}^{[l_1]} & h_{2,2}^{[l_1]} \end{pmatrix} \begin{pmatrix} f_{2,1}^{[g]} & f_{3,1}^{[g]} \\ f_{2,2}^{[g]} & f_{3,2}^{[g]} \end{pmatrix} \tag{3.33}$$

(By analogy with crystallography, the basis frequencies represent "reciprocal lattice vectors" and the harmonic indices are analogous to "Miller indices".) For a biperiodic stratum, $\vec{f}_1^{[s,l_1]}$ and $\vec{f}_2^{[s,l_1]}$ are non-zero and linearly independent; for a uniperiodic stratum, $\vec{f}_1^{[s,l_1]}$ is non-zero and $\vec{f}_2^{[s,l_1]}$ is zero; and for a homogeneous stratum $\vec{f}_1^{[s,l_1]}$ and $\vec{f}_2^{[s,l_1]}$ are both zero.

The grating structure within biperiodic stratum l_1 comprises rectangular blocks whose walls are parallel and perpendicular to $\vec{d}_2^{[s,l_1]}$ (see Figure 2). The stratum geometry is defined by first partitioning the stratum into infinite-length "stripes" parallel to $\vec{d}_2^{[s,l_1]}$, and then partitioning each stripe into blocks. For example, Figure 3 illustrates the partitioning of stratum 1 from the example of Figures 1 and 2. More complicated grating geometries can also be approximated as block-partitioned structures, e.g., Figure 4 illustrates a possible representation for a circular structure[2].

The stripes are numbered sequentially (e.g., "stripe 0", "stripe 1", "stripe 2", etc.) in the order corresponding to the $\vec{d}_1^{[s,l_1]}$ direction. The blocks within each stripe are numbered sequentially (e.g.,

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[2] The preceding cautionary footnote regarding stratification also applies to block-partitioning of curved-wall structures such as circular posts and holes. Increasing the number of stripes might not improve calculation accuracy unless the number of diffraction orders is also significantly increased.

"block 0", "block 1", etc.), with the block index order corresponding to the $\vec{d}_2^{[s,l_1]}$ direction. Each block is optically homogeneous, and the permittivity in block l_3 of stripe l_2, stratum l_1 is denoted as $\varepsilon 3^{[l_1,l_2,l_3]}$,

$$\varepsilon[\vec{x}] = \varepsilon 3^{[l_1,l_2,l_3]} \quad \text{for } \vec{x} \text{ in block } l_3 \text{ of stripe } l_2, \text{stratum } l_1 \tag{3.34}$$

(The "l_2" index is generally used as a stripe index, and "l_3" is used as a block index.)

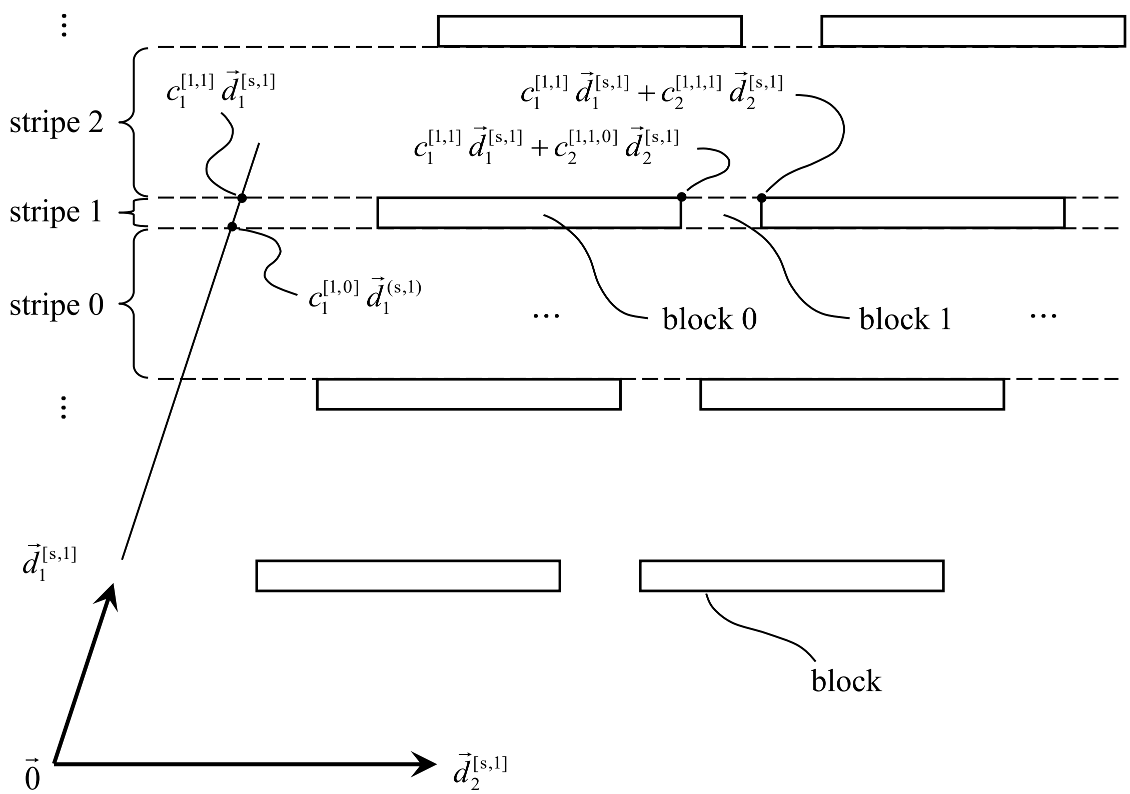

Figure 3. Stratum partitioning geometry.

The stripe boundary positions in stratum l_1 are defined in terms of a set of parameters $c_1^{[l_1,l_2]}$ $(l_2 = 1 \ldots L_2[l_1])$, where $L_2[l_1]$ is the number of stripes per period in the stratum. These values should satisfy the relation

$$c_1^{[l_1,L_2[l_1]]} - 1 \le c_1^{[l_1,1]} \le c_1^{[l_1,2]} \le \ldots \le c_1^{[l_1,L_2[l_1]]} \tag{3.35}$$

The l_2 range is implicitly extended to $\pm\infty$ by the condition

$$c_1^{[l_1,l_2+L_2[l_1]]} = c_1^{[l_1,l_2]} + 1 \tag{3.36}$$

(e.g., the left-hand value in relation 3.35 represents $c_1^{[l_1,0]}$). A ray from the coordinate origin ("$\vec{0}$" in Figure 3) in the $\vec{d}_1^{[s,l_1]}$ direction intercepts the boundaries of stripe l_2 at points $c_1^{[l_1,l_2-1]}\,\vec{d}_1^{[s,l_1]}$ and $c_1^{[l_1,l_2]}\,\vec{d}_1^{[s,l_1]}$.

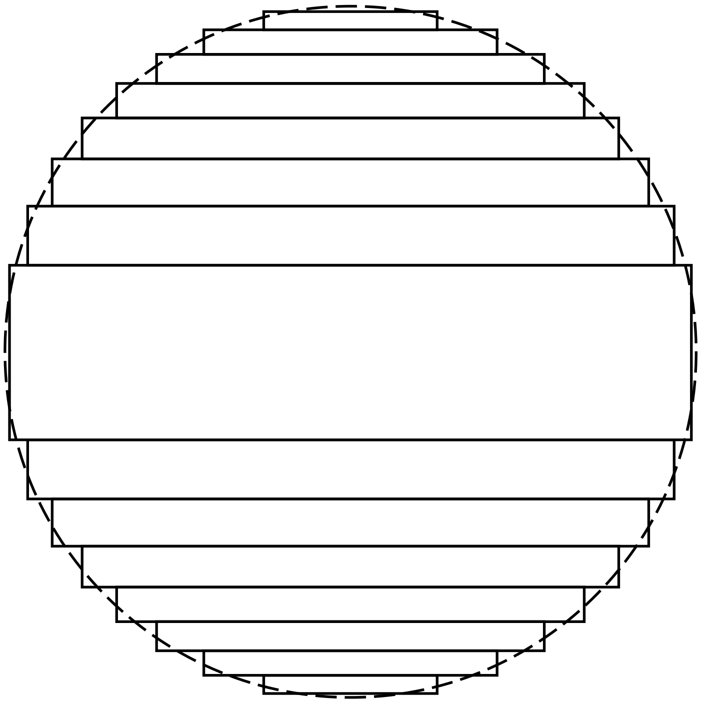

Figure 4. Block-partitioned circular structure.

The block boundary positions in stripe l_2 of stratum l_1 are defined in terms of a set of parameters $c_2^{[l_1,l_2,l_3]}$ ($l_2 = 1\ldots L_2[l_1]$, $l_3 = 1\ldots L_3[l_1,l_2]$), where $L_3[l_1,l_2]$ is the number of blocks per period in the stripe. These values should satisfy the relation

$$c_2^{[l_1,l_2,L_3[l_1,l_2]]} - 1 \le c_2^{[l_1,l_2,1]} \le c_2^{[l_1,l_2,2]} \le \ldots \le c_2^{[l_1,l_2,L_3[l_1,l_2]]} \tag{3.37}$$

The l_2 and l_3 ranges are implicitly extended to $\pm\infty$ by the conditions

$$c_2^{[l_1,l_2,l_3+L_3[l_1,l_2]]} = c_2^{[l_1,l_2,l_3]} + 1 \tag{3.38}$$

$$c_2^{[l_1,l_2+L_2[l_1],l_3]} = c_2^{[l_1,l_2,l_3]} \tag{3.39}$$

$$L_3[l_1,l_2+L_2[l_1]] = L_3[l_1,l_2] \tag{3.40}$$

(e.g., the left-hand value in relation 3.37 represents $c_2^{[l_1,l_2,0]}$). The boundaries of block l_3 in stripe l_2 intercept the interface between stripe l_2 and stripe l_2+1 at points $c_1^{[l_1,l_2]}\,\vec{d}_1^{[s,l_1]}+c_2^{[l_1,l_2,l_3-1]}\,\vec{d}_2^{[s,l_1]}$ and $c_1^{[l_1,l_2]}\,\vec{d}_1^{[s,l_1]}+c_2^{[l_1,l_2,l_3]}\,\vec{d}_2^{[s,l_1]}$.

A homogeneous stripe (e.g., stripe 0 in Figure 3) does not require any c_2 parameter specification; it only requires a c_1 parameter and a permittivity value. A uniperiodic stratum's stripes are all homogeneous and are aligned perpendicular to its $\vec{d}_1^{[s,l_1]}$ vector. A homogeneous stratum does not require any c_1 or c_2 specification; it requires only a permittivity specification.

A grating specification can contain include a coordinate break comprising lateral shift parameters Δx_2 and Δx_3, which laterally translate strata above the break by the displacement vector

$$\Delta\vec{x}=\hat{e}_2\,\Delta x_2+\hat{e}_3\,\Delta x_3 \tag{3.41}$$

The coordinate break is associated with a lateral plane at a particular x_1 height in the grating. The translational shift is only applied to strata above the coordinate break plane. Multiple coordinate breaks may be specified, and the total translation applied to any particular stratum is the sum of the $\Delta\vec{x}$ shifts specified by all the coordinate breaks below the stratum. (To apply a lateral translation to just a single stratum, a shift of $\Delta\vec{x}$ is applied immediately below the stratum and a shift of $-\Delta\vec{x}$ is applied immediately above the stratum.)

4. Electric field description

The electric field $\vec{E}$ includes an incident field $\vec{E}^{[\mathrm{Inc}]}$ and reflected field $\vec{E}^{[\mathrm{R}]}$ in the superstrate, and a transmitted field $\vec{E}^{[\mathrm{T}]}$ in the substrate. The incident field is a plane wave,

$$\vec{E}^{[\mathrm{Inc}]}[\vec{x}]=\vec{A}^{[\mathrm{Inc}]}\exp[i\,2\pi\,\vec{f}^{[\mathrm{Inc}]}\bullet\vec{x}] \tag{4.1}$$

where $\vec{A}^{[\mathrm{Inc}]}$ is a constant vector and $\vec{f}^{[\mathrm{Inc}]}$ is the incident field's spatial-frequency vector,

$$\vec{f}^{[\mathrm{Inc}]}=\hat{e}_1\,f_1^{[\mathrm{Inc}]}+\hat{e}_2\,f_2^{[\mathrm{Inc}]}+\hat{e}_3\,f_3^{[\mathrm{Inc}]} \tag{4.2}$$

The reflected field $\vec{E}^{[\mathrm{R}]}$ is a superposition of plane-wave Fourier orders $\mathit{ff}\vec{E}_{m_1,m_2}^{[\mathrm{R}]}[\vec{x}]$ with spatial-frequency vectors $\vec{f}_{m_1,m_2}^{[\mathrm{R}]}$, which are labeled by two diffraction order indices m_1 and m_2,

$$\vec{E}^{[\mathrm{R}]}[\vec{x}]=\sum_{m_1,m_2}\mathit{ff}\vec{E}_{m_1,m_2}^{[\mathrm{R}]}[\vec{x}] \tag{4.3}$$

$$ff\vec{E}^{[R]}_{m_1,m_2}[\vec{x}] = \vec{A}^{[R]}_{m_1,m_2} \exp[i\,2\pi\,\vec{f}^{[R]}_{m_1,m_2} \bullet \vec{x}] \tag{4.4}$$

(The " f " prefix connotes a Fourier expansion, and " ff " connotes a two-dimensional Fourier expansion.) The transmitted field similarly consists of plane-wave Fourier orders $ff\vec{E}^{[T]}_{m_1,m_2}[\vec{x}]$ with spatial-frequency vectors $\vec{f}^{[T]}_{m_1,m_2}$,

$$\vec{E}^{[T]}[\vec{x}] = \sum_{m_1,\,m_2} ff\vec{E}^{[T]}_{m_1,m_2}[\vec{x}] \tag{4.5}$$

$$ff\vec{E}^{[T]}_{m_1,m_2}[\vec{x}] = \vec{A}^{[T]}_{m_1,m_2} \exp[i\,2\pi\,\vec{f}^{[T]}_{m_1,m_2} \bullet \vec{x}] \tag{4.6}$$

The diffracted field's grating-tangential spatial frequencies (i.e., the $\hat{e}_2$ and $\hat{e}_3$ projections of $\vec{f}^{[R]}_{m_1,m_2}$ and $\vec{f}^{[T]}_{m_1,m_2}$) differ from that of the incident field by integer multiples of the grating's fundamental frequencies $\vec{f}^{[g]}_1$ and $\vec{f}^{[g]}_2$ (cf. Eq's. 3.27 and 3.28),

$$\begin{aligned} &\left(f^{[R]}_{2,m_1,m_2},\quad f^{[R]}_{3,m_1,m_2}\right) = \left(f^{[T]}_{2,m_1,m_2},\quad f^{[T]}_{3,m_1,m_2}\right) \\ &= \left(f^{[Inc]}_2,\quad f^{[Inc]}_3\right) + m_1\left(f^{[g]}_{2,1},\quad f^{[g]}_{3,1}\right) + m_2\left(f^{[g]}_{2,2},\quad f^{[g]}_{3,2}\right) \end{aligned} \tag{4.7}$$

where

$$f^{[R]}_{j,m_1,m_2} = \hat{e}_j \bullet \vec{f}^{[R]}_{m_1,m_2}, \quad f^{[T]}_{j,m_1,m_2} = \hat{e}_j \bullet \vec{f}^{[T]}_{m_1,m_2} \quad (j = 1,2,3) \tag{4.8}$$

The plane waves' grating-normal spatial frequencies ($\hat{e}_1$ frequency projections) are determined from the tangential frequencies,

$$f^{[Inc]}_1 = -\sqrt{\frac{\varepsilon^{[sup]}}{\lambda^2} - \left(f^{[Inc]}_2\right)^2 - \left(f^{[Inc]}_3\right)^2} \tag{4.9}$$

$$f^{[R]}_{1,m_1,m_2} = +\sqrt{\frac{\varepsilon^{[sup]}}{\lambda^2} - \left(f^{[R]}_{2,m_1,m_2}\right)^2 - \left(f^{[R]}_{3,m_1,m_2}\right)^2} \tag{4.10}$$

$$f^{[T]}_{1,m_1,m_2} = -\sqrt{\frac{\varepsilon^{[sub]}}{\lambda^2} - \left(f^{[T]}_{2,m_1,m_2}\right)^2 - \left(f^{[T]}_{3,m_1,m_2}\right)^2} \tag{4.11}$$

The square root branch is chosen so that the square root's imaginary part is non-negative, and the square root signs in Eq's. 4.9-4.11 are chosen so that the incident field propagates toward the grating and the diffracted fields propagate away from the grating. Eq's. 4.7-4.11 define all of the field's spatial frequencies, based on a specification of $f^{[Inc]}_2$, $f^{[Inc]}_3$ and the grating frequencies $\vec{f}^{[g]}_1$, $\vec{f}^{[g]}_2$.

In general, the order indices m_1 and m_2 range from $-\infty$ to $+\infty$, but for computational applications only a finite number of orders is retained. The retained orders are defined by the index limit sets $\mathcal{M}_1$ (which limits m_1) and $\mathcal{M}_2$ (which limits m_2),

$$m_2 \in \mathcal{M}_2 \tag{4.12}$$

$$m_1 \in \mathcal{M}_1[m_2] \tag{4.13}$$

The m_1 limit set $\mathcal{M}_1$ is a function of m_2. For example, Figure 5 illustrates a particular diffracted field's tangential frequencies (indicated as dots), as defined by Eq. 4.7. The integer pairs represent diffraction order indices (m_1, m_2), and if only the labeled orders are intended to be retained then the index limit sets would be defined as follows,

$$\mathcal{M}_2 = \{-2, -1, 0, 1, 2\} \tag{4.14}$$

$$\left.\begin{array}{l} \mathcal{M}_1[-2] = \{0, 1, 2\} \\ \mathcal{M}_1[-1] = \{-1, 0, 1, 2\} \\ \mathcal{M}_1[\ 0\ ] = \{-2, -1, 0, 1, 2\} \\ \mathcal{M}_1[\ 1\ ] = \{-2, -1, 0, 1\} \\ \mathcal{M}_1[\ 2\ ] = \{-2, -1, 0\} \end{array}\right\} \tag{4.15}$$

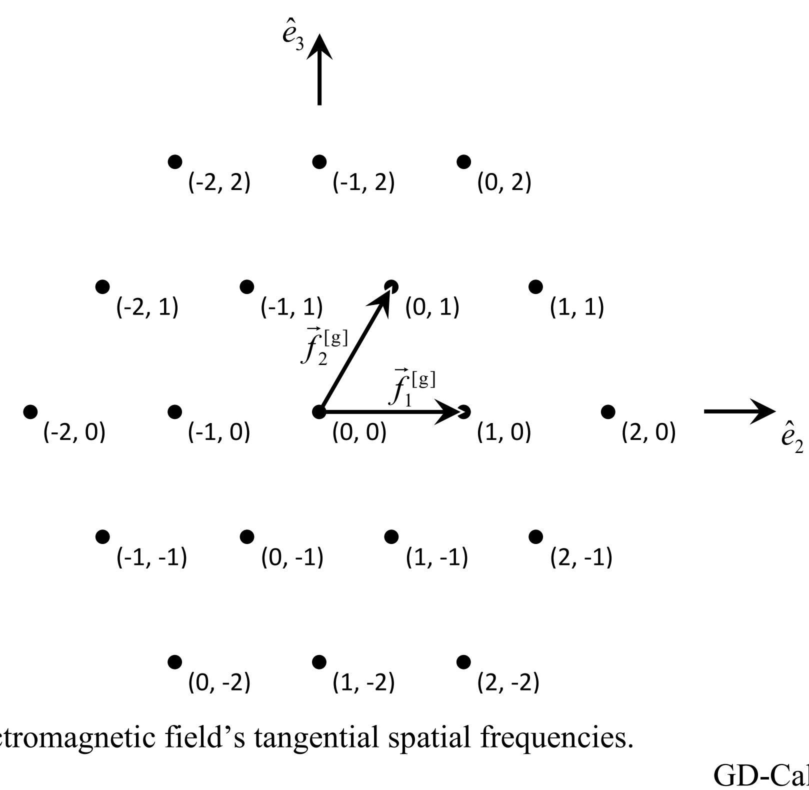

Figure 5. Electromagnetic field's tangential spatial frequencies.

The incident field amplitude is orthogonal to $\vec{f}^{[\mathrm{Inc}]}$,

$$\vec{f}^{[\mathrm{Inc}]} \bullet \vec{E}^{[\mathrm{Inc}]} = 0 \tag{4.16}$$

$\vec{E}^{[\mathrm{Inc}]}$ is specified in terms of its projections onto two unit vectors $\hat{s}^{[\mathrm{Inc}]}$ and $\hat{p}^{[\mathrm{Inc}]}$, where $\hat{s}^{[\mathrm{Inc}]}$ is orthogonal to $\hat{e}_1$, and $\hat{s}^{[\mathrm{Inc}]}$ and $\hat{p}^{[\mathrm{Inc}]}$ are both orthogonal to $\vec{f}^{[\mathrm{Inc}]}$,

$$\hat{s}^{[\mathrm{Inc}]} = \hat{e}_2\, s_2^{[\mathrm{Inc}]} + \hat{e}_3\, s_3^{[\mathrm{Inc}]} \tag{4.17}$$

$$\hat{p}^{[\mathrm{Inc}]} = \hat{e}_1\, p_1^{[\mathrm{Inc}]} + \hat{e}_2\, p_2^{[\mathrm{Inc}]} + \hat{e}_3\, p_3^{[\mathrm{Inc}]} \tag{4.18}$$

$$\left(s_2^{[\mathrm{Inc}]}, \quad s_3^{[\mathrm{Inc}]} \right) = \begin{cases} \dfrac{\left(-f_3^{[\mathrm{Inc}]}, \quad f_2^{[\mathrm{Inc}]} \right)}{\sqrt{(f_2^{[\mathrm{Inc}]})^2 + (f_3^{[\mathrm{Inc}]})^2}} & \text{if } (f_2^{[\mathrm{Inc}]})^2 + (f_3^{[\mathrm{Inc}]})^2 \neq 0 \\ \dfrac{\left(-f_{3,1}^{[\mathrm{g}]}, \quad f_{2,1}^{[\mathrm{g}]} \right)}{\sqrt{(f_{2,1}^{[\mathrm{g}]})^2 + (f_{3,1}^{[\mathrm{g}]})^2}} & \text{if } (f_2^{[\mathrm{Inc}]})^2 + (f_3^{[\mathrm{Inc}]})^2 = 0 \end{cases} \tag{4.19}$$

$$\hat{p}^{[\mathrm{Inc}]} = -\hat{s}^{[\mathrm{Inc}]} \times \vec{f}^{[\mathrm{Inc}]}\, \lambda / \sqrt{\varepsilon^{[\mathrm{sup}]}} \tag{4.20}$$

($\hat{p}^{[\mathrm{Inc}]}$ is a unit vector because $\vec{f}^{[\mathrm{Inc}]} \bullet \vec{f}^{[\mathrm{Inc}]} = \sqrt{\varepsilon^{[\mathrm{sup}]}} / \lambda$, Eq. 4.9.) The incident field is represented as

$$\vec{E}^{[\mathrm{Inc}]}[\vec{x}] = \hat{s}^{[\mathrm{Inc}]}\, E_s^{[\mathrm{Inc}]}[\vec{x}] + \hat{p}^{[\mathrm{Inc}]}\, E_p^{[\mathrm{Inc}]}[\vec{x}] \tag{4.21}$$

$\hat{s}$ and $\hat{p}$ basis vectors are similarly defined for the reflected and transmitted orders, and the diffracted field amplitudes are projected onto these bases. For the reflected waves, the following definitions apply,

$$\hat{s}_{m_1,m_2}^{[\mathrm{R}]} = \hat{e}_2\, s_{2,m_1,m_2}^{[\mathrm{R}]} + \hat{e}_3\, s_{3,m_1,m_2}^{[\mathrm{R}]} \tag{4.22}$$

$$\hat{p}_{m_1,m_2}^{[\mathrm{R}]} = \hat{e}_1\, p_{1,m_1,m_2}^{[\mathrm{R}]} + \hat{e}_2\, p_{2,m_1,m_2}^{[\mathrm{R}]} + \hat{e}_3\, p_{3,m_1,m_2}^{[\mathrm{R}]} \tag{4.23}$$

$$\left(s^{[\mathrm{R}]}_{2,m_1,m_2}, \quad s^{[\mathrm{R}]}_{3,m_1,m_2} \right) = \begin{cases} \dfrac{\left(-f^{[\mathrm{R}]}_{3,m_1,m_2}, \quad f^{[\mathrm{R}]}_{2,m_1,m_2} \right)}{\sqrt{(f^{[\mathrm{R}]}_{2,m_1,m_2})^2 + (f^{[\mathrm{R}]}_{3,m_1,m_2})^2}} & \text{if } (f^{[\mathrm{R}]}_{2,m_1,m_2})^2 + (f^{[\mathrm{R}]}_{3,m_1,m_2})^2 \neq 0 \\ \dfrac{\left(-f^{[\mathrm{g}]}_{3,1}, \quad f^{[\mathrm{g}]}_{2,1} \right)}{\sqrt{(f^{[\mathrm{g}]}_{2,1})^2 + (f^{[\mathrm{g}]}_{3,1})^2}} & \text{if } (f^{[\mathrm{R}]}_{2,m_1,m_2})^2 + (f^{[\mathrm{R}]}_{3,m_1,m_2})^2 = 0 \end{cases} \tag{4.24}$$

$$\hat{p}^{[\mathrm{R}]}_{m_1,m_2} = +\hat{s}^{[\mathrm{R}]}_{m_1,m_2} \times \vec{f}^{[\mathrm{R}]}_{m_1,m_2} \, \lambda / \sqrt{\varepsilon^{[\mathrm{sup}]}} \tag{4.25}$$

$$f\!f\vec{E}^{[\mathrm{R}]}_{m_1,m_2}[\vec{x}] = \hat{s}^{[\mathrm{R}]}_{m_1,m_2} \; f\!fE^{[\mathrm{R}]}_{\mathrm{s},m_1,m_2}[\vec{x}] + \hat{p}^{[\mathrm{R}]}_{m_1,m_2} \; f\!fE^{[\mathrm{R}]}_{\mathrm{p},m_1,m_2}[\vec{x}] \tag{4.26}$$

For the transmitted waves, the definitions are

$$\hat{s}^{[\mathrm{T}]}_{m_1,m_2} = \hat{e}_2 \, s^{[\mathrm{T}]}_{2,m_1,m_2} + \hat{e}_3 \, s^{[\mathrm{T}]}_{3,m_1,m_2} \tag{4.27}$$

$$\hat{p}^{[\mathrm{T}]}_{m_1,m_2} = \hat{e}_1 \, p^{[\mathrm{T}]}_{1,m_1,m_2} + \hat{e}_2 \, p^{[\mathrm{T}]}_{2,m_1,m_2} + \hat{e}_3 \, p^{[\mathrm{T}]}_{3,m_1,m_2} \tag{4.28}$$

$$\left(s^{[\mathrm{T}]}_{2,m_1,m_2}, \quad s^{[\mathrm{T}]}_{3,m_1,m_2} \right) = \left(s^{[\mathrm{R}]}_{2,m_1,m_2}, \quad s^{[\mathrm{R}]}_{3,m_1,m_2} \right) \tag{4.29}$$

$$\hat{p}^{[\mathrm{T}]}_{m_1,m_2} = -\hat{s}^{[\mathrm{T}]}_{m_1,m_2} \times \vec{f}^{[\mathrm{T}]}_{m_1,m_2} \, \lambda / \sqrt{\varepsilon^{[\mathrm{sub}]}} \tag{4.30}$$

$$f\!f\vec{E}^{[\mathrm{T}]}_{m_1,m_2}[\vec{x}] = \hat{s}^{[\mathrm{T}]}_{m_1,m_2} \; f\!fE^{[\mathrm{T}]}_{\mathrm{s},m_1,m_2}[\vec{x}] + \hat{p}^{[\mathrm{T}]}_{m_1,m_2} \; f\!fE^{[\mathrm{T}]}_{\mathrm{p},m_1,m_2}[\vec{x}] \tag{4.31}$$

$\hat{s}^{[\mathrm{T}]}$ is equal to $\hat{s}^{[\mathrm{R}]}$ (Eq. 4.29) because all the terms on the right side of Eq. 4.24 would be the same with $\vec{f}^{[\mathrm{T}]}$ substituted for $\vec{f}^{[\mathrm{R}]}$ (Eq. 4.7). Note the sign convention for $\hat{p}$: The definitions for downward-directed waves (Eq's. 4.20 and 4.30) include a minus sign, whereas the definition for upward-directed waves (Eq. 4.25) does not.

The diffracted fields are linearly dependent on the incident field, and the linear coefficients for order-(m_1, m_2) reflected and transmitted waves are represented by reflection and transmission matrices R_{m_1,m_2} and T_{m_1,m_2},

$$R_{m_1,m_2} = \begin{pmatrix} R_{\mathrm{s,s},m_1,m_2} & R_{\mathrm{s,p},m_1,m_2} \\ R_{\mathrm{p,s},m_1,m_2} & R_{\mathrm{p,p},m_1,m_2} \end{pmatrix} \tag{4.32}$$

$$T_{m_1,m_2} = \begin{pmatrix} T_{\mathrm{s,s},m_1,m_2} & T_{\mathrm{s,p},m_1,m_2} \\ T_{\mathrm{p,s},m_1,m_2} & T_{\mathrm{p,p},m_1,m_2} \end{pmatrix} \tag{4.33}$$

In defining these matrices, the incident and reflected amplitudes are evaluated at point $\vec{x} = \hat{e}_1\, b_1^{[L_1]}$ on the grating's top surface (Eq. 3.3), and the transmitted amplitudes are evaluated at point $\vec{x} = \hat{e}_1\, b_1^{[0]}$ on the grating's bottom surface (Eq. 3.2),

$$\begin{pmatrix} f\!f E^{[\mathrm{R}]}_{\mathrm{s},m_1,m_2}[\hat{e}_1\, b_1^{[L_1]}] \\ f\!f E^{[\mathrm{R}]}_{\mathrm{p},m_1,m_2}[\hat{e}_1\, b_1^{[L_1]}] \end{pmatrix} = \begin{pmatrix} R_{\mathrm{s},\mathrm{s},m_1,m_2} & R_{\mathrm{s},\mathrm{p},m_1,m_2} \\ R_{\mathrm{p},\mathrm{s},m_1,m_2} & R_{\mathrm{p},\mathrm{p},m_1,m_2} \end{pmatrix} \begin{pmatrix} E^{[\mathrm{Inc}]}_{\mathrm{s}}[\hat{e}_1\, b_1^{[L_1]}] \\ E^{[\mathrm{Inc}]}_{\mathrm{p}}[\hat{e}_1\, b_1^{[L_1]}] \end{pmatrix} \tag{4.34}$$

$$\begin{pmatrix} f\!f E^{[\mathrm{T}]}_{\mathrm{s},m_1,m_2}[\hat{e}_1\, b_1^{[0]}] \\ f\!f E^{[\mathrm{T}]}_{\mathrm{p},m_1,m_2}[\hat{e}_1\, b_1^{[0]}] \end{pmatrix} = \begin{pmatrix} T_{\mathrm{s},\mathrm{s},m_1,m_2} & T_{\mathrm{s},\mathrm{p},m_1,m_2} \\ T_{\mathrm{p},\mathrm{s},m_1,m_2} & T_{\mathrm{p},\mathrm{p},m_1,m_2} \end{pmatrix} \begin{pmatrix} E^{[\mathrm{Inc}]}_{\mathrm{s}}[\hat{e}_1\, b_1^{[L_1]}] \\ E^{[\mathrm{Inc}]}_{\mathrm{p}}[\hat{e}_1\, b_1^{[L_1]}] \end{pmatrix} \tag{4.35}$$

If $f_1^{[\mathrm{Inc}]}$ is real-valued then the incident power $P^{[\mathrm{Inc}]}$ propagating toward the grating (i.e., in the $-\hat{e}_1$ direction) is (within a dimensional constant)

$$P^{[\mathrm{Inc}]} = -\lambda\, f_1^{[\mathrm{Inc}]} \left(|\, E^{[\mathrm{Inc}]}_{\mathrm{s}} \,|^2 + |\, E^{[\mathrm{Inc}]}_{\mathrm{p}} \,|^2 \right) \quad (\text{when } \operatorname{Im}[f_1^{[\mathrm{Inc}]}] = 0) \tag{4.36}$$

The reflected power $P^{[\mathrm{R}]}_{m_1,m_2}$ propagating away from the grating (in the $+\hat{e}_1$ direction) in the order-(m_1, m_2) reflected wave is

$$P^{[\mathrm{R}]}_{m_1,m_2} = \operatorname{Re}[\lambda\, f^{[\mathrm{R}]}_{1,m_1,m_2}] \left(|\, f\!f E^{[\mathrm{R}]}_{\mathrm{s},m_1,m_2}[\hat{e}_1\, b_1^{[L_1]}] \,|^2 + |\, f\!f E^{[\mathrm{R}]}_{\mathrm{p},m_1,m_2}[\hat{e}_1\, b_1^{[L_1]}] \,|^2 \right) \tag{4.37}$$

(For the case $[m_1, m_2] = [0,0]$ Eq. 4.37 also assumes $\operatorname{Im}[f_1^{[\mathrm{Inc}]}] = 0$.) The transmitted power $P^{[\mathrm{T}]}_{m_1,m_2}$ propagating away from the grating (in the $-\hat{e}_1$ direction) in the order-(m_1, m_2) transmitted wave is

$$P^{[\mathrm{T}]}_{m_1,m_2} = -\operatorname{Re}[\lambda\, f^{[\mathrm{T}]}_{1,m_1,m_2}] \left(|\, f\!f E^{[\mathrm{T}]}_{\mathrm{s},m_1,m_2}[\hat{e}_1\, b_1^{[0]}] \,|^2 + |\, f\!f E^{[\mathrm{T}]}_{\mathrm{p},m_1,m_2}[\hat{e}_1\, b_1^{[0]}] \,|^2 \right) \tag{4.38}$$

The incident and reflected field amplitudes are evaluated at $\vec{x} = \hat{e}_1\, b_1^{[L_1]}$ in Eq's. 4.36 and 4.37, and the transmitted amplitudes are evaluated at $\vec{x} = \hat{e}_1\, b_1^{[0]}$ in Eq. 4.38. The signs in Eq's. 4.36-4.38 make the power positive (cf. Eq's. 4.9-4.11).

Eq's. 4.36-4.38 are derived in Appendix A, along with additional formulas for diffraction efficiency. When $f_1^{[\mathrm{Inc}]}$ is not real-valued, the incident power $P^{[\mathrm{Inc}]}$ and diffraction efficiencies are ill-defined because the zero-order power in the superstrate is not additively separable between incident and reflected waves (Eq. A.9). The assumption that $f_1^{[\mathrm{Inc}]}$ is real-valued implies that the superstrate is lossless ($\operatorname{Im}\left[\varepsilon^{[\mathrm{sup}]}\right] = 0$, Eq. 4.9) and that $f^{[\mathrm{R}]}_{1,m_1,m_2}$ and $f^{[\mathrm{T}]}_{1,m_1,m_2}$ are ether real-valued or pure complex (Eq's 4.10-4.11); in the latter case the corresponding power flux $P^{[\mathrm{R}]}_{m_1,m_2}$ or $P^{[\mathrm{T}]}_{m_1,m_2}$ is zero.

The above formalism assumes a single, plane-wave incident beam, but can be generalized to accommodate multiple incident orders. Eq. 4.1, 4.7, and 4.9 generalize to

$$\vec{E}^{[\mathrm{Inc}]}[\vec{x}] = \sum_{m_1,m_2} f\!f\vec{E}^{[\mathrm{Inc}]}_{m_1,m_2}[\vec{x}] \tag{4.39}$$

where

$$f\!f\vec{E}^{[\mathrm{Inc}]}_{m_1,m_2}[\vec{x}] = \vec{A}^{[\mathrm{Inc}]}_{m_1,m_2} \exp[i\,2\pi\,\vec{f}^{[\mathrm{Inc}]}_{m_1,m_2} \bullet \vec{x}] \tag{4.40}$$

$$\begin{aligned} &\left(f^{[\mathrm{Inc}]}_{2,m_1,m_2}, \quad f^{[\mathrm{Inc}]}_{3,m_1,m_2} \right) = \left(f^{[\mathrm{R}]}_{2,m_1,m_2}, \quad f^{[\mathrm{R}]}_{3,m_1,m_2} \right) = \left(f^{[\mathrm{T}]}_{2,m_1,m_2}, \quad f^{[\mathrm{T}]}_{3,m_1,m_2} \right) \\ &= \left(f^{[\mathrm{Inc}]}_{2,0,0}, \quad f^{[\mathrm{Inc}]}_{3,0,0} \right) + m_1 \left(f^{[\mathrm{g}]}_{2,1}, \quad f^{[\mathrm{g}]}_{3,1} \right) + m_2 \left(f^{[\mathrm{g}]}_{2,2}, \quad f^{[\mathrm{g}]}_{3,2} \right) \end{aligned} \tag{4.41}$$

$$f^{[\mathrm{Inc}]}_{1,m_1,m_2} = -\sqrt{\frac{\varepsilon^{[\mathrm{sup}]}}{\lambda^2} - \left(f^{[\mathrm{Inc}]}_{2,m_1,m_2} \right)^2 - \left(f^{[\mathrm{Inc}]}_{3,m_1,m_2} \right)^2} \tag{4.42}$$

(Eq. 4.1 only includes the zero-order incident amplitude $f\!f\vec{E}^{[\mathrm{Inc}]}_{0,0}$ with wave vector $\vec{f}^{[\mathrm{Inc}]} = \vec{f}^{[\mathrm{Inc}]}_{0,0}$.) The incident field's projection onto polarization basis vectors (Eq's. 4.17-4.21) generalizes in a manner similar to the transmitted orders (Eq's. 4.27-4.31):

$$\hat{s}^{[\mathrm{Inc}]}_{m_1,m_2} = \hat{s}^{[\mathrm{R}]}_{m_1,m_2} \tag{4.43}$$

$$\hat{p}^{[\mathrm{Inc}]}_{m_1,m_2} = -\hat{s}^{[\mathrm{Inc}]}_{m_1,m_2} \times \vec{f}^{[\mathrm{Inc}]}_{m_1,m_2}\, \lambda / \sqrt{\varepsilon^{[\mathrm{sup}]}} \tag{4.44}$$

$$f\!f\vec{E}^{[\mathrm{Inc}]}_{m_1,m_2}[\vec{x}] = \hat{s}^{[\mathrm{Inc}]}_{m_1,m_2}\, f\!fE^{[\mathrm{Inc}]}_{\mathrm{s},m_1,m_2}[\vec{x}] + \hat{p}^{[\mathrm{Inc}]}_{m_1,m_2}\, f\!fE^{[\mathrm{Inc}]}_{\mathrm{p},m_1,m_2}[\vec{x}] \tag{4.45}$$

The linear mappings from incident to diffracted orders (Eq's. 4.34 and 4.35) generalize to summations over incident orders,

$$\begin{pmatrix} f\!fE^{[\mathrm{R}]}_{\mathrm{s},m_1,m_2}[\hat{e}_1\, b^{[0]}_1] \\ f\!fE^{[\mathrm{R}]}_{\mathrm{p},m_1,m_2}[\hat{e}_1\, b^{[0]}_1] \end{pmatrix} = \sum_{m'_1,m'_2} \begin{pmatrix} R_{\mathrm{s},\mathrm{s},m_1,m_2,m'_1,m'_2} & R_{\mathrm{s},\mathrm{p},m_1,m_2,m'_1,m'_2} \\ R_{\mathrm{p},\mathrm{s},m_1,m_2,m'_1,m'_2} & R_{\mathrm{p},\mathrm{p},m_1,m_2,m'_1,m'_2} \end{pmatrix} \begin{pmatrix} E^{[\mathrm{Inc}]}_{\mathrm{s},m'_1,m'_2}[\hat{e}_1\, b^{[L_1]}_1] \\ E^{[\mathrm{Inc}]}_{\mathrm{p},m'_1,m'_2}[\hat{e}_1\, b^{[L_1]}_1] \end{pmatrix} \tag{4.46}$$

$$\begin{pmatrix} f\!fE^{[\mathrm{T}]}_{\mathrm{s},m_1,m_2}[\hat{e}_1\, b^{[0]}_1] \\ f\!fE^{[\mathrm{T}]}_{\mathrm{p},m_1,m_2}[\hat{e}_1\, b^{[0]}_1] \end{pmatrix} = \sum_{m'_1,m'_2} \begin{pmatrix} T_{\mathrm{s},\mathrm{s},m_1,m_2,m'_1,m'_2} & T_{\mathrm{s},\mathrm{p},m_1,m_2,m'_1,m'_2} \\ T_{\mathrm{p},\mathrm{s},m_1,m_2,m'_1,m'_2} & T_{\mathrm{p},\mathrm{p},m_1,m_2,m'_1,m'_2} \end{pmatrix} \begin{pmatrix} E^{[\mathrm{Inc}]}_{\mathrm{s},m'_1,m'_2}[\hat{e}_1\, b^{[L_1]}_1] \\ E^{[\mathrm{Inc}]}_{\mathrm{p},m'_1,m'_2}[\hat{e}_1\, b^{[L_1]}_1] \end{pmatrix} \tag{4.47}$$

In the GD-Calc software interface, the order index pairs (m_1, m_2) are serialized by a scalar enumeration index k ,

$$(m_1, m_2) \;\to\; (m_1[k], m_2[k]) \tag{4.48}$$

Eq's. 4.46 and 4.47 translate to summations over the incident orders' serialization index k',

$$\begin{pmatrix} ffE^{[\mathrm{R}]}_{\mathrm{s},m_1[k],m_2[k]}[\hat{e}_1\, b_1^{[0]}] \\ ffE^{[\mathrm{R}]}_{\mathrm{p},m_1[k],m_2[k]}[\hat{e}_1\, b_1^{[0]}] \end{pmatrix} = \sum_{k'} \begin{pmatrix} R_{\mathrm{s,s},m_1[k],m_2[k],m_1[k'],m_2[k']} & R_{\mathrm{s,p},m_1[k],m_2[k],m_1[k'],m_2[k']} \\ R_{\mathrm{p,s},m_1[k],m_2[k],m_1[k'],m_2[k']} & R_{\mathrm{p,p},m_1[k],m_2[k],m_1[k'],m_2[k']} \end{pmatrix} \begin{pmatrix} E^{[\mathrm{Inc}]}_{\mathrm{s},m_1[k'],m_2[k']}[\hat{e}_1\, b_1^{[L_1]}] \\ E^{[\mathrm{Inc}]}_{\mathrm{p},m_1[k'],m_2[k']}[\hat{e}_1\, b_1^{[L_1]}] \end{pmatrix} \tag{4.49}$$

$$\begin{pmatrix} ffE^{[\mathrm{T}]}_{\mathrm{s},m_1[k],m_2[k]}[\hat{e}_1\, b_1^{[0]}] \\ ffE^{[\mathrm{T}]}_{\mathrm{p},m_1[k],m_2[k]}[\hat{e}_1\, b_1^{[0]}] \end{pmatrix} = \sum_{k'} \begin{pmatrix} T_{\mathrm{s,s},m_1[k],m_2[k],m_1[k'],m_2[k']} & T_{\mathrm{s,p},m_1[k],m_2[k],m_1[k'],m_2[k']} \\ T_{\mathrm{p,s},m_1[k],m_2[k],m_1[k'],m_2[k']} & T_{\mathrm{p,p},m_1[k],m_2[k],m_1[k'],m_2[k']} \end{pmatrix} \begin{pmatrix} E^{[\mathrm{Inc}]}_{\mathrm{s},m_1[k'],m_2[k']}[\hat{e}_1\, b_1^{[L_1]}] \\ E^{[\mathrm{Inc}]}_{\mathrm{p},m_1[k'],m_2[k']}[\hat{e}_1\, b_1^{[L_1]}] \end{pmatrix} \tag{4.50}$$

In gdc.m the indices k and k' are denoted as **`k`** and **`k_inc`**, the data associated with incident order $(m_1[\texttt{k\_inc}], m_2[\texttt{k\_inc}])$ is encapsulated in struct **`inc_field(k_inc)`**, and the data associated with the diffraction order $(m_1[\texttt{k}], m_2[\texttt{k}])$ generated by incident order $(m_1[\texttt{k\_inc}], m_2[\texttt{k\_inc}])$ is encapsulated in struct **`scat_field(k_inc,k)`**. Table 4.1 summarizes the data included in these structs. (**`inc_field`** is the gdc.m output argument, which includes more information than the **`inc_field`** input argument.)

$(m_1[\texttt{k\_inc}], m_2[\texttt{k\_inc}])$	**`inc_field(k_inc).m1_inc`** and **`m2_inc`**, **`scat_field(k_inc,k).m1_inc`** and **`m2_inc`**
$(m_1[\texttt{k}], m_2[\texttt{k}])$	**`scat_field(k_inc,k).m1`** and **`m2`**
$f^{[\mathrm{Inc}]}_{j,m_1[\texttt{k\_inc}],m_2[\texttt{k\_inc}]}$ $(j=1,2,3)$	**`inc_field(k_inc).f1`**, **`f2`**, and **`f3`**
$s^{[\mathrm{Inc}]}_{j,m_1[\texttt{k\_inc}],m_2[\texttt{k\_inc}]}$ $(j=2,3)$	**`inc_field(k_inc).s2`** and **`s3`**
$p^{[\mathrm{Inc}]}_{j,m_1[\texttt{k\_inc}],m_2[\texttt{k\_inc}]}$ $(j=1,2,3)$	**`inc_field(k_inc).p1`**, **`p2`**, and **`p3`**
$f^{[\mathrm{R}]}_{j,m_1[\texttt{k}],m_2[\texttt{k}]}$ and $f^{[\mathrm{T}]}_{j,m_1[\texttt{k}],m_2[\texttt{k}]}$ $(j=2,3)$	**`scat_field(k_inc,k).f2`** and **`f3`**
$f^{[\mathrm{R}]}_{1,m_1[\texttt{k}],m_2[\texttt{k}]}$	**`scat_field(k_inc,k).f1r`**
$f^{[\mathrm{T}]}_{1,m_1[\texttt{k}],m_2[\texttt{k}]}$	**`scat_field(k_inc,k).f1t`**
$s^{[\mathrm{R}]}_{j,m_1[\texttt{k}],m_2[\texttt{k}]}$ and $s^{[\mathrm{T}]}_{j,m_1[\texttt{k}],m_2[\texttt{k}]}$ $(j=2,3)$	**`scat_field(k_inc,k).s2`** and **`s3`**
$p^{[\mathrm{R}]}_{j,m_1[\texttt{k}],m_2[\texttt{k}]}$ $(j=1,2,3)$	**`scat_field(k_inc,k).p1r`**, **`p2r`**, and **`p3r`**
$p^{[\mathrm{T}]}_{j,m_1[\texttt{k}],m_2[\texttt{k}]}$ $(j=1,2,3)$	**`scat_field(k_inc,k).p1t`**, **`p2t`**, and **`p3t`**
$R_{\mathrm{s,s},m_1[\texttt{k}],m_2[\texttt{k}],m_1[\texttt{k\_inc}],m_2[\texttt{k\_inc}]}$, etc.	**`scat_field(k_inc,k).Rss`**, etc.
$T_{\mathrm{s,s},m_1[\texttt{k}],m_2[\texttt{k}],m_1[\texttt{k\_inc}],m_2[\texttt{k\_inc}]}$, etc.	**`scat_field(k_inc,k).Tss`**, etc.

Table 4.1

Part 2: Theory and Methods

5. Fourier expansion of the electromagnetic field

The total electromagnetic field consists of the incident field (which has the form described by Eq. 4.1 for $\vec{E}$, and a similar form for $\vec{H}$), and the diffracted field (which includes the reflected and transmitted fields as well as the internal field within the grating). The grating is invariant under translation by period $\vec{d}_1^{[\mathrm{g}]}$ (Eq. 3.8), so a translation of the incident field by $\vec{d}_1^{[\mathrm{g}]}$ will have no effect on the resulting diffracted field other than to translate it by the same offset. A translation of the incident field by $\vec{d}_1^{[\mathrm{g}]}$ has the same effect as multiplying the field by a constant factor of $\exp[i\,2\pi\,\vec{f}^{[\mathrm{Inc}]}\bullet\vec{d}_1^{[\mathrm{g}]}]$,

$$\vec{E}^{[\mathrm{Inc}]}[\vec{x}+\vec{d}_1^{[\mathrm{g}]}]=\vec{E}^{[\mathrm{Inc}]}[\vec{x}]\exp[i\,2\pi\,\vec{f}^{[\mathrm{Inc}]}\bullet\vec{d}_1^{[\mathrm{g}]}] \tag{5.1}$$

(from Eq. 4.1). The diffracted field has a linear dependence on the incident field, so the resulting diffracted field is also scaled by the same factor. Hence, a translation of the diffracted field by $\vec{d}_1^{[\mathrm{g}]}$ is similarly equivalent to applying the above scaling factor, and the above relation thus applies to the total (incident plus diffracted) field,

$$\vec{E}[\vec{x}+\vec{d}_1^{[\mathrm{g}]}]=\vec{E}[\vec{x}]\exp[i\,2\pi\,\vec{f}^{[\mathrm{Inc}]}\bullet\vec{d}_1^{[\mathrm{g}]}] \tag{5.2}$$

Since $\vec{d}_1^{[\mathrm{g}]}$ has no $\hat{e}_1$ component (Eq. 3.5), the scale factor in Eq. 5.2 only depends on the projection of $\vec{f}^{[\mathrm{Inc}]}$ parallel to the grating surface, denoted as $\vec{f}^{[\mathrm{Inc}\|]}$,

$$\vec{f}^{[\mathrm{Inc}\|]}=\hat{e}_2\,f_2^{[\mathrm{Inc}]}+\hat{e}_3\,f_3^{[\mathrm{Inc}]} \tag{5.3}$$

$$\vec{E}[\vec{x}+\vec{d}_1^{[\mathrm{g}]}]=\vec{E}[\vec{x}]\exp[i\,2\pi\,\vec{f}^{[\mathrm{Inc}\|]}\bullet\vec{d}_1^{[\mathrm{g}]}] \tag{5.4}$$

(The "$\|$" superscript annotation connotes "parallel".) This implies that the total field divided by $\exp[i\,2\pi\,\vec{f}^{[\mathrm{Inc}\|]}\bullet\vec{x}]$ is periodic with period $\vec{d}_1^{[\mathrm{g}]}$,

$$\vec{E}[\vec{x}+\vec{d}_1^{[\mathrm{g}]}]/\exp[i\,2\pi\,\vec{f}^{[\mathrm{Inc}\|]}\bullet(\vec{x}+\vec{d}_1^{[\mathrm{g}]})]=\vec{E}[\vec{x}]/\exp[i\,2\pi\,\vec{f}^{[\mathrm{Inc}\|]}\bullet\vec{x}] \tag{5.5}$$

The same type of condition also holds for the grating's second fundamental period, $\vec{d}_2^{[\mathrm{g}]}$,

$$\vec{E}[\vec{x}+\vec{d}_2^{[\mathrm{g}]}]/\exp[i\,2\pi\,\vec{f}^{[\mathrm{Inc}\|]}\bullet(\vec{x}+\vec{d}_2^{[\mathrm{g}]})]=\vec{E}[\vec{x}]/\exp[i\,2\pi\,\vec{f}^{[\mathrm{Inc}\|]}\bullet\vec{x}] \tag{5.6}$$

The displacement periods $\vec{d}_1^{[\mathrm{g}]}$ and $\vec{d}_2^{[\mathrm{g}]}$ in Eq's. 5.5 and 5.6 are in the $\hat{e}_2$, $\hat{e}_3$ plane (Eq's. 3.5, 3.6), so the right-hand expression in these equations can be represented as a biperiodic Fourier series in

x_2 and x_3. Denoting the order-(m_1, m_2) Fourier coefficient as $ff\vec{E}_{m_1,m_2}[x_1]$, the following $\vec{E}$-field Fourier expansion is obtained,

$$\vec{E}[\vec{x}] = \sum_{m_1,m_2} ff\vec{E}_{m_1,m_2}[x_1] \exp[i\,2\pi\,\vec{f}^{[||]}_{m_1,m_2} \bullet \vec{x}] \tag{5.7}$$

where the field's grating-tangential (parallel) spatial frequencies $\vec{f}^{[||]}_{m_1,m_2}$ are

$$\vec{f}^{[||]}_{m_1,m_2} = \vec{f}^{[\mathrm{Inc}||]} + m_1\,\vec{f}^{[\mathrm{g}]}_1 + m_2\,\vec{f}^{[\mathrm{g}]}_2 \tag{5.8}$$

(The fundamental grating frequencies $\vec{f}^{[\mathrm{g}]}_1$ and $\vec{f}^{[\mathrm{g}]}_2$ are defined by Eq's. 3.27-3.29, and the periodicity conditions, Eq's. 5.5 and 5.6, can be verified directly using Eq's. 5.7 and 3.29.) The coordinate representation of $\vec{f}^{[||]}_{m_1,m_2}$ is

$$\vec{f}^{[||]}_{m_1,m_2} = \hat{e}_2\, f_{2,m_1,m_2} + \hat{e}_3\, f_{3,m_1,m_2} \tag{5.9}$$

$$f_{2,m_1,m_2} = f^{[\mathrm{Inc}]}_2 + m_1\, f^{[\mathrm{g}]}_{2,1} + m_2\, f^{[\mathrm{g}]}_{2,2} \tag{5.10}$$

$$f_{3,m_1,m_2} = f^{[\mathrm{Inc}]}_3 + m_1\, f^{[\mathrm{g}]}_{3,1} + m_2\, f^{[\mathrm{g}]}_{3,2} \tag{5.11}$$

The magnetic field $\vec{H}$ is represented by a similar Fourier expansion,

$$\vec{H}[\vec{x}] = \sum_{m_1,m_2} ff\vec{H}_{m_1,m_2}[x_1] \exp[i\,2\pi\,\vec{f}^{[||]}_{m_1,m_2} \bullet \vec{x}] \tag{5.12}$$

Based on the order limit conditions, Eq's. 4.12 and 4.13, the field expansions in Eq's. 5.7 and 5.12 are truncated as follows,

$$\vec{E}[\vec{x}] \cong \sum_{m_2 \in \mathcal{M}_2} \sum_{m_1 \in \mathcal{M}_1[m_2]} ff\vec{E}_{m_1,m_2}[x_1] \exp[i\,2\pi\,\vec{f}^{[||]}_{m_1,m_2} \bullet \vec{x}] \tag{5.13}$$

$$\vec{H}[\vec{x}] \cong \sum_{m_2 \in \mathcal{M}_2} \sum_{m_1 \in \mathcal{M}_1[m_2]} ff\vec{H}_{m_1,m_2}[x_1] \exp[i\,2\pi\,\vec{f}^{[||]}_{m_1,m_2} \bullet \vec{x}] \tag{5.14}$$

6. The Maxwell Equations and homogeneous-medium solutions

The Maxwell Equations (in Gaussian units) for a time-periodic electromagnetic field in a linear, isotropic, non-magnetic medium are

$$\nabla \times \vec{E} = i\,\tfrac{2\pi}{\lambda}\,\vec{H} \tag{6.1}$$

$$\nabla\times\vec{H}=-i\tfrac{2\pi}{\lambda}\,\varepsilon\,\vec{E} \tag{6.2}$$

where λ is the wavelength in vacuum and ε is the complex permittivity. An implicit time-separable factor of $\exp[-i\,2\pi\,c\,t\,/\,\lambda]$ is assumed. (t is time and c is the speed of light in vacuum.) The minus sign in this time factor implies $\operatorname{Im}[\varepsilon]\geq 0$ (relation 3.4), assuming nonnegative conductivity. Scattered fields in an absorbing medium decay exponentially away from the grating (Eq's. 4.4, 4.6, 4.9-4.11).

Considering the case where ε is equal to a constant $\varepsilon^{[c]}$ (within some x_1 range),

$$\varepsilon[\vec{x}]=\varepsilon^{[c]} \tag{6.3}$$

substitution from Eq's. 5.7 and 5.12 in 6.1 and 6.2 yields

$$i\,2\pi\,\vec{f}^{[||]}_{m_1,m_2}\times ff\vec{E}_{m_1,m_2}[x_1]+\hat{e}_1\times\partial_1 ff\vec{E}_{m_1,m_2}[x_1]=i\tfrac{2\pi}{\lambda}\,ff\vec{H}_{m_1,m_2}[x_1] \tag{6.4}$$

$$i\,2\pi\,\vec{f}^{[||]}_{m_1,m_2}\times ff\vec{H}_{m_1,m_2}[x_1]+\hat{e}_1\times\partial_1 ff\vec{H}_{m_1,m_2}[x_1]=-i\tfrac{2\pi}{\lambda}\,\varepsilon^{[c]}\,ff\vec{E}_{m_1,m_2}[x_1] \tag{6.5}$$

(∂_1 represents the derivative with respect to x_1.) Particular solutions of these equations are of the form

$$ff\vec{E}_{m_1,m_2}[x_1]=\vec{A}^{[E]}\exp[i\,2\pi\,f_1\,x_1] \tag{6.6}$$

$$ff\vec{H}_{m_1,m_2}[x_1]=\vec{A}^{[H]}\exp[i\,2\pi\,f_1\,x_1] \tag{6.7}$$

where $\vec{A}^{[E]}$, $\vec{A}^{[H]}$, and f_1 are undetermined constants. Define

$$\vec{f}=\hat{e}_1\,f_1+\hat{e}_2\,f_2+\hat{e}_3\,f_3 \tag{6.8}$$

with

$$f_2=f_{2,m_1,m_2} \tag{6.9}$$

$$f_3=f_{3,m_1,m_2} \tag{6.10}$$

(cf. Eq. 5.9). Eq's. 6.4 and 6.5 reduce to

$$\vec{f}\times\vec{A}^{[E]}=\tfrac{1}{\lambda}\,\vec{A}^{[H]} \tag{6.11}$$

$$\vec{f}\times\vec{A}^{[H]}=-\tfrac{1}{\lambda}\,\varepsilon^{[c]}\,\vec{A}^{[E]} \tag{6.12}$$

The unit vector $\hat{s}$ is defined by[3]

$$\hat{s} = \hat{e}_2\, s_2 + \hat{e}_3\, s_3 \tag{6.13}$$

$$(s_2, \quad s_3) = \begin{cases} \dfrac{(-f_3, \quad f_2)}{\sqrt{(f_2)^2 + (f_3)^2}} & \text{if } (f_2)^2 + (f_3)^2 \neq 0 \\ \dfrac{\left(-f_{3,1}^{[g]}, \quad f_{2,1}^{[g]}\right)}{\sqrt{(f_{2,1}^{[g]})^2 + (f_{3,1}^{[g]})^2}} & \text{if } (f_2)^2 + (f_3)^2 = 0 \end{cases} \tag{6.14}$$

$\vec{f}$, $\hat{s}$, and $\hat{s} \times \vec{f}$ form an orthogonal set of basis vectors, and projecting Eq's. 6.11 and 6.12 onto these bases yields

$$\vec{f} \bullet \vec{A}^{[H]} = 0 \tag{6.15}$$

$$\vec{f} \bullet \vec{A}^{[E]} = 0 \tag{6.16}$$

$$(\hat{s} \times \vec{f}) \bullet \vec{A}^{[E]} = \tfrac{1}{\lambda}\, \hat{s} \bullet \vec{A}^{[H]} \tag{6.17}$$

$$(\hat{s} \times \vec{f}) \bullet \vec{A}^{[H]} = -\tfrac{1}{\lambda}\, \varepsilon^{[c]}\, \hat{s} \bullet \vec{A}^{[E]} \tag{6.18}$$

$$(\vec{f} \bullet \vec{f})(\hat{s} \bullet \vec{A}^{[E]}) = -\tfrac{1}{\lambda} (\hat{s} \times \vec{f}) \bullet \vec{A}^{[H]} \tag{6.19}$$

$$(\vec{f} \bullet \vec{f})(\hat{s} \bullet \vec{A}^{[H]}) = \tfrac{1}{\lambda}\, \varepsilon^{[c]} (\hat{s} \times \vec{f}) \bullet \vec{A}^{[E]} \tag{6.20}$$

By substituting Eq's. 6.17 and 6.18 on the right sides of 6.20 and 6.19, the following condition is obtained,

$$\vec{f} \bullet \vec{f} = \varepsilon^{[c]} / \lambda^2 \tag{6.21}$$

This condition determines the possible values for f_1,

$$f_1 = \pm \sqrt{\frac{\varepsilon^{[c]}}{\lambda^2} - (f_2)^2 - (f_3)^2} \tag{6.22}$$

(It is assumed here that f_1 is nonzero, although this limitation will later be removed.)

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[3] For the case $(f_2)^2 + (f_3)^2 = 0$, $\hat{s}$ could be just as well defined as any unit vector orthogonal to $\hat{e}_1$. Eq's. 6.14 makes the choice independent of the coordinate bases $\hat{e}_2$ and $\hat{e}_3$.

Define the unit vector

$$\hat{p} = \pm \hat{s} \times \left(\frac{\lambda}{\sqrt{\varepsilon^{[\mathrm{c}]}}} \vec{f} \right) = \pm \frac{\lambda}{\sqrt{\varepsilon^{[\mathrm{c}]}}} (\hat{e}_1 (s_2 f_3 - s_3 f_2) + (\hat{e}_2 s_3 - \hat{e}_3 s_2) f_1) \tag{6.23}$$

$\vec{A}^{[\mathrm{E}]}$ and $\vec{A}^{[\mathrm{H}]}$ are represented as

$$\vec{A}^{[\mathrm{E}]} = \hat{s} A_{\mathrm{s}}^{[\mathrm{E}]} + \hat{p} A_{\mathrm{p}}^{[\mathrm{E}]} \tag{6.24}$$

$$\vec{A}^{[\mathrm{H}]} = \pm(\hat{s} A_{\mathrm{s}}^{[\mathrm{H}]} + \hat{p} A_{\mathrm{p}}^{[\mathrm{H}]}) \tag{6.25}$$

This representation automatically satisfies Eq's. 6.15 and 6.16, and Eq's. 6.17 and 6.18 reduce to

$$A_{\mathrm{s}}^{[\mathrm{H}]} = \sqrt{\varepsilon^{[\mathrm{c}]}} A_{\mathrm{p}}^{[\mathrm{E}]} \tag{6.26}$$

$$A_{\mathrm{p}}^{[\mathrm{H}]} = -\sqrt{\varepsilon^{[\mathrm{c}]}} A_{\mathrm{s}}^{[\mathrm{E}]} \tag{6.27}$$

The "$\pm$" signs in Eq's. 6.23 and 6.25 are, by definition, correlated with the f_1 sign in Eq. 6.22. The definitions include these signs as a notational convenience, to make the equations symmetric with respect to inversion of the x_1 coordinate ($x_1 \leftarrow -x_1$). Normally, equations involving cross products would only be valid in a right-handed coordinate system, whereas the coordinate inversion makes the coordinate system left-handed. However, the equations are preserved by changing the signs of all cross products in the left-handed system. The $\pm$ sign in Eq. 6.23 makes this equation valid under x_1 inversion, and the $\pm$ sign in Eq. 6.25 implicitly changes the sign of $\vec{A}^{[\mathrm{H}]}$ under x_1 inversion (without changing $A_{\mathrm{s}}^{[\mathrm{H}]}$ or $A_{\mathrm{p}}^{[\mathrm{H}]}$) so that the cross-product relations 6.11 and 6.12 remain valid.

A plane wave is fully specified by its $\vec{E}$ field because its $\vec{H}$ field is determined by Eq's. 6.26 and 6.27. However, an alternative approach that will be more convenient in the analyses to follow is to specify the electromagnetic field in terms of the $\vec{E}$ and $\vec{H}$ fields' $\hat{s}$ projections ($A_{\mathrm{s}}^{[\mathrm{E}]}$ and $A_{\mathrm{s}}^{[\mathrm{H}]}$), and let the $\hat{p}$ projections ($A_{\mathrm{p}}^{[\mathrm{E}]}$ and $A_{\mathrm{p}}^{[\mathrm{H}]}$) be determined from Eq's. 6.26 and 6.27. This approach is advantageous because continuity conditions between strata are applied to the surface-tangential projections of $\vec{E}$ and $\vec{H}$, of which the fields' $\hat{s}$ projections are a component. The surface-tangential projections also include the projections onto vector $\hat{q}$, which are defined as

$$\hat{q} = \pm \hat{s} \times \hat{e}_1 = \pm(\hat{e}_2 s_3 - \hat{e}_3 s_2) \tag{6.28}$$

($\hat{q}$ is a surface-tangential unit vector orthogonal to $\hat{s}$, and a "$\pm$" sign is again included to make the definition invariant under x_1 sign inversion.) Using the following relation,

$$\hat{q}\bullet\hat{p} = \frac{\lambda}{\sqrt{\varepsilon^{[c]}}} f_1 \tag{6.29}$$

(from Eq's. 6.23 and 6.28) the following expressions for the surface-tangential fields are obtained from Eq's. 6.24-6.27,

$$\hat{s}\bullet\vec{A}^{[E]} = A_s^{[E]} \tag{6.30}$$

$$\hat{s}\bullet\vec{A}^{[H]} = \pm A_s^{[H]} \tag{6.31}$$

$$\hat{q}\bullet\vec{A}^{[E]} = \frac{\lambda}{\varepsilon^{[c]}} f_1\, A_s^{[H]} \tag{6.32}$$

$$\hat{q}\bullet\vec{A}^{[H]} = \mp\lambda\, f_1\, A_s^{[E]} \tag{6.33}$$

The surface-normal field projections are

$$\hat{e}_1\bullet\vec{A}^{[E]} = \hat{e}_1\bullet\hat{p}\, A_p^{[E]} = \mp\frac{\lambda}{\varepsilon^{[c]}}\sqrt{(f_2)^2+(f_3)^2}\, A_s^{[H]} \tag{6.34}$$

$$\hat{e}_1\bullet\vec{A}^{[H]} = \pm\hat{e}_1\bullet\hat{p}\, A_p^{[H]} = \lambda\sqrt{(f_2)^2+(f_3)^2}\, A_s^{[E]} \tag{6.35}$$

The above plane-wave equations can be restated in the context of general solutions of Eq's. 6.4 and 6.5. $\vec{f}$ is rewritten as $\vec{f}_{m_1,m_2}^{[\pm]}$ to indicate explicitly its dependence on the diffraction order indices and the sign choice in Eq. 6.22,

$$\vec{f}_{m_1,m_2}^{[\pm]} = \hat{e}_1\, f_{1,m_1,m_2}^{[\pm]} + \hat{e}_2\, f_{2,m_1,m_2}^{[\pm]} + \hat{e}_3\, f_{3,m_1,m_2}^{[\pm]} \tag{6.36}$$

$$f_{1,m_1,m_2}^{[\pm]} = \pm\sqrt{\frac{\varepsilon^{[c]}}{\lambda^2} - (f_{2,m_1,m_2})^2 - (f_{3,m_1,m_2})^2} \tag{6.37}$$

$$f_{2,m_1,m_2}^{[+]} = f_{2,m_1,m_2}^{[-]} = f_{2,m_1,m_2} \tag{6.38}$$

$$f_{3,m_1,m_2}^{[+]} = f_{3,m_1,m_2}^{[-]} = f_{3,m_1,m_2} \tag{6.39}$$

(cf. Eq's. 6.9, 6.10, and 6.22). $\hat{s}$, $\hat{p}$ and $\hat{q}$ are similarly rewritten as $\hat{s}_{m_1,m_2}$, $\hat{p}_{m_1,m_2}^{[\pm]}$ and $\hat{q}_{m_1,m_2}^{[\pm]}$,

$$\hat{s}_{m_1,m_2} = \hat{e}_2\, s_{2,m_1,m_2} + \hat{e}_3\, s_{3,m_1,m_2} \tag{6.40}$$

$$\left(s_{2,m_1,m_2},\quad s_{3,m_1,m_2}\right)=\begin{cases}\dfrac{\left(-f_{3,m_1,m_2},\quad f_{2,m_1,m_2}\right)}{\sqrt{(f_{2,m_1,m_2})^2+(f_{3,m_1,m_2})^2}} & \text{if } (f_{2,m_1,m_2})^2+(f_{3,m_1,m_2})^2\neq 0\\ \dfrac{\left(-f_{3,1}^{[\mathrm{g}]},\quad f_{2,1}^{[\mathrm{g}]}\right)}{\sqrt{(f_{2,1}^{[\mathrm{g}]})^2+(f_{3,1}^{[\mathrm{g}]})^2}} & \text{if } (f_{2,m_1,m_2})^2+(f_{3,m_1,m_2})^2=0\end{cases}\tag{6.41}$$

$$\begin{aligned}\hat{p}_{m_1,m_2}^{[\pm]}&=\pm\hat{s}_{m_1,m_2}\times\left(\frac{\lambda}{\sqrt{\varepsilon^{[\mathrm{c}]}}}\vec{f}_{m_1,m_2}^{[\pm]}\right)\\&=\frac{\lambda}{\sqrt{\varepsilon^{[\mathrm{c}]}}}\left(\pm\hat{e}_1\left(s_{2,m_1,m_2}\,f_{3,m_1,m_2}-s_{3,m_1,m_2}\,f_{2,m_1,m_2}\right)+\left(\hat{e}_2\,s_{3,m_1,m_2}-\hat{e}_3\,s_{2,m_1,m_2}\right)f_{1,m_1,m_2}^{[+]}\right)\end{aligned}\tag{6.42}$$

$$\hat{q}_{m_1,m_2}^{[\pm]}=\pm\hat{s}_{m_1,m_2}\times\hat{e}_1=\pm(\hat{e}_2\,s_{3,m_1,m_2}-\hat{e}_3\,s_{2,m_1,m_2})\tag{6.43}$$

(cf. Eq's. 6.13, 6.14, 6.23, and 6.28). General solutions of Eq's. 6.4 and 6.5 comprise "up" and "down" waves, which are identified by "+" and "–" labels,

$$f\!f\vec{E}_{m_1,m_2}[x_1]=f\!f\vec{E}_{m_1,m_2}^{[+]}[x_1]+f\!f\vec{E}_{m_1,m_2}^{[-]}[x_1]\tag{6.44}$$

$$f\!f\vec{H}_{m_1,m_2}[x_1]=f\!f\vec{H}_{m_1,m_2}^{[+]}[x_1]+f\!f\vec{H}_{m_1,m_2}^{[-]}[x_1]\tag{6.45}$$

where $f\!f\vec{E}_{m_1,m_2}^{[\pm]}[x_1]$ and $f\!f\vec{H}_{m_1,m_2}^{[\pm]}[x_1]$ have the functional form

$$f\!f\vec{E}_{m_1,m_2}^{[\pm]}[x_1]=\vec{A}_{m_1,m_2}^{[\mathrm{E},\pm]}\exp[i\,2\pi\,f_{1,m_1,m_2}^{[\pm]}\,x_1]\tag{6.46}$$

$$f\!f\vec{H}_{m_1,m_2}^{[\pm]}[x_1]=\vec{A}_{m_1,m_2}^{[\mathrm{H},\pm]}\exp[i\,2\pi\,f_{1,m_1,m_2}^{[\pm]}\,x_1]\tag{6.47}$$

(cf. Eq's. 6.6 and 6.7). These functions can be represented in terms of their $\hat{s}$ and $\hat{p}$ projections,

$$f\!f\vec{E}_{m_1,m_2}^{[\pm]}[x_1]=\hat{s}_{m_1,m_2}\;f\!fE_{\mathrm{s},m_1,m_2}^{[\pm]}[x_1]+\hat{p}_{m_1,m_2}^{[\pm]}\;f\!fE_{\mathrm{p},m_1,m_2}^{[\pm]}[x_1]\tag{6.48}$$

$$f\!f\vec{H}_{m_1,m_2}^{[\pm]}[x_1]=\pm(\hat{s}_{m_1,m_2}\;f\!fH_{\mathrm{s},m_1,m_2}^{[\pm]}[x_1]+\hat{p}_{m_1,m_2}^{[\pm]}\;f\!fH_{\mathrm{p},m_1,m_2}^{[\pm]}[x_1])\tag{6.49}$$

(As with Eq. 6.25, the $\pm$ sign factor in Eq. 6.49 is included as a notational convenience, to preserve invariance of cross-product relationships under x_1 sign inversion.) The $\hat{s}$ and $\hat{p}$ projections satisfy the following relationships,

$$f\!fH_{\mathrm{s},m_1,m_2}^{[\pm]}[x_1]=\sqrt{\varepsilon^{[\mathrm{c}]}}\;f\!fE_{\mathrm{p},m_1,m_2}^{[\pm]}[x_1]\tag{6.50}$$

$$ffH^{[\pm]}_{\mathrm{p},m_1,m_2}[x_1] = -\sqrt{\varepsilon^{[\mathrm{c}]}}\; ffE^{[\pm]}_{\mathrm{s},m_1,m_2}[x_1] \tag{6.51}$$

(cf. Eq's. 6.26 and 6.27); hence only the $\hat{s}$ projections need be specified. Surface continuity conditions between strata apply to the fields' projections onto $\hat{s}$ and $\hat{q}$, which are defined as

$$\hat{s}_{m_1,m_2} \bullet ff\vec{E}_{m_1,m_2}[x_1] = ffE^{[+]}_{\mathrm{s},m_1,m_2}[x_1] + ffE^{[-]}_{\mathrm{s},m_1,m_2}[x_1] \tag{6.52}$$

$$\hat{s}_{m_1,m_2} \bullet ff\vec{H}_{m_1,m_2}[x_1] = ffH^{[+]}_{\mathrm{s},m_1,m_2}[x_1] - ffH^{[-]}_{\mathrm{s},m_1,m_2}[x_1] \tag{6.53}$$

$$\hat{q}^{[+]}_{m_1,m_2} \bullet ff\vec{E}_{m_1,m_2}[x_1] = \frac{\lambda}{\varepsilon^{[\mathrm{c}]}} f^{[+]}_{1,m_1,m_2}\,(ffH^{[+]}_{\mathrm{s},m_1,m_2}[x_1] + ffH^{[-]}_{\mathrm{s},m_1,m_2}[x_1]) \tag{6.54}$$

$$\hat{q}^{[+]}_{m_1,m_2} \bullet ff\vec{H}_{m_1,m_2}[x_1] = -\lambda\, f^{[+]}_{1,m_1,m_2}\,(ffE^{[+]}_{\mathrm{s},m_1,m_2}[x_1] - ffE^{[-]}_{\mathrm{s},m_1,m_2}[x_1]) \tag{6.55}$$

(cf. Eq's. 6.30-6.33). Generalizing from Eq's. 6.34 and 6.35, the following expressions for the surface-normal fields are obtained from Eq's. 6.48 and 6.49.

$$\begin{aligned} ffE^{[\pm]}_{1,m_1,m_2}[x_1] &= \mp\frac{\lambda}{\varepsilon^{[\mathrm{c}]}}\sqrt{(f_{2,m_1,m_2})^2 + (f_{3,m_1,m_2})^2}\; ffH^{[\pm]}_{\mathrm{s},m_1,m_2}[x_1] \\ &= -\frac{\lambda}{\varepsilon^{[\mathrm{c}]}}(f_{2,m_1,m_2}\; ffH^{[\pm]}_{3,m_1,m_2}[x_1] - f_{3,m_1,m_2}\; ffH^{[\pm]}_{2,m_1,m_2}[x_1]) \end{aligned} \tag{6.56}$$

$$\begin{aligned} ffH^{[\pm]}_{1,m_1,m_2}[x_1] &= \lambda\sqrt{(f_{2,m_1,m_2})^2 + (f_{3,m_1,m_2})^2}\; ffE^{[\pm]}_{\mathrm{s},m_1,m_2}[x_1] \\ &= \lambda\,(f_{2,m_1,m_2}\; ffE^{[\pm]}_{3,m_1,m_2}[x_1] - f_{3,m_1,m_2}\; ffE^{[\pm]}_{2,m_1,m_2}[x_1]) \end{aligned} \tag{6.57}$$

where

$$ffE^{[\pm]}_{j,m_1,m_2}[x_1] = \hat{e}_j \bullet ff\vec{E}^{[\pm]}_{m_1,m_2}[x_1], \quad ffH^{[\pm]}_{j,m_1,m_2}[x_1] = \hat{e}_j \bullet ff\vec{H}^{[\pm]}_{m_1,m_2}[x_1], \quad j = 1,2,3 \tag{6.58}$$

7. S matrices

Although the plane-wave equations of Section 6 only apply in a homogeneous region, they can be formally adopted to apply throughout the grating structure. An infinitesimally thin, homogeneous layer of permittivity $\varepsilon^{[\mathrm{c}]}$ is interposed in the grating structure at any particular x_1 level. The layer is too thin to significantly affect the electromagnetic field outside the layer, but within the layer the field comprises up and down waves, as described above. The up/down field decomposition could lead to numerical indeterminacy or instability when $f^{[\pm]}_{1,m_1,m_2}$ is zero or close to zero for some particular order (cf. Eq. 6.37), but this possibility is avoided by defining $\varepsilon^{[\mathrm{c}]}$ to have a positive imaginary part.

The electromagnetic field transformation across a plane-bounded region sandwiched between two homogeneous layers is described in terms of an "S matrix", which represents the linear relationship between the fields entering and exiting the region. ("S" connotes "scattering".) This is illustrated conceptually in Figure 6. In this figure, $F^{[+]}[x_1]$ represents a column vector that includes all of the up-wave amplitudes $\mathit{ff}E^{[+]}_{\mathrm{s},m_1,m_2}[x_1]$ and $\mathit{ff}H^{[+]}_{\mathrm{s},m_1,m_2}[x_1]$, and $F^{(-)}[x_1]$ is a column vector including all of the down-wave amplitudes $\mathit{ff}E^{[-]}_{\mathrm{s},m_1,m_2}[x_1]$ and $\mathit{ff}H^{[-]}_{\mathrm{s},m_1,m_2}[x_1]$. (The ordering of the amplitudes in $F^{[+]}$ and $F^{[-]}$ is described in Section 9.) The S matrix characterizes a grating region in the x_1 interval $x_1^{[0]} < x_1 < x_1^{[1]}$, and it defines a linear mapping between fields at the stratum boundaries. The fields entering the region include the up waves entering from the bottom $(F^{[+]}[x_1^{[0]}])$ and the down waves entering from the top $(F^{[-]}[x_1^{[1]}])$, and the fields exiting the region include the down waves at the bottom $(F^{[-]}[x_1^{[0]}])$ and the up waves at the top $(F^{[+]}[x_1^{[1]}])$. The S matrix comprises submatrices ("quadrants") $S^{[++]}$, $S^{[+-]}$, $S^{[-+]}$, and $S^{[--]}$ ("S-up-up", "S-up-down", etc.), and the mapping between the entering and exiting fields is

$$\begin{pmatrix} F^{[+]}[x_1^{[1]}] \\ F^{[-]}[x_1^{[0]}] \end{pmatrix} = \begin{pmatrix} S^{[++]} & S^{[+-]} \\ S^{[-+]} & S^{[--]} \end{pmatrix} \begin{pmatrix} F^{[+]}[x_1^{[0]}] \\ F^{[-]}[x_1^{[1]}] \end{pmatrix} \tag{7.1}$$

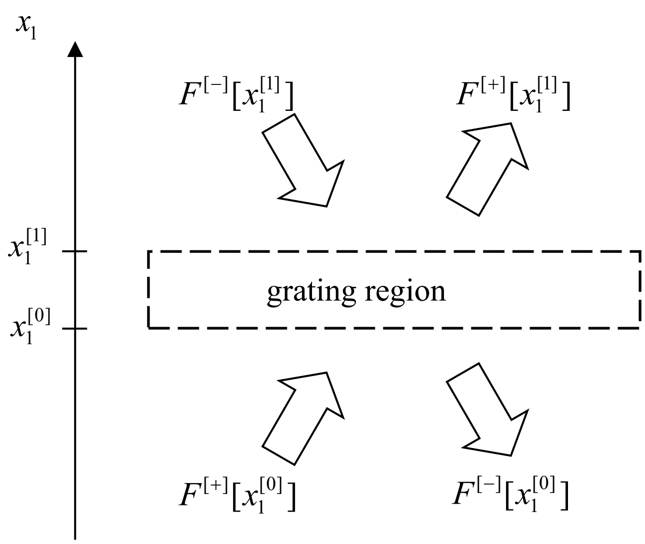

Figure 6. Up and down waves entering and exiting a grating region.

The grating analysis represents all stratum interfaces as infinitesimally thin, homogeneous layers ("fictitious layers"), with the permittivity constant ($\varepsilon^{[\mathrm{c}]}$ in Section 6, Eq. 6.3) denoted as $\varepsilon^{[\mathrm{f}]}$ in the fictitious layers. (The "f" superscript connotes "fictitious".) Separate S matrices are computed for all strata and for the substrate and superstrate boundary interfaces. A "stacking" algorithm described in Section 8 is used to combine these S matrices into a composite S matrix for the entire grating structure (i.e., with $x_1^{[0]} = b_1^{[0]} - 0$ and $x_1^{[1]} = b_1^{[L_1]} + 0$ in Eq. 7.1, where "-0" and "$+0$" mean x_1 limits from below and above, respectively, and the b_1 values define the grating boundaries, Eq's. 3.2 and 3.3).

The stacking is performed from bottom to top. The initial value of the S matrix below the grating (i.e., with $x_1^{[1]} = x_1^{[0]} = b_1[0] - 0$) is given by the condition

$$x_1^{[1]} = x_1^{[0]} \quad \to \quad S^{[++]} = S^{[--]} = \mathbf{I}, \quad S^{[+-]} = S^{[-+]} = \mathbf{0} \tag{7.2}$$

where "$\mathbf{0}$" is a zero matrix and "$\mathbf{I}$" is an identity matrix. The stacking operations progressively move $x_1^{[1]}$ up through the grating until $x_1^{[1]} = b_1^{[L_1]} + 0$. At each stage of the stacking operation only $S^{[+-]}$ and $S^{[--]}$ need to be calculated because $F^{[+]}[x_1^{[0]}]$ is zero with $x_1^{[0]} = b_1^{[0]} - 0$ in Eq. 7.1 (i.e., there is no incident field entering the grating from the substrate side):

$$\begin{pmatrix} F^{[+]}[x_1^{[1]}] \\ F^{[-]}[x_1^{[0]}] \end{pmatrix} = \begin{pmatrix} S^{[+-]} \\ S^{[--]} \end{pmatrix} F^{[-]}[x_1^{[1]}] \quad \left(\text{with } F^{[+]}[x_1^{[0]}] = \mathbf{0}\right) \tag{7.3}$$

The S matrix computation for an individual stratum is simplified somewhat by taking advantage of the following symmetry relations,

$$\left.\begin{array}{l} S^{[++]} = S^{[--]} \\ S^{[+-]} = S^{[-+]} \end{array}\right\} \text{ for a stratum} \tag{7.4}$$

This is a consequence of the x_1-independence of the permittivity within the stratum, and the identical permittivities $\varepsilon^{[\mathrm{f}]}$ above and below the stratum. Also, this condition relies on the magnetic field sign convention represented by the "$\pm$" in Eq's. 6.25 and 6.49. (Eq's. 7.4 are proved in Section 13.)

The stacking operation described above can be used to efficiently compute the diffracted field outside the grating, but if the field inside the grating must be determined a slightly different approach, outlined in Appendix B, is used.

The S-matrix quadrants $S^{[++]}$, $S^{[+-]}$, $S^{[-+]}$, and $S^{[--]}$ are diagonal or block-diagonal for some stratum types, and Section 9 outlines how the S matrix calculations are structured to take advantage of the matrix sparsity. Sections 10 through 16 derive algorithms for computing S matrices specifically for boundary surfaces, coordinate breaks, homogeneous strata, uniperiodic strata, and biperiodic strata.

8. S matrix stacking

The S-matrices across two adjacent x_1 intervals are "stacked" to determine a composite S matrix covering both intervals, as follows. An S matrix Sa covers the interval from $x_1 = x_1^{[0]}$ to $x_1 = x_1^{[1]}$, and a second S matrix Sb covers the interval from $x_1 = x_1^{[1]}$ to $x_1 = x_1^{[2]}$,

$$\begin{pmatrix} F^{[+]}[x_1^{[1]}] \\ F^{[-]}[x_1^{[0]}] \end{pmatrix} = \begin{pmatrix} Sa^{[++]} & Sa^{[+-]} \\ Sa^{[-+]} & Sa^{[--]} \end{pmatrix} \begin{pmatrix} F^{[+]}[x_1^{[0]}] \\ F^{[-]}[x_1^{[1]}] \end{pmatrix} \tag{8.1}$$

$$\begin{pmatrix} F^{[+]}[x_1^{[2]}] \\ F^{[-]}[x_1^{[1]}] \end{pmatrix} = \begin{pmatrix} Sb^{[++]} & Sb^{[+-]} \\ Sb^{[-+]} & Sb^{[--]} \end{pmatrix} \begin{pmatrix} F^{[+]}[x_1^{[1]}] \\ F^{[-]}[x_1^{[2]}] \end{pmatrix} \tag{8.2}$$

(from Eq. 7.1). Sa and Sb determine a composite S matrix covering the combined interval from $x_1 = x_1^{[0]}$ to $x_1 = x_1^{[2]}$,

$$\begin{pmatrix} F^{[+]}[x_1^{[2]}] \\ F^{[-]}[x_1^{[0]}] \end{pmatrix} = \begin{pmatrix} S^{[++]} & S^{[+-]} \\ S^{[-+]} & S^{[--]} \end{pmatrix} \begin{pmatrix} F^{[+]}[x_1^{[0]}] \\ F^{[-]}[x_1^{[2]}] \end{pmatrix} \tag{8.3}$$

Eq’s. 8.1 and 8.2 are stated equivalently as

$$\begin{pmatrix} \mathbf{I} & -Sa^{[+-]} \\ \mathbf{0} & Sa^{[--]} \end{pmatrix} \begin{pmatrix} F^{[+]}[x_1^{[1]}] \\ F^{[-]}[x_1^{[1]}] \end{pmatrix} = \begin{pmatrix} Sa^{[++]} & \mathbf{0} \\ -Sa^{[-+]} & \mathbf{I} \end{pmatrix} \begin{pmatrix} F^{[+]}[x_1^{[0]}] \\ F^{[-]}[x_1^{[0]}] \end{pmatrix} \tag{8.4}$$

$$\begin{pmatrix} \mathbf{I} & -Sb^{[+-]} \\ \mathbf{0} & Sb^{[--]} \end{pmatrix} \begin{pmatrix} F^{[+]}[x_1^{[2]}] \\ F^{[-]}[x_1^{[2]}] \end{pmatrix} = \begin{pmatrix} Sb^{[++]} & \mathbf{0} \\ -Sb^{[-+]} & \mathbf{I} \end{pmatrix} \begin{pmatrix} F^{[+]}[x_1^{[1]}] \\ F^{[-]}[x_1^{[1]}] \end{pmatrix} \tag{8.5}$$

$F^{[\pm]}[x_1^{[1]}]$ is eliminated from these equations,

$$\begin{aligned} &\begin{pmatrix} \mathbf{I} & Sa^{[+-]}\,(Sa^{[--]})^{-1} \\ \mathbf{0} & (Sa^{[--]})^{-1} \end{pmatrix} \begin{pmatrix} Sa^{[++]} & \mathbf{0} \\ -Sa^{[-+]} & \mathbf{I} \end{pmatrix} \begin{pmatrix} F^{[+]}[x_1^{[0]}] \\ F^{[-]}[x_1^{[0]}] \end{pmatrix} = \begin{pmatrix} F^{[+]}[x_1^{[1]}] \\ F^{[-]}[x_1^{[1]}] \end{pmatrix} \\ &= \begin{pmatrix} (Sb^{[++]})^{-1} & \mathbf{0} \\ Sb^{[-+]}\,(Sb^{[++]})^{-1} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{I} & -Sb^{[+-]} \\ \mathbf{0} & Sb^{[--]} \end{pmatrix} \begin{pmatrix} F^{[+]}[x_1^{[2]}] \\ F^{[-]}[x_1^{[2]}] \end{pmatrix} \end{aligned} \tag{8.6}$$

The incoming and outgoing field amplitudes are separated on opposite sides of the equation,

$$\begin{aligned} &\begin{pmatrix} \mathbf{I} & -Sa^{[+-]} \\ -Sb^{[-+]} & \mathbf{I} \end{pmatrix} \begin{pmatrix} (Sb^{[++]})^{-1} & \mathbf{0} \\ \mathbf{0} & (Sa^{[--]})^{-1} \end{pmatrix} \begin{pmatrix} F^{[+]}[x_1^{[2]}] \\ F^{[-]}[x_1^{[0]}] \end{pmatrix} \\ &= \left(\begin{pmatrix} Sa^{[++]} & \mathbf{0} \\ \mathbf{0} & Sb^{[--]} \end{pmatrix} + \begin{pmatrix} \mathbf{I} & -Sa^{[+-]} \\ -Sb^{[-+]} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{0} & (Sb^{[++]})^{-1}\,Sb^{[+-]} \\ (Sa^{[--]})^{-1}\,Sa^{[-+]} & \mathbf{0} \end{pmatrix} \right) \begin{pmatrix} F^{[+]}[x_1^{[0]}] \\ F^{[-]}[x_1^{[2]}] \end{pmatrix} \end{aligned} \tag{8.7}$$

Comparing this with Eq. 8.3, the combined S matrix is

$$\begin{pmatrix} S^{[++]} & S^{[+-]} \\ S^{[-+]} & S^{[--]} \end{pmatrix} = \left(\begin{pmatrix} Sb^{[++]} & \mathbf{0} \\ \mathbf{0} & Sa^{[--]} \end{pmatrix} \begin{pmatrix} \mathbf{I} & -Sa^{[+-]} \\ -Sb^{[-+]} & \mathbf{I} \end{pmatrix}^{-1} \left(\begin{pmatrix} Sa^{[++]} & \mathbf{0} \\ \mathbf{0} & Sb^{[--]} \end{pmatrix} + \begin{pmatrix} \mathbf{I} & -Sa^{[+-]} \\ -Sb^{[-+]} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{0} & (Sb^{[++]})^{-1} Sb^{[+-]} \\ (Sa^{[--]})^{-1} Sa^{[-+]} & \mathbf{0} \end{pmatrix} \right) \right)$$

$$= \begin{pmatrix} Sb^{[++]} (\mathbf{I} - Sa^{[+-]} Sb^{[-+]})^{-1} Sa^{[++]} & Sb^{[+-]} + Sb^{[++]} Sa^{[+-]} (\mathbf{I} - Sb^{[-+]} Sa^{[+-]})^{-1} Sb^{[--]} \\ Sa^{[-+]} + Sa^{[--]} Sb^{[-+]} (\mathbf{I} - Sa^{[+-]} Sb^{[-+]})^{-1} Sa^{[++]} & Sa^{[--]} (\mathbf{I} - Sb^{[-+]} Sa^{[+-]})^{-1} Sb^{[--]} \end{pmatrix} \tag{8.8}$$

As noted in Section 7, only $S^{[+-]}$ and $S^{[--]}$ need to be calculated when the S matrix stacking is performed from bottom to top. Eq. 8.8 is applied with Sa representing a multilayer stack and Sb representing an individual stratum added to the top of the stack. Note that in Eq. 8.8 $S^{[+-]}$ and $S^{[--]}$ do not depend on $Sa^{[++]}$ or $Sa^{[-+]}$. Thus, $Sa^{[++]}$ and $Sa^{[-+]}$ need not be specified, and $S^{[++]}$ and $S^{[-+]}$ are not calculated. If $S^{[++]}$ and $S^{[-+]}$ are required, they can be efficiently calculated using top-to-bottom stacking operations because $S^{[++]}$ and $S^{[-+]}$ do not depend on $Sb^{[+-]}$ or $Sb^{[--]}$.

$S^{[++]}$ and $S^{[-+]}$ share the common subexpression $(\mathbf{I} - Sa^{[+-]} Sb^{[-+]})^{-1} Sa^{[++]}$ in Eq. 8.8, while $S^{[+-]}$ and $S^{[--]}$ share the common subexpression $(\mathbf{I} - Sb^{[-+]} Sa^{[+-]})^{-1} Sb^{[--]}$. A slightly different but equivalent form of Eq. 8.8 is obtained by using the identities

$$Sb^{[-+]} (\mathbf{I} - Sa^{[+-]} Sb^{[-+]})^{-1} = (\mathbf{I} - Sb^{[-+]} Sa^{[+-]})^{-1} Sb^{[-+]} \tag{8.9}$$

$$Sa^{[+-]} (\mathbf{I} - Sb^{[-+]} Sa^{[+-]})^{-1} = (\mathbf{I} - Sa^{[+-]} Sb^{[-+]})^{-1} Sa^{[+-]} \tag{8.10}$$

These are applied in Eq. 8.8 to obtain

$$\begin{pmatrix} S^{[++]} & S^{[+-]} \\ S^{[-+]} & S^{[--]} \end{pmatrix} = \begin{pmatrix} Sb^{[++]} (\mathbf{I} - Sa^{[+-]} Sb^{[-+]})^{-1} Sa^{[++]} & Sb^{[+-]} + Sb^{[++]} (\mathbf{I} - Sa^{[+-]} Sb^{[-+]})^{-1} Sa^{[+-]} Sb^{[--]} \\ Sa^{[-+]} + Sa^{[--]} (\mathbf{I} - Sb^{[-+]} Sa^{[+-]})^{-1} Sb^{[-+]} Sa^{[++]} & Sa^{[--]} (\mathbf{I} - Sb^{[-+]} Sa^{[+-]})^{-1} Sb^{[--]} \end{pmatrix} \tag{8.11}$$

In this equation $S^{[++]}$ and $S^{[+-]}$ share the subexpression $Sb^{[++]} (\mathbf{I} - Sa^{[+-]} Sb^{[-+]})^{-1}$, while $S^{[-+]}$ and $S^{[--]}$ share the subexpression $Sa^{[--]} (\mathbf{I} - Sb^{[-+]} Sa^{[+-]})^{-1}$. This form of the equation is used for internal field calculations (Appendix B).

9. Order enumeration and index partitioning

In principle, the $F^{[\pm]}[x_1]$ column vectors in Eq. 7.1 contain an infinite number of elements including all of the wave amplitudes $f\!fE^{[\pm]}_{\mathrm{s},m_1,m_2}[x_1]$ and $f\!fH^{[\pm]}_{\mathrm{s},m_1,m_2}[x_1]$ for diffraction order indices m_1 and m_2 ranging from $-\infty$ to ∞. Each element of $F^{[\pm]}[x_1]$ represents a wave amplitude $f\!fE^{[\pm]}_{\mathrm{s},m_1,m_2}[x_1]$ or $f\!fH^{[\pm]}_{\mathrm{s},m_1,m_2}[x_1]$ for some order index triple (m_1, m_2, P) including the order indices m_1 and m_2, and a "polarization index" P, which is either 'E' or 'H'. In practice, the order indices are limited to a finite set $\boldsymbol{\mathcal{M}}$ defined by Eq's. 4.12 and 4.13.

$$\boldsymbol{\mathcal{M}} = \{(m_1, m_2) : m_2 \in \boldsymbol{\mathcal{M}}_2,\, m_1 \in \boldsymbol{\mathcal{M}}_1[m_2]\} \tag{9.1}$$

The $F^{[\pm]}$ elements are denoted as $F^{[\pm]}_{(m_1,m_2,P)}$, where

$$F^{[\pm]}_{(m_1,m_2,\mathrm{E})}[x_1] = f\!fE^{[\pm]}_{\mathrm{s},m_1,m_2}[x_1], \quad F^{[\pm]}_{(m_1,m_2,\mathrm{H})}[x_1] = f\!fH^{[\pm]}_{\mathrm{s},m_1,m_2}[x_1] \tag{9.2}$$

The parenthetical grouping of the subscripts (m_1, m_2, P) indicates that $F^{[\pm]}$ is to be viewed as a partitioned vector (a column), not as a multidimensional array. The S matrix quadrants $S^{[\pm,\pm']}$ are correspondingly structured as partitioned matrices with the matrix element coupling $F^{[\pm]}_{(m_1,m_2,P)}$ and $F^{[\pm']}_{(m_1',m_2',P')}$ denoted as $S^{[\pm,\pm']}_{(m_1,m_2,P),(m_1',m_2',P')}$. In practice the multi-level indices can be replaced by scalar enumeration indices 1, 2, …, which serialize the (m_1, m_2, P) index triplets.

The index set $\boldsymbol{\mathcal{M}}$ can often be partitioned into multiple disjoint subsets $\boldsymbol{\mathcal{M}}^{[1]}$, $\boldsymbol{\mathcal{M}}^{[2]}$, … ("decoupled index sets") such that there is no amplitude coupling between wave amplitudes of different sets within a particular grating layer. (The index partitioning generally differs for different layers.) Eq. 7.1 represents a summation relation of the general form

$$\begin{pmatrix} F^{[+]}_{(m_1,m_2,P)}[x_1^{[1]}] \\ F^{[-]}_{(m_1,m_2,P)}[x_1^{[0]}] \end{pmatrix} = \sum_{\substack{(m_1',m_2')\in\boldsymbol{\mathcal{M}} \\ P'\in\{\mathrm{E},\mathrm{H}\}}} \begin{pmatrix} S^{[++]}_{(m_1,m_2,P),(m_1',m_2',P')} & S^{[+-]}_{(m_1,m_2,P),(m_1',m_2',P')} \\ S^{[-+]}_{(m_1,m_2,P),(m_1',m_2',P')} & S^{[--]}_{(m_1,m_2,P),(m_1',m_2',P')} \end{pmatrix} \begin{pmatrix} F^{[+]}_{(m_1',m_2',P')}[x_1^{[0]}] \\ F^{[-]}_{(m_1',m_2',P')}[x_1^{[1]}] \end{pmatrix}$$
$$\text{for } (m_1, m_2) \in \boldsymbol{\mathcal{M}},\ P \in \{\mathrm{E},\mathrm{H}\} \tag{9.3}$$

But with decoupling this relation separates into equations of the following form in which all order indices are limited to one index set $\boldsymbol{\mathcal{M}}^{[j]}$,

$$\begin{pmatrix} F^{[+]}_{(m_1,m_2,P)}[x_1^{[1]}] \\ F^{[-]}_{(m_1,m_2,P)}[x_1^{[0]}] \end{pmatrix} = \sum_{\substack{(m_1',m_2')\in\boldsymbol{\mathcal{M}}^{[j]} \\ P'\in\{\mathrm{E},\mathrm{H}\}}} \begin{pmatrix} S^{[++]}_{(m_1,m_2,P),(m_1',m_2',P')} & S^{[+-]}_{(m_1,m_2,P),(m_1',m_2',P')} \\ S^{[-+]}_{(m_1,m_2,P),(m_1',m_2',P')} & S^{[--]}_{(m_1,m_2,P),(m_1',m_2',P')} \end{pmatrix} \begin{pmatrix} F^{[+]}_{(m_1',m_2',P')}[x_1^{[0]}] \\ F^{[-]}_{(m_1',m_2',P')}[x_1^{[1]}] \end{pmatrix}$$
$$\text{for } (m_1, m_2) \in \boldsymbol{\mathcal{M}}^{[j]},\ P \in \{\mathrm{E},\mathrm{H}\} \tag{9.4}$$

In applying the stacking operation (Eq. 8.8) to combine S matrices Sa and Sb into a single matrix S, the decoupled index sets $\mathcal{M}^{[j]}$ of Sa and Sb are merged, if necessary, so that the same index partitioning is used for Sa, Sb, and S.

10. The S matrix for a boundary surface

In defining the S matrix for a boundary surface between two homogeneous regions via Eq. 7.1, $x_1^{[0]}$ is immediately below the surface and $x_1^{[1]}$ is immediately above it; see Figure 7. (The difference $x_1^{[1]} - x_1^{[0]}$ is infinitesimal.) The permittivity below the surface is denoted $\varepsilon^{[0]}$, and the permittivity above the surface is denoted $\varepsilon^{[1]}$.

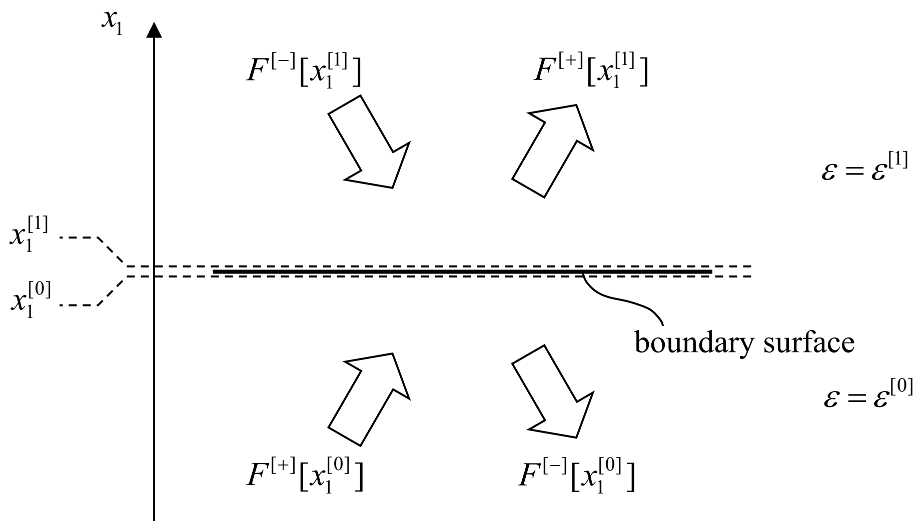

Figure 7. Up and down waves crossing a boundary surface.

The $\vec{E}$ and $\vec{H}$ fields' surface-tangential projections are continuous across the boundary surface. These projections are defined by Eq's. 6.52-6.55 for Fourier order (m_1, m_2). In Eq. 6.54 and in the definition of $f_1^{[+]}$ (Eq. 6.37) $\varepsilon^{[c]}$ is equal to $\varepsilon^{[0]}$ below the surface and is $\varepsilon^{[1]}$ above the surface, and the two corresponding $f_1^{[+]}$ values are indicated as $f_1^{[0,+]}$ and $f_1^{[1,+]}$.

$$f_{1,m_1,m_2}^{[0,+]} = +\sqrt{\frac{\varepsilon^{[0]}}{\lambda^2} - (f_{2,m_1,m_2})^2 - (f_{3,m_1,m_2})^2} \tag{10.1}$$

$$f_{1,m_1,m_2}^{[1,+]} = +\sqrt{\frac{\varepsilon^{[1]}}{\lambda^2} - (f_{2,m_1,m_2})^2 - (f_{3,m_1,m_2})^2} \tag{10.2}$$

(In the present context, either of the above values could be zero.) With these notational substitutions, the continuity conditions are, from Eq's. 6.52-6.55,

$$ffE_{s,m_1,m_2}^{[+]}[x_1^{[1]}] + ffE_{s,m_1,m_2}^{[-]}[x_1^{[1]}] = ffE_{s,m_1,m_2}^{[+]}[x_1^{[0]}] + ffE_{s,m_1,m_2}^{[-]}[x_1^{[0]}] \tag{10.3}$$

$$ffH_{s,m_1,m_2}^{[+]}[x_1^{[1]}] - ffH_{s,m_1,m_2}^{[-]}[x_1^{[1]}] = ffH_{s,m_1,m_2}^{[+]}[x_1^{[0]}] - ffH_{s,m_1,m_2}^{[-]}[x_1^{[0]}] \tag{10.4}$$

$$\frac{f_{1,m_1,m_2}^{[1,+]}}{\varepsilon^{[1]}}(ffH_{s,m_1,m_2}^{[+]}[x_1^{[1]}] + ffH_{s,m_1,m_2}^{[-]}[x_1^{[1]}]) = \frac{f_{1,m_1,m_2}^{[0,+]}}{\varepsilon^{[0]}}(ffH_{s,m_1,m_2}^{[+]}[x_1^{[0]}] + ffH_{s,m_1,m_2}^{[-]}[x_1^{[0]}]) \tag{10.5}$$

$$f_{1,m_1,m_2}^{[1,+]}(ffE_{s,m_1,m_2}^{[+]}[x_1^{[1]}] - ffE_{s,m_1,m_2}^{[-]}[x_1^{[1]}]) = f_{1,m_1,m_2}^{[0,+]}(ffE_{s,m_1,m_2}^{[+]}[x_1^{[0]}] - ffE_{s,m_1,m_2}^{[-]}[x_1^{[0]}]) \tag{10.6}$$

These conditions are equivalently restated as following,

$$\begin{pmatrix} ffE_{s,m_1,m_2}^{[+]}[x_1^{[1]}] \\ ffE_{s,m_1,m_2}^{[-]}[x_1^{[0]}] \end{pmatrix} = \frac{1}{f_{1,m_1,m_2}^{[1,+]} + f_{1,m_1,m_2}^{[0,+]}} \cdot \begin{pmatrix} 2\,f_{1,m_1,m_2}^{[0,+]} & f_{1,m_1,m_2}^{[1,+]} - f_{1,m_1,m_2}^{[0,+]} \\ f_{1,m_1,m_2}^{[0,+]} - f_{1,m_1,m_2}^{[+,1]} & 2\,f_{1,m_1,m_2}^{[1,+]} \end{pmatrix} \begin{pmatrix} ffE_{s,m_1,m_2}^{[+]}[x_1^{[0]}] \\ ffE_{s,m_1,m_2}^{[-]}[x_1^{[1]}] \end{pmatrix} \tag{10.7}$$

$$\begin{pmatrix} ffH_{s,m_1,m_2}^{[+]}[x_1^{[1]}] \\ ffH_{s,m_1,m_2}^{[-]}[x_1^{[0]}] \end{pmatrix} = \frac{1}{\dfrac{f_{1,m_1,m_2}^{[1,+]}}{\varepsilon^{[1]}} + \dfrac{f_{1,m_1,m_2}^{[0,+]}}{\varepsilon^{[0]}}} \cdot \begin{pmatrix} \dfrac{2\,f_{1,m_1,m_2}^{[0,+]}}{\varepsilon^{[0]}} & \dfrac{f_{1,m_1,m_2}^{[0,+]}}{\varepsilon^{[0]}} - \dfrac{f_{1,m_1,m_2}^{[1,+]}}{\varepsilon^{[1]}} \\ \dfrac{f_{1,m_1,m_2}^{[1,+]}}{\varepsilon^{[1]}} - \dfrac{f_{1,m_1,m_2}^{[0,+]}}{\varepsilon^{[0]}} & \dfrac{2\,f_{1,m_1,m_2}^{[1,+]}}{\varepsilon^{[1]}} \end{pmatrix} \begin{pmatrix} ffH_{s,m_1,m_2}^{[+]}[x_1^{[0]}] \\ ffH_{s,m_1,m_2}^{[-]}[x_1^{[1]}] \end{pmatrix} \tag{10.8}$$

The boundary surface does not induce any coupling between Fourier orders or between polarization modes; thus the S-matrix quadrants $S^{[++]}$, $S^{[+-]}$, $S^{[-+]}$, and $S^{[--]}$ are diagonal and each index set $\mathcal{M}^{[j]}$ in Eq. 9.4 consists of a single index pair (m_1, m_2). The nonzero elements of the S-matrix quadrants $S^{[\pm\pm']}$ are obtained from Eq's. 10.7 and 10.8 (cf. Eq's. 9.2 and 9.4),

$$\begin{aligned} S_{(m_1,m_2,\mathrm{E}),(m_1,m_2,\mathrm{E})}^{[+-]} &= -S_{(m_1,m_2,\mathrm{E}),(m_1,m_2,\mathrm{E})}^{[-+]} = 1 - S_{(m_1,m_2,\mathrm{E}),(m_1,m_2,\mathrm{E})}^{[++]} = S_{(m_1,m_2,\mathrm{E}),(m_1,m_2,\mathrm{E})}^{[--]} - 1 \\ &= \frac{f_{1,m_1,m_2}^{[1,+]} - f_{1,m_1,m_2}^{[0,+]}}{f_{1,m_1,m_2}^{[1,+]} + f_{1,m_1,m_2}^{[0,+]}} \end{aligned} \tag{10.9}$$

$$\begin{aligned} & S_{(m_1,m_2,\mathrm{H}),(m_1,m_2,\mathrm{H})}^{[+-]} = -S_{(m_1,m_2,\mathrm{H}),(m_1,m_2,\mathrm{H})}^{[-+]} = S_{(m_1,m_2,\mathrm{H}),(m_1,m_2,\mathrm{H})}^{[++]} - 1 = 1 - S_{(m_1,m_2,\mathrm{H}),(m_1,m_2,\mathrm{H})}^{[--]} \\ & = \frac{\dfrac{f_{1,m_1,m_2}^{[0,+]}}{\varepsilon^{[0]}} - \dfrac{f_{1,m_1,m_2}^{[1,+]}}{\varepsilon^{[1]}}}{\dfrac{f_{1,m_1,m_2}^{[1,+]}}{\varepsilon^{[1]}} + \dfrac{f_{1,m_1,m_2}^{[0,+]}}{\varepsilon^{[0]}}} \end{aligned} \tag{10.10}$$

If the denominator in either Eq. 10.9 or 10.10 is zero, then the entire expression is set to zero. (This condition should not occur unless $f^{[1,+]}_{1,m_1,m_2}$ and $f^{[0,+]}_{1,m_1,m_2}$ are both zero, implying that $\varepsilon^{[0]}$ and $\varepsilon^{[1]}$ are real-valued and equal and the S matrix is an identity matrix.)

11. The S matrix for a homogeneous stratum (without surfaces)

The S matrix for a homogeneous stratum (excluding its boundary surfaces) is determined from Eq's. 6.46 and 6.47. These equations imply

$$ffE^{[\pm]}_{\mathrm{s},m_1,m_2}[x_1^{[1]}] = \exp[\pm i\,\varphi_{m_1,m_2}]\, ffE^{[\pm]}_{\mathrm{s},m_1,m_2}[x_1^{[0]}] \tag{11.1}$$

$$ffH^{[\pm]}_{\mathrm{s},m_1,m_2}[x_1^{[1]}] = \exp[\pm i\,\varphi_{m_1,m_2}]\, ffH^{[\pm]}_{\mathrm{s},m_1,m_2}[x_1^{[0]}] \tag{11.2}$$

where the phase shift φ_{m_1,m_2} is

$$\varphi_{m_1,m_2} = 2\pi\, f^{[+]}_{1,m_1,m_2}\,(x_1^{[1]} - x_1^{[0]}) \tag{11.3}$$

The stratum boundaries are at $x_1 = x_1^{[0]}$ and $x_1 = x_1^{[1]}$ ($x_1^{[1]} \ge x_1^{[0]}$, see Figure 8). $f^{[+]}_{1,m_1,m_2}$ is defined by Eq. 6.37. (The stratum permittivity is $\varepsilon^{[\mathrm{c}]}$ in Eq. 6.37.)

Eq's. 11.1 and 11.2 are equivalently stated as follows,

$$\begin{pmatrix} ffE^{[+]}_{\mathrm{s},m_1,m_2}[x_1^{[1]}] \\ ffE^{[-]}_{\mathrm{s},m_1,m_2}[x_1^{[0]}] \end{pmatrix} = \begin{pmatrix} \exp[i\,\varphi_{m_1,m_2}] & 0 \\ 0 & \exp[i\,\varphi_{m_1,m_2}] \end{pmatrix} \begin{pmatrix} ffE^{[+]}_{\mathrm{s},m_1,m_2}[x_1^{[0]}] \\ ffE^{[-]}_{\mathrm{s},m_1,m_2}[x_1^{[1]}] \end{pmatrix} \tag{11.4}$$

$$\begin{pmatrix} ffH^{[+]}_{\mathrm{s},m_1,m_2}[x_1^{[1]}] \\ ffH^{[-]}_{\mathrm{s},m_1,m_2}[x_1^{[0]}] \end{pmatrix} = \begin{pmatrix} \exp[i\,\varphi_{m_1,m_2}] & 0 \\ 0 & \exp[i\,\varphi_{m_1,m_2}] \end{pmatrix} \begin{pmatrix} ffH^{[+]}_{\mathrm{s},m_1,m_2}[x_1^{[0]}] \\ ffH^{[-]}_{\mathrm{s},m_1,m_2}[x_1^{[1]}] \end{pmatrix} \tag{11.5}$$

There is no diffractive coupling or polarization coupling within the stratum; thus the S-matrix quadrants $S^{[++]}$, $S^{[+-]}$, $S^{[-+]}$, and $S^{[--]}$ are diagonal and each index set $\mathcal{M}^{[j]}$ in Eq. 9.4 consists of a single index pair (m_1, m_2). The nonzero elements of the S-matrix quadrants $S^{[\pm\pm']}$ are obtained from Eq's. 11.4 and 11.5 (cf. Eq's. 9.2 and 9.4),

$$\begin{aligned} &S^{[++]}_{(m_1,m_2,\mathrm{E}),(m_1,m_2,\mathrm{E})} = S^{[--]}_{(m_1,m_2,\mathrm{E}),(m_1,m_2,\mathrm{E})} = S^{[++]}_{(m_1,m_2,\mathrm{H}),(m_1,m_2,\mathrm{H})} = S^{[--]}_{(m_1,m_2,\mathrm{H}),(m_1,m_2,\mathrm{H})} \\ &= \exp[i\,\varphi_{m_1,m_2}] \end{aligned} \tag{11.6}$$

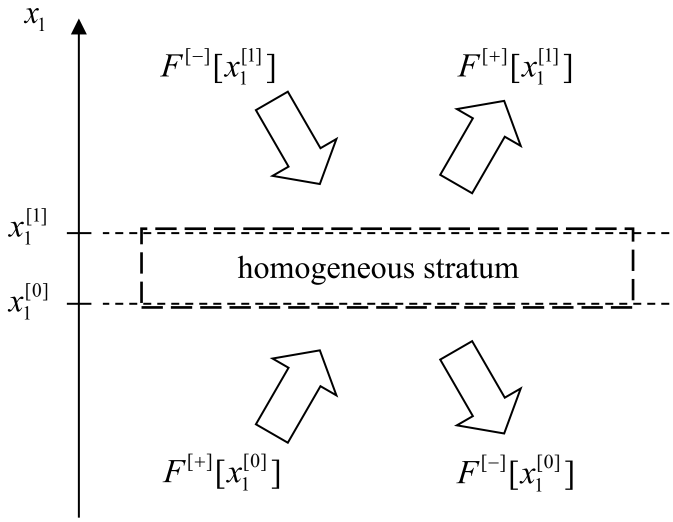

Figure 8. Up and down waves traversing a homogeneous stratum.

The stratum's S matrix defined by Eq. 11.6 could be combined with the stratum's boundary-surface S matrices (Eq's. 10.9-10.10) via stacking (Eq. 8.8). The resulting composite S matrix can contain indeterminacies when a Fourier order's grating-normal frequency (f_1) is zero in the stratum or in either of its bounding layers. However, this problem is avoided by describing the layer in terms of an S matrix representing the electromagnetic field transitions between two fictitious layers of permittivity $\varepsilon^{[f]}$ bounding the stratum. (The S matrix includes the bounding surfaces.) S matrices for periodic strata are similarly defined in relation to fictitious bounding layers, and Section 16 derives the S matrix for a homogeneous layer as a specialization of the periodic case.

12. The S matrix for a coordinate break

A coordinate break applies a translational offset to the x_2, x_3 coordinates at a particular height x_1 in the grating stack. The coordinate break is represented by an S matrix, as in Eq. 7.1, where $x_1^{[0]}$ represents the x_1 height immediately below the break and $x_1^{[1]}$ represents the height immediately above it. (The difference $x_1^{[1]} - x_1^{[0]}$ is infinitesimal.) The column vectors $F^{[\pm]}[x_1]$ in Eq. 7.1 represent field quantities evaluated at $(x_2, x_3) = (0,0)$ below the break ($x_1 < x_1^{[0]}$), and at $(x_2', x_3') = (0,0)$ above the break ($x_1 > x_1^{[1]}$), where the primed coordinates are defined by

$$(x_2', x_3') = (x_2, x_3) - (\Delta x_2, \Delta x_3) \tag{12.1}$$

Δx_2 and Δx_3 are the translational offsets. For example, Figure 9 conceptually illustrates a break applied to the x_2 coordinate, with offset Δx_2. Inserting a coordinate break has the effect of repositioning all layers above the break by displacement vector $(\Delta x_2, \Delta x_3)$.

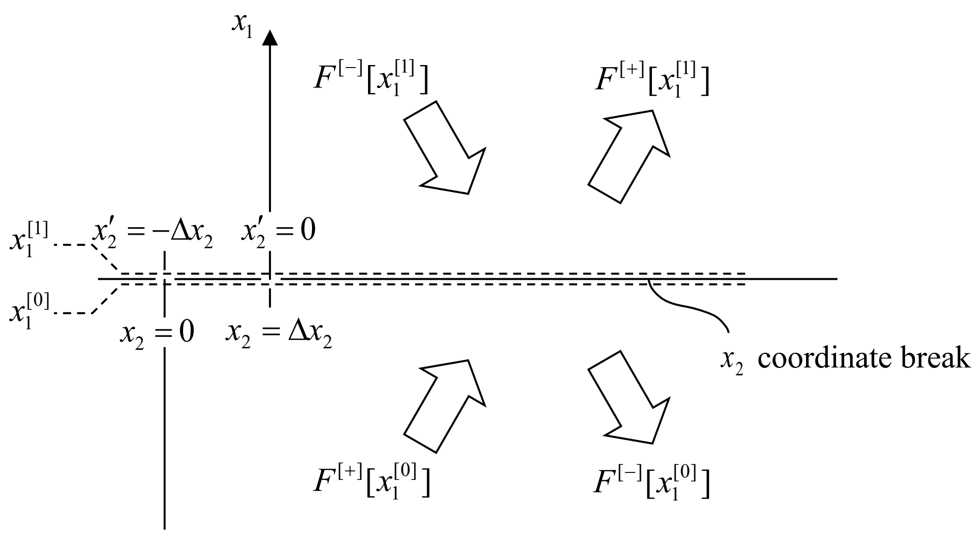

Figure 9. Up and down waves with a coordinate break ($x_2' = x_2 - \Delta x_2$).

The offset vector $\Delta\vec{x}$ is defined as in Eq. 3.41,

$$\Delta\vec{x} = \hat{e}_2\, \Delta x_2 + \hat{e}_3\, \Delta x_3 \tag{12.2}$$

The electric field representation $\vec{E}[\hat{e}_1\, x_1^{[0]} + \hat{e}_2\, x_2 + \hat{e}_3\, x_3]$ below the break is transformed into the representation $\vec{E}[\hat{e}_1\, x_1^{[1]} + \hat{e}_2\, x_2' + \hat{e}_3\, x_3']$ above the break, where

$$\vec{E}[\hat{e}_1\, x_1^{[1]} + \hat{e}_2\, x_2' + \hat{e}_3\, x_3'] = \vec{E}[\hat{e}_1\, x_1^{[0]} + \hat{e}_2\, x_2 + \hat{e}_3\, x_3] = \vec{E}[\hat{e}_1\, x_1^{[0]} + \hat{e}_2\, x_2' + \hat{e}_3\, x_3' + \Delta\vec{x}] \tag{12.3}$$

Substituting the field's Fourier expansion 5.7 in 12.3 and using the condition $\hat{e}_1 \bullet \vec{f}^{[||]}_{m_1,m_2} = 0$ (from Eq. 5.9), the following relationship is obtained,

$$\begin{aligned}&\sum_{m_1,m_2} ff\vec{E}_{m_1,m_2}[x_1^{[1]}] \exp[i\, 2\pi\, \vec{f}^{[||]}_{m_1,m_2} \bullet (\hat{e}_2\, x_2' + \hat{e}_3\, x')] = \\ &\quad \sum_{m_1,m_2} ff\vec{E}_{m_1,m_2}[x_1^{[0]}] \exp[i\, 2\pi\, \vec{f}^{[||]}_{m_1,m_2} \bullet (\hat{e}_2\, x_2' + \hat{e}_3\, x_3' + \Delta\vec{x})]\end{aligned} \tag{12.4}$$

Hence the coordinate translation induces the following phase shift in the field's Fourier coefficients,

$$ff\vec{E}_{m_1,m_2}[x_1^{[1]}] = ff\vec{E}_{m_1,m_2}[x_1^{[0]}] \exp[i\, \varphi_{m_1,m_2}] \tag{12.5}$$

where

$$\varphi_{m_1,m_2} = 2\pi\, \vec{f}^{[||]}_{m_1,m_2} \bullet \Delta\vec{x} \tag{12.6}$$

A similar phase shift is applied to the $ff\vec{H}$ coefficients in Eq. 5.12, and to the $ffE_{\rm s}^{[\pm]}$ and $ffH_{\rm s}^{[\pm]}$ functions defined by Eq's. 6.52-6.55. The phase-shift relations are expressed as follows,

$$\begin{pmatrix} ffE_{{\rm s},m_1,m_2}^{[+]}[x_1^{[1]}] \\ ffE_{{\rm s},m_1,m_2}^{[-]}[x_1^{[0]}] \end{pmatrix} = \begin{pmatrix} \exp[i\,\varphi_{m_1,m_2}] & 0 \\ 0 & \exp[-i\,\varphi_{m_1,m_2}] \end{pmatrix} \begin{pmatrix} ffE_{{\rm s},m_1,m_2}^{[+]}[x_1^{[0]}] \\ ffE_{{\rm s},m_1,m_2}^{[-]}[x_1^{[1]}] \end{pmatrix} \tag{12.7}$$

$$\begin{pmatrix} ffH_{{\rm s},m_1,m_2}^{[+]}[x_1^{[1]}] \\ ffH_{{\rm s},m_1,m_2}^{[-]}[x_1^{[0]}] \end{pmatrix} = \begin{pmatrix} \exp[i\,\varphi_{m_1,m_2}] & 0 \\ 0 & \exp[-i\,\varphi_{m_1,m_2}] \end{pmatrix} \begin{pmatrix} ffH_{{\rm s},m_1,m_2}^{[+]}[x_1^{[0]}] \\ ffH_{{\rm s},m_1,m_2}^{[-]}[x_1^{[1]}] \end{pmatrix} \tag{12.8}$$

There is no diffractive coupling or polarization coupling induced by the coordinate break; thus the S-matrix quadrants $S^{[++]}$, $S^{[+-]}$, $S^{[-+]}$, and $S^{[--]}$ are diagonal and each index set $\mathcal{M}^{[j]}$ in Eq. 9.4 consists of a single index pair (m_1, m_2). The nonzero elements of the S-matrix quadrants $S^{[\pm\pm']}$ corresponding to (m_1, m_2) are obtained from Eq's. 12.7 and 12.8 (cf. Eq's. 9.2 and 9.4),

$$S_{(m_1,m_2,{\rm E}),(m_1,m_2,{\rm E})}^{[++]} = S_{(m_1,m_2,{\rm H}),(m_1,m_2,{\rm H})}^{[++]} = \exp[i\,\varphi_{m_1,m_2}] \tag{12.9}$$

$$S_{(m_1,m_2,{\rm E}),(m_1,m_2,{\rm E})}^{[--]} = S_{(m_1,m_2,{\rm H}),(m_1,m_2,{\rm H})}^{[--]} = \exp[-i\,\varphi_{m_1,m_2}] \tag{12.10}$$

13. The S matrix for a biperiodic stratum

As a consequence of the grating periodicity, Eq's. 3.17 and 3.18, the permittivity in stratum l_1 (Eq. 3.10) has a Fourier series representation of the form,

$$\varepsilon[\vec{x}] = \varepsilon 1^{[l_1]}[x_2, x_3] = \sum_{n_1,n_2} ff\,\varepsilon 1_{n_1,n_2}^{[l_1]} \exp[i\,2\pi\,(n_1\,\vec{f}_1^{[{\rm s},l_1]} + n_2\,\vec{f}_2^{[{\rm s},l_1]})\bullet\vec{x}] \tag{13.1}$$

The stratum's basis frequencies $\vec{f}_1^{[{\rm s},l_1]}$ and $\vec{f}_2^{[{\rm s},l_1]}$ are defined by Eq's. 3.30-3.32, and the periodicity conditions, Eq's. 3.17 and 3.18, can be verified directly using Eq's. 13.1 and 3.32. Appendix C describes the explicit form of the Fourier coefficients $ff\,\varepsilon 1_{n_1,n_2}^{[l_1]}$, based on the grating geometry specification outlined in Section 3.

The stratum's basis frequencies $\vec{f}_1^{[{\rm s},l_1]}$ and $\vec{f}_2^{[{\rm s},l_1]}$ are linear combinations of the grating's fundamental basis frequencies $\vec{f}_1^{[{\rm g}]}$ and $\vec{f}_2^{[{\rm g}]}$,

$$\vec{f}_1^{[{\rm s},l_1]} = h_{1,1}^{[l_1]}\,\vec{f}_1^{[{\rm g}]} + h_{1,2}^{[l_1]}\,\vec{f}_2^{[{\rm g}]} \tag{13.2}$$

$$\vec{f}_2^{[\mathrm{s},l_1]} = h_{2,1}^{[l_1]}\,\vec{f}_1^{[\mathrm{g}]} + h_{2,2}^{[l_1]}\,\vec{f}_2^{[\mathrm{g}]} \tag{13.3}$$

(cf. Eq. 3.33). The diffraction order indices (m_1, m_2) of any particular Fourier order in the electromagnetic field expansions 5.7 and 5.12 are represented as

$$(m_1, m_2) = (m_1^{[\mathrm{base}]}, m_2^{[\mathrm{base}]}) + (n_1, n_2)\begin{pmatrix} h_{1,1}^{[l_1]} & h_{1,2}^{[l_1]} \\ h_{2,1}^{[l_1]} & h_{2,2}^{[l_1]} \end{pmatrix} \tag{13.4}$$

n_1, and n_2 will be termed "suborder indices" corresponding to order (m_1, m_2) in stratum l_1, defined by

$$(n_1, n_2) = \mathrm{floor}\left[(m_1, m_2)\begin{pmatrix} h_{1,1}^{[l_1]} & h_{1,2}^{[l_1]} \\ h_{2,1}^{[l_1]} & h_{2,2}^{[l_1]} \end{pmatrix}^{-1} \right] \tag{13.5}$$

(The "floor" function rounds toward $-\infty$.) $m_1^{[\mathrm{base}]}$ and $m_2^{[\mathrm{base}]}$ are "base indices" in the range

$$0 \le (m_1^{[\mathrm{base}]}, m_2^{[\mathrm{base}]})\begin{pmatrix} h_{1,1}^{[l_1]} & h_{1,2}^{[l_1]} \\ h_{2,1}^{[l_1]} & h_{2,2}^{[l_1]} \end{pmatrix}^{-1} < 1 \tag{13.6}$$

The set of all order index pairs (m_1, m_2) in $\mathcal{M}$ corresponding to a particular base index pair $(m_1^{[\mathrm{base}]}, m_2^{[\mathrm{base}]})$ in Eq. 13.4 defines a decoupled index set $\mathcal{M}^{[j]}$ in Eq. 9.4. ($\mathcal{M}$ is the union of $\mathcal{M}^{[1]}$, $\mathcal{M}^{[2]}$, … .) The set of all base index pairs $(m_1^{[\mathrm{base}]}, m_2^{[\mathrm{base}]})$ satisfying Eq's. 13.4 and 13.6 for some $(m_1, m_2) \in \mathcal{M}$ are enumerated and denoted as $(m_1^{[\mathrm{base},j]}, m_2^{[\mathrm{base},j]})$ for $\mathcal{M}^{[j]}$. In Eq's. 5.7 and 5.12 the field amplitudes $f\!f\vec{E}_{m_1,m_2}$ and $f\!f\vec{H}_{m_1,m_2}$ corresponding to $\mathcal{M}^{[j]}$ and suborder indices (n_1, n_2) are represented as follows

$$\begin{gathered} f\!f\vec{E}_{n_1,n_2}^{[j]}[x_1] = f\!f\vec{E}_{m_1,m_2}[x_1], \quad f\!f\vec{H}_{n_1,n_2}^{[j]}[x_1] = f\!f\vec{H}_{m_1,m_2}[x_1] \\ \text{with } (m_1, m_2) = (m_1^{[\mathrm{base},j]}, m_2^{[\mathrm{base},j]}) + (n_1, n_2)\begin{pmatrix} h_{1,1}^{[l_1]} & h_{1,2}^{[l_1]} \\ h_{2,1}^{[l_1]} & h_{2,2}^{[l_1]} \end{pmatrix} \end{gathered} \tag{13.7}$$

The up/down fields $f\!f\vec{E}^{[\pm]}$ and $f\!f\vec{H}^{[\pm]}$ in Eq's. 6.48 and 6.49, $F^{[\pm]}$ amplitudes in Eq. 9.2, and S-matrix quadrants $S^{[++]}$, $S^{[+-]}$, $S^{[-+]}$, and $S^{[--]}$ in Eq. 9.4, similarly separate into decoupled matrix partitions identified by j superscripts corresponding to $\mathcal{M}^{[j]}$:

$$\left.\begin{aligned} F^{[\pm,j]}_{(n_1,n_2,\mathrm{E})}[x_1] &= \mathit{ff}\vec{E}^{[\pm,j]}_{n_1,n_2}[x_1] = \mathit{ff}\vec{E}^{[\pm]}_{m_1,m_2}[x_1] \\ F^{[\pm,j]}_{(n_1,n_2,\mathrm{H})}[x_1] &= \mathit{ff}\vec{H}^{[\pm,j]}_{n_1,n_2}[x_1] = \mathit{ff}\vec{H}^{[\pm]}_{m_1,m_2}[x_1] \end{aligned}\right\}$$
$$\text{with } (m_1,m_2) = (m_1^{[\mathrm{base},j]}, m_2^{[\mathrm{base},j]}) + (n_1,n_2)\begin{pmatrix} h^{[l_1]}_{1,1} & h^{[l_1]}_{1,2} \\ h^{[l_1]}_{2,1} & h^{[l_1]}_{2,2} \end{pmatrix} \tag{13.8}$$

$$S^{[\pm\pm',j]}_{(n_1,n_2,P),(n'_1,n'_2,P')} = S^{[\pm\pm']}_{(m_1,m_2,P),(m'_1,m'_2,P')}$$
$$\text{with } (m_1,m_2) = (m_1^{[\mathrm{base},j]}, m_2^{[\mathrm{base},j]}) + (n_1,n_2)\begin{pmatrix} h^{[l_1]}_{1,1} & h^{[l_1]}_{1,2} \\ h^{[l_1]}_{2,1} & h^{[l_1]}_{2,2} \end{pmatrix}, \tag{13.9}$$
$$(m'_1,m'_2) = (m_1^{[\mathrm{base},j]}, m_2^{[\mathrm{base},j]}) + (n'_1,n'_2)\begin{pmatrix} h^{[l_1]}_{1,1} & h^{[l_1]}_{1,2} \\ h^{[l_1]}_{2,1} & h^{[l_1]}_{2,2} \end{pmatrix}$$

The following grating-tangential spatial frequencies are also defined for $\mathcal{M}^{[j]}$,

$$\vec{f}^{[\mathrm{Inc}\|,j]} = \vec{f}^{[\mathrm{Inc}\|]} + m_1^{[\mathrm{base},j]}\,\vec{f}_1^{[\mathrm{g}]} + m_2^{[\mathrm{base},j]}\,\vec{f}_2^{[\mathrm{g}]} = \hat{e}_2\,f_2^{[\mathrm{Inc},j]} + \hat{e}_3\,f_3^{[\mathrm{Inc},j]} \tag{13.10}$$

$$\vec{f}^{[\|,j]}_{n_1,n_2} = \vec{f}^{[\mathrm{Inc}\|,j]} + n_1\,\vec{f}_1^{[\mathrm{s},l_1]} + n_2\,\vec{f}_2^{[\mathrm{s},l_1]} = \hat{e}_2\,f^{[j]}_{2,n_1,n_2} + \hat{e}_3\,f^{[j]}_{3,n_1,n_2}$$
$$= \vec{f}^{[\|]}_{m_1,m_2} \quad \text{with } (m_1,m_2) = (m_1^{[\mathrm{base},j]}, m_2^{[\mathrm{base},j]}) + (n_1,n_2)\begin{pmatrix} h^{[l_1]}_{1,1} & h^{[l_1]}_{1,2} \\ h^{[l_1]}_{2,1} & h^{[l_1]}_{2,2} \end{pmatrix} \tag{13.11}$$

(from Eq's. 13.2, 13.3, 5.9). With these definitions along with Eq's. 13.7 and 5.8, the field expansions 5.7 and 5.12 (with the sums truncated to $(m_1,m_2)\in\mathcal{M}$) are reformulated as follows,

$$\vec{E}[\vec{x}] = \sum_j \sum_{(n_1,n_2)\in\mathcal{N}^{[j]}} \mathit{ff}\vec{E}^{[j]}_{n_1,n_2}[x_1]\exp[i\,2\pi\,\vec{f}^{[\|,j]}_{n_1,n_2}\bullet\vec{x}] \tag{13.12}$$

$$\vec{H}[\vec{x}] = \sum_j \sum_{(n_1,n_2)\in\mathcal{N}^{[j]}} \mathit{ff}\vec{H}^{[j]}_{n_1,n_2}[x_1]\exp[i\,2\pi\,\vec{f}^{[\|,j]}_{n_1,n_2}\bullet\vec{x}] \tag{13.13}$$

where $\mathcal{N}^{[j]}$ is the set of suborder index pairs (n_1,n_2) for which (m_1,m_2), as defined by Eq. 13.4 with $(m_1^{[\mathrm{base}]}, m_2^{[\mathrm{base}]}) = (m_1^{[\mathrm{base},j]}, m_2^{[\mathrm{base},j]})$, is in $\mathcal{M}^{[j]}$,

$$\mathcal{N}^{[j]} = \left\{ (n_1,n_2):\ (m_1^{[\mathrm{base},j]}, m_2^{[\mathrm{base},j]}) + (n_1,n_2)\begin{pmatrix} h^{[l_1]}_{1,1} & h^{[l_1]}_{1,2} \\ h^{[l_1]}_{2,1} & h^{[l_1]}_{2,2} \end{pmatrix} \in \mathcal{M}^{[j]} \right\} \tag{13.14}$$

The union of all $\mathcal{N}^{[j]}$ sets is denoted as $\mathcal{N}$,

$$\boldsymbol{\mathcal{N}} = \boldsymbol{\mathcal{N}}^{[1]} \cup \boldsymbol{\mathcal{N}}^{[2]} \cup \ldots \tag{13.15}$$

The set of n_2 indices in $\boldsymbol{\mathcal{N}}^{[j]}$ is denoted as $\boldsymbol{\mathcal{N}}_2^{[j]}$,

$$\boldsymbol{\mathcal{N}}_2^{[j]} = \left\{ n_2 : \, (n_1, n_2) \in \boldsymbol{\mathcal{N}}^{[j]} \text{ for some } n_1 \right\} \tag{13.16}$$

The set of n_1 indices for which $(n_1, n_2) \in \boldsymbol{\mathcal{N}}^{[j]}$ is denoted as $\boldsymbol{\mathcal{N}}_1^{[j]}[n_2]$:

$$\text{For each } n_2 \in \boldsymbol{\mathcal{N}}_2^{[j]}, \, \boldsymbol{\mathcal{N}}_1^{[j]}[n_2] = \left\{ n_1 : \, (n_1, n_2) \in \boldsymbol{\mathcal{N}}^{[j]} \right\} \tag{13.17}$$

In developing the S matrix for stratum l_1, the $\hat{e}_2$, $\hat{e}_3$ coordinate orientation is chosen so that $\hat{e}_2$ is parallel to $\vec{f}_1^{[\mathrm{s},l_1]}$ (Eq. 3.30),

$$f_{3,1}^{[\mathrm{s},l_1]} = 0; \quad \vec{f}_1^{[\mathrm{s},l_1]} = \hat{e}_2 \, f_{2,1}^{[\mathrm{s},l_1]} \tag{13.18}$$

(The S matrix definition is independent of the $\hat{e}_2$, $\hat{e}_3$ coordinate orientation because the definition of $ffE_{\mathrm{s}}^{[\pm]}$ and $ffH_{\mathrm{s}}^{[\pm]}$ implicit in Eq's. 6.48 and 6.49 is coordinate-independent. Thus, the choice of coordinate orientation has no effect on the S matrix.) The permittivity expansion, Eq. 13.1, then takes the form of a one-dimensional Fourier series in x_3 (the coordinate parallel to the grating stripes),

$$\varepsilon[\vec{x}] = \varepsilon 1^{[l_1]}[x_2, x_3] = \sum_{n_2} f\varepsilon 1_{n_2}^{[l_1]}[x_2] \exp[i \, 2\pi \, n_2 \, f_{3,2}^{[\mathrm{s},l_1]} \, x_3] \tag{13.19}$$

where each Fourier coefficient $f\varepsilon 1_{n_2}^{[l_1]}[x_2]$ is a one-dimensional Fourier series in x_2 (the stripe-transverse coordinate),

$$f\varepsilon 1_{n_2}^{[l_1]}[x_2] = \sum_{n_1} ff\varepsilon 1_{n_1,n_2}^{[l_1]} \exp[i \, 2\pi \, (n_1 \, f_{2,1}^{[\mathrm{s},l_1]} + n_2 \, f_{2,2}^{[\mathrm{s},l_1]}) \, x_2] \tag{13.20}$$

($\varepsilon 1^{[l_1]}[x_2, x_3]$ and $f\varepsilon 1_{n_2}^{[l_1]}[x_2]$ are independent of x_2 within each stripe, and $\varepsilon 1^{[l_1]}[x_2, x_3]$ is independent of both x_2 and x_3 within each block.) The truncated electromagnetic field expansions 13.12 and 13.13 are similarly represented as nested one-dimensional expansions,

$$\vec{E}[\vec{x}] = \sum_j \sum_{n_2 \in \boldsymbol{\mathcal{N}}_2^{[j]}} f\vec{E}_{n_2}^{[j]}[x_1, x_2] \exp[i \, 2\pi \, (f_3^{[\mathrm{Inc},j]} + n_2 \, f_{3,2}^{[\mathrm{s},l_1]}) \, x_3] \tag{13.21}$$

$$\vec{H}[\vec{x}] = \sum_j \sum_{n_2 \in \boldsymbol{\mathcal{N}}_2^{[j]}} f\vec{H}_{n_2}^{[j]}[x_1, x_2] \exp[i \, 2\pi \, (f_3^{[\mathrm{Inc},j]} + n_2 \, f_{3,2}^{[\mathrm{s},l_1]}) \, x_3] \tag{13.22}$$

where

$$f\vec{E}_{n_2}^{[j]}[x_1,x_2]=\sum_{n_1\in\mathcal{N}_1^{[j]}[n_2]} ff\vec{E}_{(n_1,n_2)}^{[j]}[x_1]\exp[i\,2\pi\,(f_2^{[\mathrm{Inc},j]}+n_1\,f_{2,1}^{[\mathrm{s},l_1]}+n_2\,f_{2,2}^{[\mathrm{s},l_1]})\,x_2] \tag{13.23}$$

$$f\vec{H}_{n_2}^{[j]}[x_1,x_2]=\sum_{n_1\in\mathcal{N}_1^{[j]}[n_2]} ff\vec{H}_{(n_1,n_2)}^{[j]}[x_1]\exp[i\,2\pi\,(f_2^{[\mathrm{Inc},j]}+n_1\,f_{2,1}^{[\mathrm{s},l_1]}+n_2\,f_{2,2}^{[\mathrm{s},l_1]})\,x_2] \tag{13.24}$$

Eq's. 13.23-13.24 are obtained from Eq's. 13.12-13.13 with substitution from Eq's. 13.11 (first equality), 13.10 (right-hand expression), 3.30-3.31, and 13.18, and with the $\mathcal{N}^{[j]}$ decomposition in Eq's. 13.16-13.17. The subscripts in $ff\vec{E}_{(n_1,n_2)}^{[j]}$ and $ff\vec{H}_{(n_1,n_2)}^{[j]}$ are parenthesized to indicate that the pair (n_1,n_2) will be used as a partitioned vector index.

The Fourier expansions over x_3, Eq's. 13.19, 13.21, and 13.22, are substituted in the Maxwell Eq's. 6.1 and 6.2, which have the explicit coordinate representation,

$$\partial_2\,E_3-\partial_3\,E_2=i\,\tfrac{2\pi}{\lambda}\,H_1 \tag{13.25}$$

$$\partial_3\,E_1-\partial_1\,E_3=i\,\tfrac{2\pi}{\lambda}\,H_2 \tag{13.26}$$

$$\partial_1\,E_2-\partial_2\,E_1=i\,\tfrac{2\pi}{\lambda}\,H_3 \tag{13.27}$$

$$\partial_2\,H_3-\partial_3\,H_2=-i\,\tfrac{2\pi}{\lambda}\,\varepsilon\,E_1 \tag{13.28}$$

$$\partial_3\,H_1-\partial_1\,H_3=-i\,\tfrac{2\pi}{\lambda}\,\varepsilon\,E_2 \tag{13.29}$$

$$\partial_1\,H_2-\partial_2\,H_1=-i\,\tfrac{2\pi}{\lambda}\,\varepsilon\,E_3 \tag{13.30}$$

where ∂_j represents the derivative with respect to x_j. In making the substitution, Laurent's product rule for Fourier series should only be applied to the right sides of Eq's. 13.28-13.30 when the product factors do not have concurrent discontinuities in x_3. Otherwise, convergence of the truncated Fourier series will be nonuniform and severe numerical instabilities might result [Ref. 4]. The $\vec{E}$ and $\vec{H}$ fields' surface-tangential components are continuous across permittivity discontinuity surfaces, and the grating walls between blocks within each stripe are parallel to $\hat{e}_1$ and $\hat{e}_2$ (Eq. C.5 in Appendix C); hence the factors E_1 and E_2 in Eq's. 13.28 and 13.29 are continuous with x_3 and there is no problem applying Laurent's rule in these equations. The factors ε and E_3 in Eq. 13.30 generally have concurrent discontinuities; however the terms H_1 and H_2 on the left side of the equation are continuous (and hence, so are their tangential derivatives $\partial_2\,H_1$ and $\partial_1\,H_2$), so Laurent's rule can be reliably applied by moving the ε factor to the left side of the equation,

$$\tfrac{1}{\varepsilon}\left(\partial_1 H_2 - \partial_2 H_1\right) = -i\tfrac{2\pi}{\lambda} E_3 \tag{13.31}$$

The reciprocal permittivity factor in Eq. 13.31 is represented by a Fourier series similar to Eq. 13.19,

$$\frac{1}{\varepsilon[\vec{x}]} = \frac{1}{\varepsilon 1^{[l_1]}[x_2, x_3]} = \sum_{n_2} fr\varepsilon 1^{[l_1]}_{n_2}[x_2] \exp[i\, 2\pi\, n_2\, f^{[\mathrm{s},l_1]}_{3,2}\, x_3] \tag{13.32}$$

(The "r" in "$fr\varepsilon 1$" connotes "reciprocal".) Substituting Eq's. 13.21, 13.22, 13.19, and 13.32 in Eq's. 13.25-13.29 and 13.31, and separating Fourier orders, the following equations are obtained (with $n_2 \in \mathcal{N}^{[j]}_2$),

$$\partial_2\, fE^{[j]}_{3,n_2}[x_1, x_2] - i\, 2\pi\, (f^{[\mathrm{Inc},j]}_3 + n_2\, f^{[\mathrm{s},l_1]}_{3,2})\, fE^{[j]}_{2,n_2}[x_1, x_2] = i\tfrac{2\pi}{\lambda}\, fH^{[j]}_{1,n_2}[x_1, x_2] \tag{13.33}$$

$$i\, 2\pi\, (f^{[\mathrm{Inc},j]}_3 + n_2\, f^{[\mathrm{s},l_1]}_{3,2})\, fE^{[j]}_{1,n_2}[x_1, x_2] - \partial_1\, fE^{[j]}_{3,n_2}[x_1, x_2] = i\tfrac{2\pi}{\lambda}\, fH^{[j]}_{2,n_2}[x_1, x_2] \tag{13.34}$$

$$\partial_1\, fE^{[j]}_{2,n_2}[x_1, x_2] - \partial_2\, fE^{[j]}_{1,n_2}[x_1, x_2] = i\tfrac{2\pi}{\lambda}\, fH^{[j]}_{3,n_2}[x_1, x_2] \tag{13.35}$$

$$\begin{aligned}&\partial_2\, fH^{[j]}_{3,n_2}[x_1, x_2] - i\, 2\pi\, (f^{[\mathrm{Inc},j]}_3 + n_2\, f^{[\mathrm{s},l_1]}_{3,2})\, fH^{[j]}_{2,n_2}[x_1, x_2] = \\ &\quad -i\tfrac{2\pi}{\lambda} \sum_{n'_2 \in \mathcal{N}^{[j]}_2} f\varepsilon 1^{[l_1]}_{n_2 - n'_2}[x_2]\, fE^{[j]}_{1,n'_2}[x_1, x_2]\end{aligned} \tag{13.36}$$

$$\begin{aligned}&i\, 2\pi\, (f^{[\mathrm{Inc},j]}_3 + n_2\, f^{[\mathrm{s},l_1]}_{3,2})\, fH^{[j]}_{1,n_2}[x_1, x_2] - \partial_1\, fH^{[j]}_{3,n_2}[x_1, x_2] = \\ &\quad -i\tfrac{2\pi}{\lambda} \sum_{n'_2 \in \mathcal{N}^{[j]}_2} f\varepsilon 1^{[l_1]}_{n_2 - n'_2}[x_2]\, fE^{[j]}_{2,n'_2}[x_1, x_2]\end{aligned} \tag{13.37}$$

$$\sum_{n'_2 \in \mathcal{N}^{[j]}_2} fr\varepsilon 1^{[l_1]}_{n_2 - n'_2}[x_2] \left(\partial_1\, fH^{[j]}_{2,n'_2}[x_1, x_2] - \partial_2\, fH^{[j]}_{1,n'_2}[x_1, x_2]\right) = -i\tfrac{2\pi}{\lambda}\, fE^{[j]}_{3,n_2}[x_1, x_2] \tag{13.38}$$

Next, the Fourier expansions in x_2, Eq's. 13.20, 13.23, and 13.24, are substituted above. Once again, Laurent's rule is applied to the products inside the summations, taking care to avoid applying the rule to products with concurrent discontinuities. The grating walls between stripes within each stratum are parallel to $\hat{e}_1$ and $\hat{e}_3$ (Eq. C.4 in Appendix C); hence the field components E_1, E_3, H_1 and H_3, and their associated Fourier coefficients $fE^{[j]}_{1,n_2}$, $fE^{[j]}_{3,n_2}$, $fH^{[j]}_{1,n_2}$ and $fH^{[j]}_{3,n_2}$ (and also the derivative $\partial_1\, fH^{[j]}_{3,n_2}$), are all continuous with x_2, whereas terms associated with E_2 and H_2 generally are not. Thus, Laurent's rule can be reliably applied to Eq. 13.36, but Eq's. 13.37 and 13.38 must be modified to move the permittivity terms to the side of each equation containing the continuous field quantities.

The modification is facilitated by making the following definitions,

$$t\varepsilon 1^{[l_1]}_{n_2,n'_2}[x_2] = f\varepsilon 1^{[l_1]}_{n_2-n'_2}[x_2] \tag{13.39}$$

$$tr\varepsilon 1^{[l_1]}_{n_2,n'_2}[x_2] = fr\varepsilon 1^{[l_1]}_{n_2-n'_2}[x_2] \tag{13.40}$$

The "t" prefix connotes a Toeplitz matrix, and the matrices $t\varepsilon 1^{[l_1]}$ and $tr\varepsilon 1^{[l_1]}$ are defined for all integer indices n_2 and n'_2. The truncated matrices, limited to $n_2, n'_2 \in \mathcal{N}_2^{[j]}$, are denoted as $t\varepsilon 1^{[l_1,j]}$ and $tr\varepsilon 1^{[l_1,j]}$, and the corresponding reciprocal matrices are denoted as $rt\varepsilon 1^{[l_1,j]}$ and $rtr\varepsilon 1^{[l_1,j]}$,

$$rt\varepsilon 1^{[l_1,j]}[x_2] = (t\varepsilon 1^{[l_1,j]}[x_2])^{-1} \tag{13.41}$$

$$rtr\varepsilon 1^{[l_1,j]}[x_2] = (tr\varepsilon 1^{[l_1,j]}[x_2])^{-1} \tag{13.42}$$

($t\varepsilon 1^{[l_1,j]}$, $tr\varepsilon 1^{[l_1,j]}$, $rt\varepsilon 1^{[l_1,j]}[x_2]$, and $rtr\varepsilon 1^{[l_1,j]}[x_2]$ are independent of x_2 within each stripe. The matrices are functions of j due to their dependence on $\mathcal{N}_2^{[j]}$, but $\mathcal{N}_2^{[j]}$ is oftentimes the same for many or all index sets, in which case the matrices need only be computed for the unique $\mathcal{N}_2^{[j]}$ sets.) With these definitions, Eq's. 13.37 and 13.38 are restated in a form that is suitable for application of Laurent's rule,

$$\begin{aligned}&\sum_{n'_2\in\mathcal{N}_2^{[j]}} rt\varepsilon 1^{[l_1,j]}_{n_2,n'_2}[x_2]\Big(i\,2\pi\,(f_3^{[\mathrm{Inc},j]} + n'_2\, f_{3,2}^{[\mathrm{s},l_1]})\, fH^{[j]}_{1,n'_2}[x_1,x_2] - \partial_1\, fH^{[j]}_{3,n'_2}[x_1,x_2]\Big) = \\ &\quad -i\,\tfrac{2\pi}{\lambda}\, fE^{[j]}_{2,n_2}[x_1,x_2]\end{aligned} \tag{13.43}$$

$$\partial_1\, fH^{[j]}_{2,n_2}[x_1,x_2] - \partial_2\, fH^{[j]}_{1,n_2}[x_1,x_2] = -i\,\tfrac{2\pi}{\lambda} \sum_{n'_2\in\mathcal{N}_2^{[j]}} rtr\varepsilon 1^{[l_1,j]}_{n_2,n'_2}[x_2]\, fE^{[j]}_{3,n'_2}[x_1,x_2] \tag{13.44}$$

Eq. 13.20 defines the Fourier expansion, with respect to x_2, of the permittivity term in Eq. 13.36. The permittivity terms in Eq's. 13.43 and 13.44 have similar Fourier expansions, which are derived from the periodicity conditions, Eq's. 3.17 and 3.18. It follows from Eq's. 3.32 and 13.18 that Eq's. 3.17 and 3.18 can be equivalently stated

$$\varepsilon 1^{[l_1]}[x_2 + 1/f_{2,1}^{[\mathrm{s},l_1]},\, x_3 - f_{2,2}^{[\mathrm{s},l_1]}/(f_{2,1}^{[\mathrm{s},l_1]}\, f_{3,2}^{[\mathrm{s},l_1]})] = \varepsilon 1^{[l_1]}[x_2, x_3] \tag{13.45}$$

$$\varepsilon 1^{[l_1]}[x_2, x_3 + 1/f_{3,2}^{[\mathrm{s},l_1]}] = \varepsilon 1^{[l_1]}[x_2, x_3] \tag{13.46}$$

The permittivity's Fourier expansion 13.19 follows from Eq. 13.46, and based on Eq's. 13.19 and 13.45 the Fourier coefficients satisfy the following x_2-periodicity condition,

$$f\varepsilon 1_{n_2}^{[l_1]}[x_2 + 1/f_{2,1}^{[s,l_1]}]\exp[-i\,2\pi\,n_2\,f_{2,2}^{[s,l_1]}\,(x_2 + 1/f_{2,1}^{[s,l_1]})] = \\ f\varepsilon 1_{n_2}^{[l_1]}[x_2]\exp[-i\,2\pi\,n_2\,f_{2,2}^{[s,l_1]}\,x_2] \tag{13.47}$$

Eq. 13.20 follows from Eq. 13.47.

Based on Eq. 13.47, the Toeplitz matrix $t\varepsilon 1$ defined by Eq. 13.39 satisfies a similar periodicity condition,

$$t\varepsilon 1_{n_2,n_2'}^{[l_1]}[x_2 + 1/f_{2,1}^{[s,l_1]}]\exp[-i\,2\pi\,(n_2 - n_2')\,f_{2,2}^{[s,l_1]}\,(x_2 + 1/f_{2,1}^{[s,l_1]})] = \\ t\varepsilon 1_{n_2,n_2'}^{[l_1]}[x_2]\exp[-i\,2\pi\,(n_2 - n_2')\,f_{2,2}^{[s,l_1]}\,x_2] \tag{13.48}$$

and the reciprocal Toeplitz matrix $rt\varepsilon 1$ defined by Eq. 13.41 has the same periodicity,

$$rt\varepsilon 1_{n_2,n_2'}^{[l_1,j]}[x_2 + 1/f_{2,1}^{[s,l_1]}]\exp[-i\,2\pi\,(n_2 - n_2')\,f_{2,2}^{[s,l_1]}\,(x_2 + 1/f_{2,1}^{[s,l_1]})] = \\ rt\varepsilon 1_{n_2,n_2'}^{[l_1,j]}[x_2]\exp[-i\,2\pi\,(n_2 - n_2')\,f_{2,2}^{[s,l_1]}\,x_2] \tag{13.49}$$

Hence, $rt\varepsilon 1$ is represented by a Fourier expansion similar to Eq. 13.20,

$$rt\varepsilon 1_{n_2,n_2'}^{[l_1,j]}[x_2] = \sum_{n_1} frt\varepsilon 1_{n_1,n_2,n_2'}^{[l_1,j]}\,\exp[i\,2\pi\,(n_1\,f_{2,1}^{[s,l_1]} + (n_2 - n_2')\,f_{2,2}^{[s,l_1]})\,x_2] \tag{13.50}$$

The matrix $rtr\varepsilon 1$ defined by Eq. 13.42 is similarly represented as

$$rtr\varepsilon 1_{n_2,n_2'}^{[l_1,j]}[x_2] = \sum_{n_1} frtr\varepsilon 1_{n_1,n_2,n_2'}^{[l_1,j]}\,\exp[i\,2\pi\,(n_1\,f_{2,1}^{[s,l_1]} + (n_2 - n_2')\,f_{2,2}^{[s,l_1]})\,x_2] \tag{13.51}$$

Substituting Eq's. 13.23, 13.24, 13.20, 13.50, and 13.51 in Eq's. 13.33-13.36, 13.43, and 13.44, and separating Fourier orders, the following equations are obtained for $(n_1, n_2) \in \mathcal{N}^{[j]}$,

$$f_{2,n_1,n_2}^{[j]}\;ffE_{3,(n_1,n_2)}^{[j]}[x_1] - f_{3,(n_1,n_2)}^{[j]}\;ffE_{2,(n_1,n_2)}^{[j]}[x_1] = \tfrac{1}{\lambda}\,ffH_{1,(n_1,n_2)}^{[j]}[x_1] \tag{13.52}$$

$$i\,2\pi\,f_{3,n_1,n_2}^{[j]}\;ffE_{1,(n_1,n_2)}^{[j]}[x_1] - \partial_1\,ffE_{3,(n_1,n_2)}^{[j]}[x_1] = i\,\tfrac{2\pi}{\lambda}\,ffH_{2,(n_1,n_2)}^{[j]}[x_1] \tag{13.53}$$

$$\partial_1\,ffE_{2,(n_1,n_2)}^{[j]}[x_1] - i\,2\pi\,f_{2,n_1,n_2}^{[j]}\;ffE_{1,(n_1,n_2)}^{[j]}[x_1] = i\,\tfrac{2\pi}{\lambda}\,ffH_{3,(n_1,n_2)}^{[j]}[x_1] \tag{13.54}$$

$$f_{2,n_1,n_2}^{[j]}\;ffH_{3,(n_1,n_2)}^{[j]}[x_1] - f_{3,n_1,n_2}^{[j]}\;ffH_{2,(n_1,n_2)}^{[j]}[x_1] = -\tfrac{1}{\lambda}\sum_{(n_1',n_2')\in\mathcal{N}^{[j]}} ff\varepsilon 1_{n_1-n_1',n_2-n_2'}^{[l_1]}\;ffE_{1,(n_1',n_2')}^{[j]}[x_1] \tag{13.55}$$

$$\sum_{(n_1',n_2')\in\mathcal{N}^{[j]}} frt\varepsilon 1^{[l_1,j]}_{n_1-n_1',n_2,n_2'} \left(i\,2\pi\, f^{[j]}_{3,n_1',n_2'}\; ffH^{[j]}_{1,(n_1',n_2')}[x_1] - \partial_1\, ffH^{[j]}_{3,(n_1',n_2')}[x_1] \right) = -i\,\tfrac{2\pi}{\lambda}\, ffE^{[j]}_{2,(n_1,n_2)}[x_1]$$

(13.56)

$$\partial_1\, ffH^{[j]}_{2,(n_1,n_2)}[x_1] - i\,2\pi\, f^{[j]}_{2,n_1,n_2}\; ffH^{[j]}_{1,(n_1,n_2)}[x_1] = -i\,\tfrac{2\pi}{\lambda} \sum_{(n_1',n_2')\in\mathcal{N}^{[j]}} frtr\varepsilon 1^{[l_1,j]}_{n_1-n_1',n_2,n_2'}\; ffE^{[j]}_{3,(n_1',n_2')}[x_1]$$

(13.57)

The permittivity terms in Eq's. 13.55-13.57 are represented by matrices defined as follows,

$$tt\varepsilon 1^{[l_1,j]}_{(n_1,n_2),(n_1',n_2')} = ff\,\varepsilon 1^{[l_1]}_{n_1-n_1',n_2-n_2'} \tag{13.58}$$

$$trt\varepsilon 1^{[l_1,j]}_{(n_1,n_2),(n_1',n_2')} = frt\varepsilon 1^{[l_1,j]}_{n_1-n_1',n_2,n_2'} \tag{13.59}$$

$$trtr\varepsilon 1^{[l_1,j]}_{(n_1,n_2),(n_1',n_2')} = frtr\varepsilon 1^{[l_1,j]}_{n_1-n_1',n_2,n_2'} \tag{13.60}$$

The parenthesized subscripts indicate that these terms represent partitioned matrices with multi-level row and column indices, (n_1, n_2) for rows and (n_1', n_2') for columns. (In practice, the multi-level row/column indices can be replaced by scalar enumeration indices 1, 2, …, which serialize the (n_1, n_2) elements of $\mathcal{N}^{[j]}$.) The " j " superscript annotation in $tt\varepsilon 1^{[l_1,j]}$ indicates that the matrix is truncated to the range $(n_1,n_2),(n_1',n_2')\in\mathcal{N}^{[j]}$. $tt\varepsilon 1^{[l_1,j]}$ is a Toeplitz matrix whereas $trt\varepsilon 1^{[l_1,j]}$ and $trtr\varepsilon 1^{[l_1,j]}$ are "quasi-Toeplitz" matrices, in that their submatrices for fixed n_2 and n_2' are Toeplitz with respect to n_1 and n_1'.

The partitioned diagonal matrices $df_2^{[j]}$ and $df_3^{[j]}$ are also defined,

$$df^{[j]}_{\nu,(n_1,n_2),(n_1',n_2')} = \begin{cases} f^{[j]}_{\nu,n_1,n_2} & \text{if } (n_1,n_2)=(n_1',n_2') \\ 0 & \text{if } (n_1,n_2)\neq(n_1',n_2') \end{cases};\quad \nu = 2,3 \tag{13.61}$$

With the above substitutions, Eq's. 13.52-13.57 are expressed in compact matrix form with the (n_1, n_2) and (n_1', n_2') row/column indices omitted,

$$df_2^{[j]}\, ffE_3^{[j]}[x_1] - df_3^{[j]}\, ffE_2^{[j]}[x_1] = \tfrac{1}{\lambda}\, ffH_1^{[j]}[x_1] \tag{13.62}$$

$$i\,2\pi\, df_3^{[j]}\, ffE_1^{[j]}[x_1] - \partial_1\, ffE_3^{[j]}[x_1] = i\,\tfrac{2\pi}{\lambda}\, ffH_2^{[j]}[x_1] \tag{13.63}$$

$$\partial_1\, ffE_2^{[j]}[x_1] - i\,2\pi\, df_2^{[j]}\, ffE_1^{[j]}[x_1] = i\,\tfrac{2\pi}{\lambda}\, ffH_3^{[j]}[x_1] \tag{13.64}$$

$$df_2^{[j]}\ ffH_3^{[j]}[x_1] - df_3^{[j]}\ ffH_2^{[j]}[x_1] = -\tfrac{1}{\lambda}\, tt\varepsilon 1^{[l_1,j]}\ ffE_1^{[j]}[x_1] \tag{13.65}$$

$$trt\varepsilon 1^{[l_1,j]} \left(i\, 2\pi\, df_3^{[j]}\ ffH_1^{[j]}[x_1] - \partial_1\ ffH_3^{[j]}[x_1] \right) = -i\,\tfrac{2\pi}{\lambda}\ ffE_2^{[j]}[x_1] \tag{13.66}$$

$$\partial_1\ ffH_2^{[j]}[x_1] - i\, 2\pi\, df_2^{[j]}\ ffH_1^{[j]}[x_1] = -i\,\tfrac{2\pi}{\lambda}\, trtr\varepsilon 1^{[l_1,j]}\ ffE_3^{[j]}[x_1] \tag{13.67}$$

The permittivity terms in Eq's. 13.65 and 13.66 are moved to the other side of each equation,

$$rtt\varepsilon 1^{[l_1,j]} \left(df_2^{[j]}\ ffH_3^{[j]}[x_1] - df_3^{[j]}\ ffH_2^{[j]}[x_1] \right) = -\tfrac{1}{\lambda}\ ffE_1^{[j]}[x_1] \tag{13.68}$$

$$i\, 2\pi\, df_3^{[j]}\ ffH_1^{[j]}[x_1] - \partial_1\ ffH_3^{[j]}[x_1] = -i\,\tfrac{2\pi}{\lambda}\, rtrt\varepsilon 1^{[l_1,j]}\ ffE_2^{[j]}[x_1] \tag{13.69}$$

where

$$rtt\varepsilon 1^{[l_1,j]} = (tt\varepsilon 1^{[l_1,j]})^{-1} \tag{13.70}$$

$$rtrt\varepsilon 1^{[l_1,j]} = (trt\varepsilon 1^{[l_1,j]})^{-1} \tag{13.71}$$

Eq's. 13.62 and 13.68 are used to eliminate $ffE_1^{[j]}[x_1]$ and $ffH_1^{[j]}[x_1]$ from Eq's. 13.63, 13.64, 13.69, and 13.67,

$$\partial_1\ ffE_3^{[j]}[x_1] = -i\, 2\pi \left(\tfrac{1}{\lambda}\ ffH_2^{[j]}[x_1] + \lambda\, df_3^{[j]}\, rtt\varepsilon 1^{[l_1,j]}\, (df_2^{[j]}\ ffH_3^{[j]}[x_1] - df_3^{[j]}\ ffH_2^{[j]}[x_1]) \right) \tag{13.72}$$

$$\partial_1\ ffE_2^{[j]}[x_1] = i\, 2\pi \left(\tfrac{1}{\lambda}\ ffH_3^{[j]}[x_1] - \lambda\, df_2^{[j]}\, rtt\varepsilon 1^{[l_1,j]}\, (df_2^{[j]}\ ffH_3^{[j]}[x_1] - df_3^{[j]}\ ffH_2^{[j]}[x_1]) \right) \tag{13.73}$$

$$\partial_1\ ffH_3^{[j]}[x_1] = i\, 2\pi \left(\tfrac{1}{\lambda}\, rtrt\varepsilon 1^{[l_1,j]}\ ffE_2^{[j]}[x_1] + \lambda\, df_3^{[j]} \left(df_2^{[j]}\ ffE_3^{[j]}[x_1] - df_3^{[j]}\ ffE_2^{[j]}[x_1] \right) \right) \tag{13.74}$$

$$\partial_1\ ffH_2^{[j]}[x_1] = -i\, 2\pi \left(\tfrac{1}{\lambda}\, trtr\varepsilon 1^{[l_1,j]}\ ffE_3^{[j]}[x_1] - \lambda\, df_2^{[j]} \left(df_2^{[j]}\ ffE_3^{[j]}[x_1] - df_3^{[j]}\ ffE_2^{[j]}[x_1] \right) \right) \tag{13.75}$$

Eq's. 13.72-13.75 are restated in terms of the fields' $\hat{s}$ and $\hat{q}$ projections, and are then separated into up and down waves relative to a fictitious homogeneous medium of permittivity $\varepsilon^{[\mathrm{f}]}$, as described in Section 6 (Eq's. 6.52-6.55). The up/down separation involves the $f_1^{[\pm]}$ terms defined in Eq. 6.37 (with $\varepsilon^{[\mathrm{c}]} = \varepsilon^{[\mathrm{f}]}$), which are specialized for index set j as follows,

$$f_{1,n_1,n_2}^{[\mathrm{f},\pm,j]} = \pm\sqrt{\frac{\varepsilon^{[\mathrm{f}]}}{\lambda^2} - (f_{2,n_1,n_2}^{[j]})^2 - (f_{3,n_1,n_2}^{[j]})^2} \tag{13.76}$$

where $f_{2,n_1,n_2}^{[j]}$ and $f_{3,n_1,n_2}^{[j]}$ are defined in Eq. 13.11. ($\varepsilon^{[\mathrm{f}]}$ has a positive imaginary part to ensure that $f_{1,n_1,n_2}^{[\mathrm{f},\pm,j]} \neq 0$.) The grating-tangential $\hat{s}$ vector defined by Eq's. 6.40 and 6.41 is similarly specialized for index set j,

$$\begin{aligned} \hat{s}_{n_1,n_2}^{[j]} &= \hat{e}_2\, s_{2,n_1,n_2}^{[j]} + \hat{e}_3\, s_{3,n_1,n_2}^{[j]} \\ &= \hat{s}_{m_1,m_2} \text{ with } (m_1,m_2) = (m_1^{[\mathrm{base},j]}, m_2^{[\mathrm{base},j]}) + (n_1,n_2)\begin{pmatrix} h_{1,1}^{[l_1]} & h_{1,2}^{[l_1]} \\ h_{2,1}^{[l_1]} & h_{2,2}^{[l_1]} \end{pmatrix} \end{aligned} \tag{13.77}$$

$$\left(s_{2,n_1,n_2}^{[j]},\quad s_{3,n_1,n_2}^{[j]} \right) = \begin{cases} \dfrac{\left(-f_{3,n_1,n_2}^{[j]},\quad f_{2,n_1,n_2}^{[j]} \right)}{\sqrt{(f_{2,n_1,n_2}^{[j]})^2 + (f_{3,n_1,n_2}^{[j]})^2}} & \text{if } (f_{2,n_1,n_2}^{[j]})^2 + (f_{3,n_1,n_2}^{[j]})^2 \neq 0 \\ \dfrac{\left(-f_{3,1}^{[\mathrm{g}]},\quad f_{2,1}^{[\mathrm{g}]} \right)}{\sqrt{(f_{2,1}^{[\mathrm{g}]})^2 + (f_{3,1}^{[\mathrm{g}]})^2}} & \text{if } (f_{2,n_1,n_2}^{[j]})^2 + (f_{3,n_1,n_2}^{[j]})^2 = 0 \end{cases} \tag{13.78}$$

(The "if … = 0" branch in this definition can be modified to preserve polarization decoupling for uniperiodic gratings – see Section 15 – but the modification has no effect on the results in this section.) The grating-tangential $\hat{q}$ vector (Eq. 6.43) is also represented as

$$\begin{aligned} \hat{q}_{n_1,n_2}^{[\pm,j]} &= \pm \hat{s}_{n_1,n_2}^{[j]} \times \hat{e}_1 = \pm(\hat{e}_2\, s_{3,n_1,n_2}^{[j]} - \hat{e}_3\, s_{2,n_1,n_2}^{[j]}) \\ &= \hat{q}_{m_1,m_2}^{[\pm]} \text{ with } (m_1,m_2) = (m_1^{[\mathrm{base},j]}, m_2^{[\mathrm{base},j]}) + (n_1,n_2)\begin{pmatrix} h_{1,1}^{[l_1]} & h_{1,2}^{[l_1]} \\ h_{2,1}^{[l_1]} & h_{2,2}^{[l_1]} \end{pmatrix} \end{aligned} \tag{13.79}$$

Eq's. 6.52-6.55 and 6.43 are adapted to define the fields' $\hat{s}$ and $\hat{q}$ projections ($\mathit{ffE}_{\mathrm{s}}^{[j]}$, $\mathit{ffE}_{\mathrm{q}}^{[j]}$, $\mathit{ffH}_{\mathrm{s}}^{[j]}$, $\mathit{ffH}_{\mathrm{q}}^{[j]}$), and also define the corresponding up/down fields' $\hat{s}$ projections ($\mathit{ffE}_{\mathrm{s}}^{[\pm,j]}$, $\mathit{ffH}_{\mathrm{s}}^{[\pm,j]}$),

$$\begin{aligned} \mathit{ffE}_{\mathrm{s},(n_1,n_2)}^{[j]}[x_1] &= \hat{s}_{n_1,n_2}^{[j]} \bullet \mathit{ff}\vec{E}_{(n_1,n_2)}^{[j]}[x_1] = s_{2,n_1,n_2}^{[j]}\, \mathit{ffE}_{2,(n_1,n_2)}^{[j]}[x_1] + s_{3,n_1,n_2}^{[j]}\, \mathit{ffE}_{3,(n_1,n_2)}^{[j]}[x_1] \\ &= \mathit{ffE}_{\mathrm{s},(n_1,n_2)}^{[+,j]}[x_1] + \mathit{ffE}_{\mathrm{s},(n_1,n_2)}^{[-,j]}[x_1] \end{aligned} \tag{13.80}$$

$$\begin{aligned} \mathit{ffH}_{\mathrm{s},(n_1,n_2)}^{[j]}[x_1] &= \hat{s}_{n_1,n_2}^{[j]} \bullet \mathit{ff}\vec{H}_{(n_1,n_2)}^{[j]}[x_1] = s_{2,n_1,n_2}^{[j]}\, \mathit{ffH}_{2,(n_1,n_2)}^{[j]}[x_1] + s_{3,n_1,n_2}^{[j]}\, \mathit{ffH}_{3,(n_1,n_2)}^{[j]}[x_1] \\ &= \mathit{ffH}_{\mathrm{s},(n_1,n_2)}^{[+,j]}[x_1] - \mathit{ffH}_{\mathrm{s},(n_1,n_2)}^{[-,j]}[x_1] \end{aligned} \tag{13.81}$$

$$\begin{aligned} \mathit{ffE}_{\mathrm{q},(n_1,n_2)}^{[j]}[x_1] &= \hat{q}_{n_1,n_2}^{[+,j]} \bullet \mathit{ff}\vec{E}_{(n_1,n_2)}^{[j]}[x_1] = s_{3,n_1,n_2}^{[j]}\, \mathit{ffE}_{2,(n_1,n_2)}^{[j]}[x_1] - s_{2,n_1,n_2}^{[j]}\, \mathit{ffE}_{3,(n_1,n_2)}^{[j]}[x_1] \\ &= \frac{\lambda}{\varepsilon^{[\mathrm{f}]}}\, f_{1,(n_1,n_2)}^{[\mathrm{f},+,j]}\, (\mathit{ffH}_{\mathrm{s},(n_1,n_2)}^{[+,j]}[x_1] + \mathit{ffH}_{\mathrm{s},(n_1,n_2)}^{[-,j]}[x_1]) \end{aligned} \tag{13.82}$$

$$\begin{aligned} ffH^{[j]}_{\mathrm{q},(n_1,n_2)}[x_1] &= \hat{q}^{[+,j]}_{(n_1,n_2)} \bullet ff\vec{H}^{[j]}_{(n_1,n_2)}[x_1] = s^{[j]}_{3,n_1,n_2}\, ffH^{[j]}_{2,(n_1,n_2)}[x_1] - s^{[j]}_{2,n_1,n_2}\, ffH^{[j]}_{3,(n_1,n_2)}[x_1] \\ &= -\lambda\, f^{[\mathrm{f},+,j]}_{1,(n_1,n_2)}\, (ffE^{(+,j)}_{\mathrm{s},(n_1,n_2)}[x_1] - ffE^{[-,j]}_{\mathrm{s},(n_1,n_2)}[x_1]) \end{aligned} \tag{13.83}$$

The following diagonal matrix notation is used for $f_1^{[\mathrm{f},\pm,j]}$ and $s_k^{[j]}$,

$$df^{[\mathrm{f},\pm,j]}_{1,(n_1,n_2),(n'_1,n'_2)} = \begin{cases} f^{[\mathrm{f},\pm,j]}_{1,n_1,n_2} & \text{if } (n_1,n_2) = (n'_1,n'_2) \\ 0 & \text{if } (n_1,n_2) \neq (n'_1,n'_2) \end{cases} \tag{13.84}$$

$$ds^{[j]}_{k,(n_1,n_2),(n'_1,n'_2)} = \begin{cases} s^{[j]}_{k,n_1,n_2} & \text{if } (n_1,n_2) = (n'_1,n'_2) \\ 0 & \text{if } (n_1,n_2) \neq (n'_1,n'_2) \end{cases}; \quad k = 2,3 \tag{13.85}$$

With these definitions, Eq’s. 13.80-13.83 are stated more compactly as

$$ffE^{[j]}_{\mathrm{s}}[x_1] = ds^{[j]}_2\, ffE^{[j]}_2[x_1] + ds^{[j]}_3\, ffE^{[j]}_3[x_1] = ffE^{[+,j]}_{\mathrm{s}}[x_1] + ffE^{[-,j]}_{\mathrm{s}}[x_1] \tag{13.86}$$

$$ffH^{[j]}_{\mathrm{s}}[x_1] = ds^{[j]}_2\, ffH^{[j]}_2[x_1] + ds^{[j]}_3\, ffH^{[j]}_3[x_1] = ffH^{[+,j]}_{\mathrm{s}}[x_1] - ffH^{[-,j]}_{\mathrm{s}}[x_1] \tag{13.87}$$

$$ffE^{[j]}_{\mathrm{q}}[x_1] = ds^{[j]}_3\, ffE^{[j]}_2[x_1] - ds^{[j]}_2\, ffE^{[j]}_3[x_1] = \frac{\lambda}{\varepsilon^{[\mathrm{f}]}}\, df^{[\mathrm{f},+,j]}_1\, (ffH^{[+,j]}_{\mathrm{s}}[x_1] + ffH^{[-,j]}_{\mathrm{s}}[x_1]) \tag{13.88}$$

$$ffH^{[j]}_{\mathrm{q}}[x_1] = ds^{[j]}_3\, ffH^{[j]}_2[x_1] - ds^{[j]}_2\, ffH^{[j]}_3[x_1] = -\lambda\, df^{[\mathrm{f},+,j]}_1\, (ffE^{[+,j]}_{\mathrm{s}}[x_1] - ffE^{[-,j]}_{\mathrm{s}}[x_1]) \tag{13.89}$$

Eq’s. 13.86-13.89 are combined with the relation $(ds^{[j]}_2)^2 + (ds^{[j]}_3)^2 = \mathbf{I}$ (from Eq. 13.78) to obtain

$$ffE^{[j]}_2[x_1] = ds^{[j]}_2\, ffE^{[j]}_{\mathrm{s}}[x_1] + ds^{[j]}_3\, ffE^{[j]}_{\mathrm{q}}[x_1] \tag{13.90}$$

$$ffE^{[j]}_3[x_1] = ds^{[j]}_3\, ffE^{[j]}_{\mathrm{s}}[x_1] - ds^{[j]}_2\, ffE^{[j]}_{\mathrm{q}}[x_1] \tag{13.91}$$

$$ffH^{[j]}_2[x_1] = ds^{[j]}_2\, ffH^{[j]}_{\mathrm{s}}[x_1] + ds^{[j]}_3\, ffH^{[j]}_{\mathrm{q}}[x_1] \tag{13.92}$$

$$ffH^{[j]}_3[x_1] = ds^{[j]}_3\, ffH^{[j]}_{\mathrm{s}}[x_1] - ds^{[j]}_2\, ffH^{[j]}_{\mathrm{q}}[x_1] \tag{13.93}$$

The above equations are used to restate differential Eq’s. 13.72-13.75 in terms of the fields’ $\hat{s}$ and $\hat{q}$ projections,

$$\partial_1\, ffE^{[j]}_{\mathrm{s}}[x_1] = -i\,\tfrac{2\pi}{\lambda}\, ffH^{[j]}_{\mathrm{q}}[x_1] \tag{13.94}$$

$$\partial_1 \, f\!f E_{\rm q}^{[j]}[x_1] = i\,2\pi \left(\tfrac{1}{\lambda}\mathbf{I} - \lambda \sqrt{(df_2^{[j]})^2 + (df_3^{[j]})^2} \; rtt\varepsilon 1^{[l_1,j]} \sqrt{(df_2^{[j]})^2 + (df_3^{[j]})^2} \right) f\!f H_{\rm s}^{[j]}[x_1] \quad (13.95)$$

$$\partial_1 \, f\!f H_{\rm s}^{[j]}[x_1] = i\,\tfrac{2\pi}{\lambda} \begin{pmatrix} ds_3^{[j]} \, rtrt\varepsilon 1^{[l_1,j]} \, (ds_2^{[j]} \, f\!f E_{\rm s}^{[j]}[x_1] + ds_3^{[j]} \, f\!f E_{\rm q}^{[j]}[x_1]) \\ - ds_2^{[j]} \, trtr\varepsilon 1^{[l_1,j]} \, (ds_3^{[j]} \, f\!f E_{\rm s}^{[j]}[x_1] - ds_2^{[j]} \, f\!f E_{\rm q}^{[j]}[x_1]) \end{pmatrix} \quad (13.96)$$

$$\partial_1 \, f\!f H_{\rm q}^{[j]}[x_1] = -i\,2\pi \begin{pmatrix} \tfrac{1}{\lambda} \begin{pmatrix} ds_2^{[j]} \, rtrt\varepsilon 1^{[l_1,j]} \left(ds_2^{[j]} \, f\!f E_{\rm s}^{[j]}[x_1] + ds_3^{[j]} \, f\!f E_{\rm q}^{[j]}[x_1] \right) \\ + ds_3^{[j]} \, trtr\varepsilon 1^{[l_1,j]} \left(ds_3^{[j]} \, f\!f E_{\rm s}^{[j]}[x_1] - ds_2^{[j]} \, f\!f E_{\rm q}^{[j]}[x_1] \right) \end{pmatrix} \\ -\lambda \left((df_2^{[j]})^2 + (df_3^{[j]})^2 \right) f\!f E_{\rm s}^{[j]}[x_1] \end{pmatrix} \quad (13.97)$$

These equations are of the form

$$\partial_1 \begin{pmatrix} F^{[\mathrm{E},j]}[x_1] \\ F^{[\mathrm{H},j]}[x_1] \end{pmatrix} = \begin{pmatrix} \mathbf{0} & DEH^{[j]} \\ DHE^{[j]} & \mathbf{0} \end{pmatrix} \begin{pmatrix} F^{[\mathrm{E},j]}[x_1] \\ F^{[\mathrm{H},j]}[x_1] \end{pmatrix} \quad (13.98)$$

where

$$F^{[\mathrm{E},j]}[x_1] = \begin{pmatrix} f\!f E_{\rm s}^{[j]}[x_1] \\ f\!f E_{\rm q}^{[j]}[x_1] \end{pmatrix} \quad (13.99)$$

$$F^{[\mathrm{H},j]}[x_1] = i \begin{pmatrix} f\!f H_{\rm s}^{[j]}[x_1] \\ f\!f H_{\rm q}^{[j]}[x_1] \end{pmatrix} \quad (13.100)$$

$$DEH^{[j]} = 2\pi \begin{pmatrix} \mathbf{0} & -\tfrac{1}{\lambda}\mathbf{I} \\ \tfrac{1}{\lambda}\boldsymbol{I} - \lambda \sqrt{(df_2^{[j]})^2 + (df_3^{[j]})^2} \; rtt\varepsilon 1^{[l_1,j]} \sqrt{(df_2^{[j]})^2 + (df_3^{[j]})^2} & \mathbf{0} \end{pmatrix} \quad (13.101)$$

$$DHE^{[j]} = -2\pi \begin{pmatrix} \tfrac{1}{\lambda} \left(\begin{pmatrix} ds_3^{[j]} \\ -ds_2^{[j]} \end{pmatrix} rtrt\varepsilon 1^{[l_1,j]} \begin{pmatrix} ds_2^{[j]} & ds_3^{[j]} \end{pmatrix} - \begin{pmatrix} ds_2^{[j]} \\ ds_3^{[j]} \end{pmatrix} trtr\varepsilon 1^{[l_1,j]} \begin{pmatrix} ds_3^{[j]} & -ds_2^{[j]} \end{pmatrix} \right) \\ + \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \lambda \left((df_2^{[j]})^2 + (df_3^{[j]})^2 \right) & \mathbf{0} \end{pmatrix} \end{pmatrix} \quad (13.102)$$

Eq. 13.98 has a solution in the form of an exponential matrix representing a linear relationship between the field quantities at $x_1 = x_1^{[0]}$ and $x_1 = x_1^{[1]}$, from which the stratum's S matrix can be determined. However, the exponential matrix computation becomes numerically unstable when Δx_1 is large [Ref. 5], so an alternative approach is used. An S matrix is calculated for a thin stratum of thickness Δx_1, which is set equal to the full stratum thickness scaled by a power of 1/2,

$$\Delta x_1 = (x_1^{[1]} - x_1^{[0]}) / 2^{sp} \tag{13.103}$$

The scaling factor's exponent sp ("scaling power") is chosen so that the S matrix can be calculated using a rational approximation. (Details of the calculation and the choice of sp are outlined in Appendix D.) Then sp stacking operations are performed (each one doubling the thickness) to obtain the S matrix for a stratum of thickness $x_1^{[1]} - x_1^{[0]}$. The rational approximation is based on a Padé ("Pah-*deh*") approximation to the exponential matrix (Appendix D),

$$\begin{pmatrix} P^{[\mathrm{E},\mathrm{E},j]} & -P^{[\mathrm{E},\mathrm{H},j]} \\ -P^{[\mathrm{H},\mathrm{E},j]} & P^{[\mathrm{H},\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} F^{[\mathrm{E},j]}[x_1^{[0]} + \Delta x_1] \\ F^{[\mathrm{H},j]}[x_1^{[0]} + \Delta x_1] \end{pmatrix} = \begin{pmatrix} P^{[\mathrm{E},\mathrm{E},j]} & P^{[\mathrm{E},\mathrm{H},j]} \\ P^{[\mathrm{H},\mathrm{E},j]} & P^{[\mathrm{H},\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} F^{[\mathrm{E},j]}[x_1^{[0]}] \\ F^{[\mathrm{H},j]}[x_1^{[0]}] \end{pmatrix} \tag{13.104}$$

The right side of Eq. 13.100 is prefixed with a factor of i so that the P matrix is real-valued under the following condition,

$$\begin{aligned} &\text{If } \varepsilon 1^{[l_1]}[-x_2, -x_3]^* = \varepsilon 1^{[l_1]}[x_2, x_3] \text{ then} \\ &\quad \mathrm{Im}[DEH^{[j]}] = 0,\ \mathrm{Im}[DHE^{[j]}] = 0, \\ &\quad \mathrm{Im}[P^{[\mathrm{E},\mathrm{E},j]}] = 0,\ \mathrm{Im}[P^{[\mathrm{E},\mathrm{H},j]}] = 0,\ \mathrm{Im}[P^{[\mathrm{H},\mathrm{E},j]}] = 0,\ \mathrm{Im}[P^{[\mathrm{H},\mathrm{H},j]}] = 0 \end{aligned} \tag{13.105}$$

In particular, Eq's. 13.105 hold for a symmetric, non-absorbing stratum ($\varepsilon 1^{[l_1]}[x_2, x_3] = \varepsilon 1^{[l_1]}[-x_2, -x_3]$ and $\mathrm{Im}[\varepsilon 1^{[l_1]}[x_2, x_3]] = 0$). In some cases, a coordinate translation can be applied, as described in Section 12, to move the (x_2, x_3) coordinate origin to the symmetry axis so that the symmetry condition holds. The condition $\varepsilon 1^{[l_1]}[-x_2, -x_3]^* = \varepsilon 1^{[l_1]}[x_2, x_3]$ in Eq. 13.105 is equivalent to $\mathrm{Im}[\mathit{ff}\varepsilon 1^{[l_1]}] = \boldsymbol{0}$ (Eq. 13.1), and it implies that the three matrices $\mathit{rtt}\varepsilon 1^{[l_1,j]}$, $\mathit{rtrt}\varepsilon 1^{[l_1,j]}$, and $\mathit{trtr}\varepsilon 1^{[l_1,j]}$ in Eq's. 13.101 and 13.102 are real-valued, thus establishing Eq's. 13.105. The first result, $\mathrm{Im}[\mathit{rtt}\varepsilon 1^{[l_1,j]}] = \boldsymbol{0}$, follows from Eq's. 13.58 and 13.70. The second result, $\mathrm{Im}[\mathit{rtrt}\varepsilon 1^{[l_1,j]}] = \boldsymbol{0}$, is derived as follows: The condition $\varepsilon 1^{[l_1]}[-x_2, -x_3]^* = \varepsilon 1^{[l_1]}[x_2, x_3]$ implies that $f\varepsilon 1^{[l_1]}[-x_2]^* = f\varepsilon 1^{[l_1]}[x_2]$ (Eq. 13.19), $t\varepsilon 1^{[l_1]}[-x_2]^* = t\varepsilon 1^{[l_1]}[x_2]$ (Eq. 13.39), $rt\varepsilon 1^{[l_1]}[-x_2]^* = rt\varepsilon 1^{[l_1]}[x_2]$ (Eq. 13.41), $\mathrm{Im}[\mathit{frt}\varepsilon 1^{[l_1,j]}] = 0$ (Eq. 13.50), $\mathrm{Im}[\mathit{trt}\varepsilon 1^{[l_1,j]}] = 0$ (Eq. 13.59), and $\mathrm{Im}[\mathit{rtrt}\varepsilon 1^{[l_1,j]}] = 0$ (Eq. 13.71). The third result ($\mathrm{Im}[\mathit{trtr}\varepsilon 1^{[l_1,j]}] = \boldsymbol{0}$) similarly follows from Eq's. 13.32, 13.40, 13.42, 13.51, and 13.60.

The following relations are obtained from Eq's. 13.86-13.89, 13.99, and 13.100,

$$\begin{pmatrix} F^{[\mathrm{E},j]}[x_1] \\ F^{[\mathrm{H},j]}[x_1] \end{pmatrix} = \begin{pmatrix} \Gamma^{[\mathrm{E},j]} & \Gamma^{[\mathrm{E},j]} \\ \Gamma^{[\mathrm{H},j]} & -\Gamma^{[\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} F^{[+,j]}[x_1] \\ F^{[-,j]}[x_1] \end{pmatrix} \tag{13.106}$$

where

$$\Gamma^{[\mathrm{E},j]} = \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & (\lambda / \varepsilon^{[\mathrm{f}]})\, df_1^{[\mathrm{f},+,j]} \end{pmatrix} \tag{13.107}$$

$$\Gamma^{[\mathrm{H},j]} = i \begin{pmatrix} \mathbf{0} & \mathbf{I} \\ -\lambda\, df_1^{[\mathrm{f},+,j]} & \mathbf{0} \end{pmatrix} \tag{13.108}$$

$$F^{[\pm,j]}[x_1] = \begin{pmatrix} ffE_{\mathrm{s}}^{[\pm,j]}[x_1] \\ ffH_{\mathrm{s}}^{[\pm,j]}[x_1] \end{pmatrix} \tag{13.109}$$

Eq’s. 13.106 are used to restate Eq. 13.104 in terms of the up/down field amplitudes, $F^{[\pm,j]}$.

$$\begin{aligned} &\begin{pmatrix} P^{[\mathrm{E,E},j]} & -P^{[\mathrm{E,H},j]} \\ -P^{[\mathrm{H,E},j]} & P^{[\mathrm{H,H},j]} \end{pmatrix} \begin{pmatrix} \Gamma^{[\mathrm{E},j]} & \Gamma^{[\mathrm{E},j]} \\ \Gamma^{[\mathrm{H},j]} & -\Gamma^{[\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} F^{[+,j]}[x_1^{[0]} + \Delta x_1] \\ F^{[-,j]}[x_1^{[0]} + \Delta x_1] \end{pmatrix} \\ &= \begin{pmatrix} P^{[\mathrm{E,E},j]} & P^{[\mathrm{E,H},j]} \\ P^{[\mathrm{H,E},j]} & P^{[\mathrm{H,H},j]} \end{pmatrix} \begin{pmatrix} \Gamma^{[\mathrm{E},j]} & \Gamma^{[\mathrm{E},j]} \\ \Gamma^{[\mathrm{H},j]} & -\Gamma^{[\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} F^{[+,j]}[x_1^{[0]}] \\ F^{[-,j]}[x_1^{[0]}] \end{pmatrix} \end{aligned} \tag{13.110}$$

The outgoing waves $F^{[+,j]}[x_1^{[0]} + \Delta x_1]$ and $F^{[-,j]}[x_1^{[0]}]$ are represented as linear functions of the incoming waves $F^{[+,j]}[x_1^{[0]}]$ and $F^{[-,j]}[x_1^{[0]} + \Delta x_1]$, with the linear coefficients encapsulated in an S matrix,

$$\begin{pmatrix} F^{[+,j]}[x_1^{[0]} + \Delta x_1] \\ F^{[-,j]}[x_1^{[0]}] \end{pmatrix} = \begin{pmatrix} S^{[++,j]} & S^{[+-,j]} \\ S^{[-+,j]} & S^{[--,j]} \end{pmatrix} \begin{pmatrix} F^{[+,j]}[x_1^{[0]}] \\ F^{[-,j]}[x_1^{[0]} + \Delta x_1] \end{pmatrix} \tag{13.111}$$

Eq. 13.111 is substituted in Eq. 13.110,

$$\begin{aligned} &\begin{pmatrix} P^{[\mathrm{E,E},j]} & -P^{[\mathrm{E,H},j]} \\ -P^{[\mathrm{H,E},j]} & P^{[\mathrm{H,H},j]} \end{pmatrix} \begin{pmatrix} \Gamma^{[\mathrm{E},j]} & \Gamma^{[\mathrm{E},j]} \\ \Gamma^{[\mathrm{H},j]} & -\Gamma^{[\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} S^{[++,j]} & S^{[+-,j]} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \begin{pmatrix} F^{[+,j]}[x_1^{[0]}] \\ F^{[-,j]}[x_1^{[0]} + \Delta x_1] \end{pmatrix} \\ &= \begin{pmatrix} P^{[\mathrm{E,E},j]} & P^{[\mathrm{E,H},j]} \\ P^{[\mathrm{H,E},j]} & P^{[\mathrm{H,H},j]} \end{pmatrix} \begin{pmatrix} \Gamma^{[\mathrm{E},j]} & \Gamma^{[\mathrm{E},j]} \\ \Gamma^{[\mathrm{H},j]} & -\Gamma^{[\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ S^{[-+,j]} & S^{[--,j]} \end{pmatrix} \begin{pmatrix} F^{[+,j]}[x_1^{[0]}] \\ F^{[-,j]}[x_1^{[0]} + \Delta x_1] \end{pmatrix} \end{aligned} \tag{13.112}$$

This equation holds for any incoming waves; hence

$$\begin{aligned} &\begin{pmatrix} P^{[\mathrm{E,E},j]} & -P^{[\mathrm{E,H},j]} \\ -P^{[\mathrm{H,E},j]} & P^{[\mathrm{H,H},j]} \end{pmatrix} \begin{pmatrix} \Gamma^{[\mathrm{E},j]} & \Gamma^{[\mathrm{E},j]} \\ \Gamma^{[\mathrm{H},j]} & -\Gamma^{[\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} S^{[++,j]} & S^{[+-,j]} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \\ &= \begin{pmatrix} P^{[\mathrm{E,E},j]} & P^{[\mathrm{E,H},j]} \\ P^{[\mathrm{H,E},j]} & P^{[\mathrm{H,H},j]} \end{pmatrix} \begin{pmatrix} \Gamma^{[\mathrm{E},j]} & \Gamma^{[\mathrm{E},j]} \\ \Gamma^{[\mathrm{H},j]} & -\Gamma^{[\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ S^{[-+,j]} & S^{[--,j]} \end{pmatrix} \end{aligned} \tag{13.113}$$

Eq. 13.113 can be rearranged as follows,

$$\begin{pmatrix} P^{[\mathrm{E},\mathrm{E},j]} & -P^{[\mathrm{E},\mathrm{H},j]} \\ -P^{[\mathrm{H},\mathrm{E},j]} & P^{[\mathrm{H},\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} \Gamma^{[\mathrm{E},j]} & \Gamma^{[\mathrm{E},j]} \\ \Gamma^{[\mathrm{H},j]} & -\Gamma^{[\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} S^{[--,j]} & S^{[-+,j]} \\ \mathbf{0} & \mathbf{I} \end{pmatrix}$$
$$= \begin{pmatrix} P^{[\mathrm{E},\mathrm{E},j]} & P^{[\mathrm{E},\mathrm{H},j]} \\ P^{[\mathrm{H},\mathrm{E},j]} & P^{[\mathrm{H},\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} \Gamma^{[\mathrm{E},j]} & \Gamma^{[\mathrm{E},j]} \\ \Gamma^{[\mathrm{H},j]} & -\Gamma^{[\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ S^{[+-,j]} & S^{[++,j]} \end{pmatrix} \tag{13.114}$$

This result is obtained by applying the following operations to the left side of Eq. 13.113, and applying a similar transformation to the right side,

$$\begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -\mathbf{I} \end{pmatrix} \begin{pmatrix} P^{[\mathrm{E},\mathrm{E},j]} & -P^{[\mathrm{E},\mathrm{H},j]} \\ -P^{[\mathrm{H},\mathrm{E},j]} & P^{[\mathrm{H},\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} \Gamma^{[\mathrm{E},j]} & \Gamma^{[\mathrm{E},j]} \\ \Gamma^{[\mathrm{H},j]} & -\Gamma^{[\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} S^{[++,j]} & S^{[+-,j]} \\ \mathbf{0} & \mathbf{I} \end{pmatrix}$$
$$= \begin{pmatrix} P^{[\mathrm{E},\mathrm{E},j]} & P^{[\mathrm{E},\mathrm{H},j]} \\ P^{[\mathrm{H},\mathrm{E},j]} & P^{[\mathrm{H},\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -\mathbf{I} \end{pmatrix} \begin{pmatrix} \Gamma^{[\mathrm{E},j]} & \Gamma^{[\mathrm{E},j]} \\ \Gamma^{[\mathrm{H},j]} & -\Gamma^{[\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} S^{[++,j]} & S^{[+-,j]} \\ \mathbf{0} & \mathbf{I} \end{pmatrix}$$
$$= \begin{pmatrix} P^{[\mathrm{E},\mathrm{E},j]} & P^{[\mathrm{E},\mathrm{H},j]} \\ P^{[\mathrm{H},\mathrm{E},j]} & P^{[\mathrm{H},\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} \Gamma^{[\mathrm{E},j]} & \Gamma^{[\mathrm{E},j]} \\ \Gamma^{[\mathrm{H},j]} & -\Gamma^{[\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} \mathbf{0} & \mathbf{I} \\ \mathbf{I} & \mathbf{0} \end{pmatrix} \begin{pmatrix} S^{[++,j]} & S^{[+-,j]} \\ \mathbf{0} & \mathbf{I} \end{pmatrix}$$
$$= \begin{pmatrix} P^{[\mathrm{E},\mathrm{E},j]} & P^{[\mathrm{E},\mathrm{H},j]} \\ P^{[\mathrm{H},\mathrm{E},j]} & P^{[\mathrm{H},\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} \Gamma^{[\mathrm{E},j]} & \Gamma^{[\mathrm{E},j]} \\ \Gamma^{[\mathrm{H},j]} & -\Gamma^{[\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ S^{[+-,j]} & S^{[++,j]} \end{pmatrix} \begin{pmatrix} \mathbf{0} & \mathbf{I} \\ \mathbf{I} & \mathbf{0} \end{pmatrix} \tag{13.115}$$

Comparing Eq's. 13.113 and 13.114, the following symmetry relations (Eq. 7.4) are obtained,

$$S^{[++,j]} = S^{[--,j]}, \quad S^{[+-,j]} = S^{[-+,j]} \tag{13.116}$$

With this simplification, only two of the four S-matrix quadrants need be determined. The first block column in Eq. 13.114 is

$$\begin{pmatrix} P^{[\mathrm{E},\mathrm{E},j]} & -P^{[\mathrm{E},\mathrm{H},j]} \\ -P^{[\mathrm{H},\mathrm{E},j]} & P^{[\mathrm{H},\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} \Gamma^{[\mathrm{E},j]} \\ \Gamma^{[\mathrm{H},j]} \end{pmatrix} S^{[--,j]} = \begin{pmatrix} P^{[\mathrm{E},\mathrm{E},j]} & P^{[\mathrm{E},\mathrm{H},j]} \\ P^{[\mathrm{H},\mathrm{E},j]} & P^{[\mathrm{H},\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} \Gamma^{[\mathrm{E},j]} & \Gamma^{[\mathrm{E},j]} \\ \Gamma^{[\mathrm{H},j]} & -\Gamma^{[\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} \mathbf{I} \\ S^{[+-,j]} \end{pmatrix} \tag{13.117}$$

For small Δx_1 the P matrix is close to an identity matrix ($P^{[\mathrm{E},\mathrm{E},j]} \cong \mathbf{I} \cong P^{[\mathrm{H},\mathrm{H},j]}$, $P^{[\mathrm{E},\mathrm{H},j]} \cong \mathbf{0} \cong P^{[\mathrm{H},\mathrm{E},j]}$), $S^{[+-,j]}$ is close to $\mathbf{0}$ and $S^{[--,j]}$ is close to $\mathbf{I}$. The numerical precision of $S^{[--,j]}$ might be limited by the large diagonal elements (close to 1), but the precision loss can be avoided by calculating $S^{[--,j]} - \mathbf{I}$ rather than $S^{[--,j]}$, using the following variant of Eq. 13.117,

$$\begin{pmatrix} P^{[\mathrm{E},\mathrm{E},j]} & -P^{[\mathrm{E},\mathrm{H},j]} \\ -P^{[\mathrm{H},\mathrm{E},j]} & P^{[\mathrm{H},\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} \Gamma^{[\mathrm{E},j]} \\ \Gamma^{[\mathrm{H},j]} \end{pmatrix} (S^{[--,j]} - \mathbf{I}) - \begin{pmatrix} P^{[\mathrm{E},\mathrm{E},j]} & P^{[\mathrm{E},\mathrm{H},j]} \\ P^{[\mathrm{H},\mathrm{E},j]} & P^{[\mathrm{H},\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} \Gamma^{[\mathrm{E},j]} \\ -\Gamma^{[\mathrm{H},j]} \end{pmatrix} S^{[+-,j]}$$
$$= 2 \begin{pmatrix} \mathbf{0} & P^{[\mathrm{E},\mathrm{H},j]} \\ P^{[\mathrm{H},\mathrm{E},j]} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \Gamma^{[\mathrm{E},j]} \\ \Gamma^{[\mathrm{H},j]} \end{pmatrix} \tag{13.118}$$

The solution of Eq. 13.118 is

$$\begin{pmatrix} S^{[+-,j]} \\ S^{[--,j]} - \mathbf{I} \end{pmatrix} = \begin{pmatrix} \mathbf{I} & \mathbf{I} \\ -\mathbf{I} & \mathbf{I} \end{pmatrix} \begin{pmatrix} (-P^{[\mathrm{E},\mathrm{E},j]}\,\Gamma^{[\mathrm{E},j]} + P^{[\mathrm{E},\mathrm{H},j]}\,\Gamma^{[\mathrm{H},j]})^{-1}\,P^{[\mathrm{E},\mathrm{H},j]}\,\Gamma^{[\mathrm{H},j]} \\ (-P^{[\mathrm{H},\mathrm{E},j]}\,\Gamma^{[\mathrm{E},j]} + P^{[\mathrm{H},\mathrm{H},j]}\,\Gamma^{[\mathrm{H},j]})^{-1}\,P^{[\mathrm{H},\mathrm{E},j]}\,\Gamma^{[\mathrm{E},j]} \end{pmatrix} \tag{13.119}$$

With the symmetry relations of Eq's. 13.116, the following self-stacking operation effectively doubles Δx_1,

$$\begin{pmatrix} S^{[+-,j]} \\ S^{[--,j]} \end{pmatrix} \leftarrow \begin{pmatrix} S^{[+-,j]} + S^{[--,j]}\,S^{[+-,j]}\,(\mathbf{I} - (S^{[+-,j]})^2)^{-1}\,S^{[--,j]} \\ S^{[--,j]}\,(\mathbf{I} - (S^{[+-,j]})^2)^{-1}\,S^{[--,j]} \end{pmatrix} \qquad (\Delta x_1 \leftarrow 2\,\Delta x_1) \tag{13.120}$$

(from Eq's. 7.4 and 8.8, with $Sa = Sb = S$). This operation is repeated sp times to build up the full S matrix for a stratum of thickness $x_1^{[1]} - x_1^{[0]} = 2^{sp}\,\Delta x_1$ (Eq. 13.103).

For small Δx_1 in Eq. 13.103, the P matrix in Eq. 13.104 is close to an identity matrix, $S^{[+-,j]}$ is close to $\boldsymbol{0}$, and $S^{[--,j]}$ is close to $\mathbf{I}$. The numeric precision of $S^{[--,j]}$ is limited by the dominating diagonal elements. Eq. 13.119 returns $S^{[--,j]}$ with $\mathbf{I}$ subtracted off, and Eq. 13.120 could be modified to operate on $S^{[--,j]} - \mathbf{I}$, rather than $S^{[--,j]}$, to avoid precision loss in the initial stages of the stacking operation. However, the cumulative $S^{[--,j]}$, after completing all sp self-stacking steps, can be very close to zero for a low-transmittance (nearly opaque) stratum. In this case the quantity $S^{[--,j]} - \mathbf{I}$ will be precision limited, and adding $\mathbf{I}$ to recover $S^{[--,j]}$ could yield numeric zero.

To minimize precision loss in $S^{[--,j]}$ at both the beginning and end of the self-stacking process, the stacking operation is applied with the diagonal of $S^{[--,j]}$ subtracted off at each step as follows:

$$
\left.\begin{array}{l}
\text{Initialize } S^{[+-,j]} \text{ and } S'^{[--,j]} = S^{[--,j]} - \operatorname{diag}[d] \text{ with} \\
\quad \Delta x_1 = (x_1^{[1]} - x_1^{[0]}) / 2^{sp} \text{ and } d = \begin{pmatrix} 1 \\ 1 \\ \vdots \end{pmatrix} \; \left(\mathbf{I} = \operatorname{diag}[d]\right) \\
\text{Repeat } sp \text{ times:} \\
\qquad (1)\; S^{[--,j]} = S'^{[--,j]} + \operatorname{diag}[d] \\
\qquad (2)\; d'_k = S^{[--,j]}_{k,k} \\
\qquad (3)\; S'^{[--,j]}_{k,k} \leftarrow S'^{[--,j]}_{k,k} - \left(d'_k - d_k\right) \\
\qquad (4)\; d \leftarrow d' \\
\qquad (5)\; \begin{pmatrix} S^{[+-,j]} \\ S'^{[--,j]} \end{pmatrix} \leftarrow \begin{pmatrix} S^{[+-,j]} + S^{[--,j]} S^{[+-,j]} (\mathbf{I} - (S^{[+-,j]})^2)^{-1} S^{[--,j]} \\ \left(S'^{[--,j]} + \operatorname{diag}[d](S^{[+-,j]})^2\right)(\mathbf{I} - (S^{[+-,j]})^2)^{-1} S^{[--,j]} + \operatorname{diag}[d] S'^{[--,j]} \end{pmatrix} \\
\qquad (6)\; d_k \leftarrow d_k{}^2 \\
S^{[--,j]} = S'^{[--,j]} + \operatorname{diag}[d]
\end{array}\right\} \tag{13.121}
$$

At step (1) in the repeat loop d is at least roughly equal to the diagonal of $S^{[--,j]}$, i.e., $d_k \cong S^{[--,j]}_{k,k}$. Step (2) recalculates the diagonal elements: $d'_k = S^{[--,j]}_{k,k} = S'^{[--,j]}_{k,k} + d_k$, although d'_k can be numerically equal to d_k when $S'^{[--,j]}_{k,k}$ very small. Step (3) recalculates the diagonal of $S'^{[--,j]}$ so that $S^{[--,j]} = S'^{[--,j]} + \operatorname{diag}[d']$, using the calculated difference $d' - d$ as a decrement offset to minimize accuracy loss in the diagonal. Step (4) restores the relation $S'^{[--,j]} = S^{[--,j]} - \operatorname{diag}[d]$. Step (5) redefines $S^{[+-,j]}$ as in Eq. 13.120 and it redefines $S'^{[--,j]} = S^{[--,j]} - \operatorname{diag}[d]^2$ (after $S^{[--,j]}$ has been transformed by Eq. 13.120). This step is based on the relation $(\mathbf{I} - A)^{-1} = \mathbf{I} + A(\mathbf{I} - A)^{-1}$ with $A = (S^{[+-,j]})^2$:

$$
\begin{aligned}
& S^{[--,j]} (\mathbf{I} - (S^{[+-,j]})^2)^{-1} S^{[--,j]} \\
& = \left(S'^{[--,j]} + \operatorname{diag}[d]\right)(\mathbf{I} - (S^{[+-,j]})^2)^{-1} S^{[--,j]} \\
& = S'^{[--,j]} (\mathbf{I} - (S^{[+-,j]})^2)^{-1} S^{[--,j]} + \operatorname{diag}[d]\left(\mathbf{I} + (S^{[+-,j]})^2 (\mathbf{I} - (S^{[+-,j]})^2)^{-1}\right) S^{[--,j]} \\
& = \left(S'^{[--,j]} + \operatorname{diag}[d](S^{[+-,j]})^2\right)(\mathbf{I} - (S^{[+-,j]})^2)^{-1} S^{[--,j]} + \operatorname{diag}[d] S'^{[--,j]} + \operatorname{diag}[d]^2
\end{aligned} \tag{13.122}
$$

Step (6) restores the relation $S'^{[--,j]} = S^{[--,j]} - \operatorname{diag}[d]$.

All term in step (5) reduce to zero in the case that the S-matrix is diagonal ($S^{[+-,j]} = \mathbf{0}$, $S^{[--,j]} = \operatorname{diag}[d]$). Thus, the precision loss due a dominant diagonal is avoided. Eq. 13.120 requires four matrix multiplies and one matrix divide per iteration. The same is true of Eq. 13.121, step (5), not counting the two diagonal matrix multiplies, so the more complex stacking operation does not entail a significant efficiency penalty.

14. The S matrix for a uniperiodic stratum

A uniperiodic stratum is treated as a special case of a biperiodic stratum, requiring just a few specializations or modifications of the equations in Section 13. In Eq. 13.1 the range of n_2 is limited to $\{0\}$,

$$\varepsilon[\vec{x}] = \varepsilon 1^{[l_1]}[x_2, x_3] = \sum_{n_1} f\!f\,\varepsilon 1^{[l_1]}_{n_1,0} \exp[i\,2\pi\, n_1\, \vec{f}_1^{[s,l_1]} \bullet \vec{x}] \tag{14.1}$$

Eq. 13.4 reduces to

$$\begin{pmatrix} m_1, & m_2 \end{pmatrix} = (m_1^{[\text{base}]}, m_2^{[\text{base}]}) + n_1 \begin{pmatrix} h_{1,1}^{[l_1]}, & h_{1,2}^{[l_1]} \end{pmatrix} \tag{14.2}$$

and Eq. 13.5 is replaced with the following definition of n_1

$$\left.\begin{array}{l} \text{If } \left|h_{1,1}^{[l_1]}\right| \geq \left|h_{1,2}^{[l_1]}\right|: \quad n_1 = \text{floor}[m_1 / h_{1,1}^{[l_1]}] \\ \text{If } \left|h_{1,1}^{[l_1]}\right| < \left|h_{1,2}^{[l_1]}\right|: \quad n_1 = \text{floor}[m_2 / h_{1,2}^{[l_1]}] \end{array}\right\} \tag{14.3}$$

($h_{1,1}^{[l_1]}$ and $h_{1,2}^{[l_1]}$ cannot both be zero; see Eq. 3.23.) Relation 13.6 is replaced by a scalar relation constraining just one of the base indices $m_1^{[\text{base}]}$ or $m_2^{[\text{base}]}$,

$$\left.\begin{array}{l} \text{If } \left|h_{1,1}^{[l_1]}\right| \geq \left|h_{1,2}^{[l_1]}\right|: \quad 0 \leq m_1^{[\text{base}]} / h_{1,1}^{[l_1]} < 1 \\ \text{If } \left|h_{1,1}^{[l_1]}\right| < \left|h_{1,2}^{[l_1]}\right|: \quad 0 \leq m_2^{[\text{base}]} / h_{1,2}^{[l_1]} < 1 \end{array}\right\} \tag{14.4}$$

Since the other base index is unconstrained, there is an infinite number of base index pairs $(m_1^{[\text{base}]}, m_2^{[\text{base}]})$ and associated decoupled index sets. But in practice the order truncation (Eq's. 4.12 and 4.13) eliminates all but a finite number of index sets.

All remaining equations containing n_2 are modified according to the restriction $n_2 = 0$. In particular, Eq's. 13.19 and 13.32 reduce to

$$\varepsilon[\vec{x}] = \varepsilon 1^{[l_1]}[x_2, x_3] = f\,\varepsilon 1_0^{[l_1]}[x_2] \tag{14.5}$$

$$\frac{1}{\varepsilon[\vec{x}]} = \frac{1}{\varepsilon 1^{[l_1]}[x_2, x_3]} = f r \varepsilon 1_0^{[l_1]}[x_2] \tag{14.6}$$

(The coordinate orientation defined by Eq's. 13.18 makes the stratum permittivity independent of x_3.) The periodicity conditions, Eq's. 13.45 and 13.46, are replaced with a single condition,

$$\varepsilon 1^{[l_1]}[x_2 + 1/f_{2,1}^{[\mathrm{s},l_1]}, x_3] = \varepsilon 1^{[l_1]}[x_2, x_3] \tag{14.7}$$

Substituting Eq. 13.18 and $n_2 = 0$ in Eq. 13.11 yields

$$\vec{f}_{n_1,0}^{[\|,j]} = \vec{f}^{[\mathrm{Inc}\|,j]} + n_1\, \hat{e}_2\, f_{2,1}^{[\mathrm{s},l_1]} = \hat{e}_2\, f_{2,n_1,0}^{[j]} + \hat{e}_3\, f_{3,n_1,0}^{[j]} \tag{14.8}$$

Hence,

$$f_{2,n_1,0}^{[j]} = f_2^{[\mathrm{Inc},j]} + n_1\, f_{2,1}^{[\mathrm{s},l_1]}, \quad f_{3,n_1,0}^{[j]} = f_3^{[\mathrm{Inc},j]} \tag{14.9}$$

Thus, with the choice of coordinate orientation defined by Eq. 13.18, all of the field's spatial frequencies share the same $\hat{e}_3$ component. If $f_3^{[\mathrm{Inc},j]} = 0$, these components are all zero and the following condition is obtained

$$f_3^{[\mathrm{Inc},j]} = 0 \quad \rightarrow \quad f_{3,n_1,0}^{[j]} = 0 \tag{14.10}$$

Based on Eq. 13.78, it also follows that if $f_3^{[\mathrm{Inc},j]} = 0$, then $s_{2,n_1,n_2}^{[j]}$ is zero, with the possible exception of the case $(f_{2,n_1,n_2}^{[j]})^2 + (f_{3,n_1,n_2}^{[j]})^2 = 0$ and $f_{3,1}^{[g]} \neq 0$. Section 15 describes a modified definition of $\hat{s}_{n_1,n_2}^{[j]}$ that avoids the exceptional condition, ensuring that $s_{2,n_1,n_2}^{[j]} = 0$ for all (n_1, n_2) (in this case with n_2 limited to $\{0\}$) when $f_3^{[\mathrm{Inc},j]} = 0$.

If $s_{2,n_1,n_2}^{[j]} = 0$ for all (n_1, n_2), then $ds_2^{[j]} = \mathbf{0}$ (Eq. 13.85) and Eq's. 13.101 and 13.102 are both block-anti-diagonal with separate TE ("Transverse Electric") and TM ("Transverse Magnetic") coupling matrices indicated below by the "TE" and "TM" superscripts,

$$\begin{gathered} ds_2^{[j]} = \mathbf{0} \quad \rightarrow \\ DEH^{[j]} = \begin{pmatrix} \mathbf{0} & DEH^{[\mathrm{TE},j]} \\ DEH^{[\mathrm{TM},j]} & \mathbf{0} \end{pmatrix}, \quad DHE^{[j]} = \begin{pmatrix} \mathbf{0} & DHE^{[\mathrm{TM},j]} \\ DHE^{[\mathrm{TE},j]} & \mathbf{0} \end{pmatrix} \end{gathered} \tag{14.11}$$

where

$$DEH^{[\mathrm{TE},j]} = -\tfrac{2\pi}{\lambda}\,\mathbf{I} \tag{14.12}$$

$$DEH^{[\mathrm{TM},j]} = 2\pi\left(\tfrac{1}{\lambda}\,\mathbf{I} - \lambda\sqrt{(df_2^{[j]})^2 + (df_3^{[j]})^2}\; rtt\varepsilon 1^{[l_1,j]}\sqrt{(df_2^{[j]})^2 + (df_3^{[j]})^2}\right) \tag{14.13}$$

$$DHE^{[\mathrm{TM},j]} = -\tfrac{2\pi}{\lambda}\, ds_3^{[j]}\, rtrt\varepsilon 1^{[l_1,j]}\, ds_3^{[j]} \tag{14.14}$$

$$DHE^{[\mathrm{TE},j]} = -2\pi\left(-\tfrac{1}{\lambda}\, ds_3^{[j]}\, trtr\varepsilon 1^{[l_1,j]}\, ds_3^{[j]} + \lambda\left((df_2^{[j]})^2 + (df_3^{[j]})^2\right)\right) \tag{14.15}$$

Eq. 13.98 separates into decoupled TE and TM equations,

$$\begin{gathered} ds_2^{[j]} = \mathbf{0} \quad \rightarrow \\ \partial_1 \begin{pmatrix} F^{[\mu,\mathrm{E},j]}[x_1] \\ F^{[\mu,\mathrm{H},j]}[x_1] \end{pmatrix} = \begin{pmatrix} \mathbf{0} & DEH^{[\mu,j]} \\ DHE^{[\mu,j]} & \mathbf{0} \end{pmatrix} \begin{pmatrix} F^{[\mu,\mathrm{E},j]}[x_1] \\ F^{[\mu,\mathrm{H},j]}[x_1] \end{pmatrix}, \quad \mu = \text{TE or TM} \end{gathered} \tag{14.16}$$

where

$$\begin{pmatrix} F^{[\mathrm{TE},\mathrm{E},j]}[x_1] \\ F^{[\mathrm{TE},\mathrm{H},j]}[x_1] \end{pmatrix} = \begin{pmatrix} ffE_{\mathrm{s}}^{[j]}[x_1] \\ i\, ffH_{\mathrm{q}}^{[j]}[x_1] \end{pmatrix}, \quad \begin{pmatrix} F^{[\mathrm{TM},\mathrm{E},j]}[x_1] \\ F^{[\mathrm{TM},\mathrm{H},j]}[x_1] \end{pmatrix} = \begin{pmatrix} ffE_{\mathrm{q}}^{[j]}[x_1] \\ i\, ffH_{\mathrm{s}}^{[j]}[x_1] \end{pmatrix} \tag{14.17}$$

Solutions to Eq’s. 14.16, in the form of Padé approximations, are obtained by the method detailed in Appendix D (cf. Eq’s. 13.98, 13.104),

$$\begin{gathered} \begin{pmatrix} P^{[\mu,\mathrm{E},\mathrm{E},j]} & -P^{[\mu,\mathrm{E},\mathrm{H},j]} \\ -P^{[\mu,\mathrm{H},\mathrm{E},j]} & P^{[\mu,\mathrm{H},\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} F^{[\mu,\mathrm{E},j]}[x_1^{[0]} + \Delta x_1] \\ F^{[\mu,\mathrm{H},j]}[x_1^{[0]} + \Delta x_1] \end{pmatrix} = \begin{pmatrix} P^{[\mu,\mathrm{E},\mathrm{E},j]} & P^{[\mu,\mathrm{E},\mathrm{H},j]} \\ P^{[\mu,\mathrm{H},\mathrm{E},j]} & P^{[\mu,\mathrm{H},\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} F^{[\mu,\mathrm{E},j]}[x_1^{[0]}] \\ F^{[\mu,\mathrm{H},j]}[x_1^{[0]}] \end{pmatrix}, \\ \mu = \text{TE or TM} \end{gathered} \tag{14.18}$$

The field separation into up/down waves, Eq’s. 13.106, is reformulated as

$$\begin{pmatrix} F^{[\mu,\mathrm{E},j]}[x_1] \\ F^{[\mu,\mathrm{H},j]}[x_1] \end{pmatrix} = \begin{pmatrix} \Gamma^{[\mu,\mathrm{E},j]} & \Gamma^{[\mu,\mathrm{E},j]} \\ \Gamma^{[\mu,\mathrm{H},j]} & -\Gamma^{[\mu,\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} F^{[\mu,+,j]}[x_1] \\ F^{[\mu,-,j]}[x_1] \end{pmatrix}, \quad \mu = \text{TE or TM} \tag{14.19}$$

where

$$\Gamma^{[\mathrm{TE},\mathrm{E},j]} = \mathbf{I}, \quad \Gamma^{[\mathrm{TM},\mathrm{E},j]} = (\lambda / \varepsilon^{[\mathrm{f}]})\, df_1^{[\mathrm{f},+,j]} \tag{14.20}$$

$$\Gamma^{[\mathrm{TE},\mathrm{H},j]} = -i\,\lambda\, df_1^{[\mathrm{f},+,j]}, \quad \Gamma^{[\mathrm{TM},\mathrm{H},j]} = i\,\mathbf{I} \tag{14.21}$$

$$F^{[\mathrm{TE},\pm,j]}[x_1] = ffE_{\mathrm{s}}^{[\pm,j]}[x_1], \quad F^{[\mathrm{TM},\pm,j]}[x_1] = ffH_{\mathrm{s}}^{[\pm,j]}[x_1] \tag{14.22}$$

The P matrices are converted to S-matrices, as outlined in Section 13 (Eq’s. 13.111, 13.119),

$$\begin{pmatrix} F^{[\mu,+,j]}[x_1^{[0]} + \Delta x_1] \\ F^{[\mu,-,j]}[x_1^{[0]}] \end{pmatrix} = \begin{pmatrix} S^{[\mu,++,j]} & S^{[\mu,+-,j]} \\ S^{[\mu,-+,j]} & S^{[\mu,--,j]} \end{pmatrix} \begin{pmatrix} F^{[\mu,+,j]}[x_1^{[0]}] \\ F^{[\mu,-,j]}[x_1^{[0]} + \Delta x_1] \end{pmatrix}, \quad \mu = \text{TE or TM} \tag{14.23}$$

$$\begin{pmatrix} S^{[\mu,+-,j]} \\ S^{[\mu,--,j]}-\mathbf{I} \end{pmatrix} = \begin{pmatrix} \mathbf{I} & \mathbf{I} \\ -\mathbf{I} & \mathbf{I} \end{pmatrix} \begin{pmatrix} (-P^{[\mu,\mathrm{E},\mathrm{E},j]}\,\Gamma^{[\mu,\mathrm{E},j]} + P^{[\mu,\mathrm{E},\mathrm{H},j]}\,\Gamma^{[\mu,\mathrm{H},j]})^{-1}\, P^{[\mu,\mathrm{E},\mathrm{H},j]}\,\Gamma^{[\mu,\mathrm{H},j]} \\ (-P^{[\mu,\mathrm{H},\mathrm{E},j]}\,\Gamma^{[\mu,\mathrm{E},j]} + P^{[\mu,\mathrm{H},\mathrm{H},j]}\,\Gamma^{[\mu,\mathrm{H},j]})^{-1}\, P^{[\mu,\mathrm{H},\mathrm{E},j]}\,\Gamma^{[\mu,\mathrm{E},j]} \end{pmatrix}, \quad \mu = \mathrm{TE}\ \text{or}\ \mathrm{TM} \tag{14.24}$$

Δx_1 is defined by Eq. 13.103 with the scaling factor of 2^{-sp} applied, and sp stacking operations are subsequently applied (as in Eq. 13.120 or 13.121) to remove the scaling factor.

15. Change of $\hat{s}$ basis to maintain polarization decoupling

As noted in Section 14, if $f_3^{[\mathrm{Inc},j]}=0$ then $s_{2,n_1,n_2}^{[j]}=0$ is zero for all (n_1,n_2), with the possible exception of the case $(f_{2,n_1,n_2}^{[j]})^2+(f_{3,n_1,n_2}^{[j]})^2=0$ (see Eq's. 13.78 and 14.10; in this case n_2 is limited to $\{0\}$). However, the second branch condition in Eq. 13.78 ("if … = 0") can be modified to avoid the exceptional condition, ensuring polarization decoupling for all diffraction orders in the j-th index set when $f_3^{[\mathrm{Inc},j]}=0$. The second branch condition is modified to make $\hat{s}_{n_1,n_2}^{[j]}$ orthogonal to the stratum's basis frequency vector $\vec{f}_1^{[\mathrm{s},l_1]}$ (in Eq's. 3.30 and 14.1), rather than the grating's basis frequency $\vec{f}_1^{[\mathrm{g}]}$. $\vec{f}_1^{[\mathrm{s},l_1]}$ is parallel to $\hat{e}_2$ (Eq. 13.18), so $\hat{s}_{n_1,n_2}^{[j]}$ is parallel to $\hat{e}_3$ in the second branch,

$$\left(s_{2,n_1,n_2}^{[j]},\quad s_{3,n_1,n_2}^{[j]}\right) = \begin{cases} \dfrac{\left(-f_{3,n_1,n_2}^{[j]},\quad f_{2,n_1,n_2}^{[j]}\right)}{\sqrt{(f_{2,n_1,n_2}^{[j]})^2+(f_{3,n_1,n_2}^{[j]})^2}} & \text{if } (f_{2,n_1,n_2}^{[j]})^2+(f_{3,n_1,n_2}^{[j]})^2 \neq 0 \\ (0,\quad 1) & \text{if } (f_{2,n_1,n_2}^{[j]})^2+(f_{3,n_1,n_2}^{[j]})^2 = 0 \end{cases} \tag{15.1}$$

None of the results of Sections 13 and 14 are affected by the adoption of Eq. 15.1 in lieu of Eq. 13.78; however, the S matrices for all strata must be modified to revert to the common definition, Eq. 13.78, before stacking them to form the grating's cumulative S matrix. The $\hat{s}$ basis redefinition is itself represented formally by an S matrix by the procedure outlined below.

No more than one of the tangential frequencies $\vec{f}_{m_1,m_2}^{[||]}$ (Eq. 5.8) can be zero because the grating basis frequencies $\vec{f}_1^{[\mathrm{g}]}$ and $\vec{f}_2^{[\mathrm{g}]}$ are linearly independent (cf. Eq's. 3.27-3.29). $\vec{f}_{m_1,m_2}^{[||]}$ is assumed to be zero for particular order indices $(m_1,m_2)=(m_1^{[\perp]},m_2^{[\perp]})$,

$$(f_{2,m_1,m_2})^2+(f_{3,m_1,m_2})^2=0 \quad \text{for } (m_1,m_2)=(m_1^{[\perp]},m_2^{[\perp]}) \tag{15.2}$$

The connotation of the "$\perp$" superscript is that the order's propagation direction is perpendicular to the substrate. In practice the zero-equality test "$\ldots=0$" in Eq's. 15.1 and 15.2 can be replaced by "smaller than or comparable to $(\delta/\lambda)^2$", where δ is the numeric precision ($\delta=2^{-52}$ for double-precision).

The electromagnetic field representation for diffraction order $(m_1,m_2)=(m_1^{[\perp]},m_2^{[\perp]})$ is based on $\hat{s}_{m_1,m_2}$ and $\hat{q}^{[\pm]}_{m_1,m_2}$ projections at a particular level $x_1=x_1^{[0]}$ in the grating, and projection vectors denoted as $\hat{s}'_{m_1,m_2}$ and $\hat{q}'^{[\pm]}_{m_1,m_2}$ projections at level $x_1=x_1^{[1]}$ infinitesimally above $x_1^{[0]}$. (These definitions of $x_1^{[0]}$ and $x_1^{[1]}$ adapt the basis change to the S matrix framework, as described in Section 7.) One of the two basis vectors $\hat{s}$ or $\hat{s}'$ is defined by the second branch condition ("if … = 0") in Eq. 6.41 (with $(m_1,m_2)=(m_1^{[\perp]},m_2^{[\perp]})$); and the other is similarly defined, but with $\vec{f}_1^{[\mathrm{s},l_1]}$ substituted for $\vec{f}_1^{[\mathrm{g}]}$ (as in Eq. 15.1). $\hat{q}^{[\pm]}$ and $\hat{q}'^{[\pm]}$ are defined according to Eq. 6.43.

The electromagnetic field is furthermore represented in terms of up and down waves in a fictitious medium of permittivity $\varepsilon^{[\mathrm{f}]}$. Based on Eq's. 6.52-6.55 (with $\varepsilon^{[\mathrm{c}]}=\varepsilon^{[\mathrm{f}]}$), the $\hat{s}$ basis change is described by the following relations,

$$
\begin{aligned}
&\text{With } (m_1,m_2)=(m_1^{[\perp]},m_2^{[\perp]}),\\
&\hat{s}_{m_1,m_2}\,(\mathit{ffE}^{[+]}_{\mathrm{s},m_1,m_2}[x_1^{[0]}]+\mathit{ffE}^{[-]}_{\mathrm{s},m_1,m_2}[x_1^{[0]}])+\hat{q}^{[+]}_{m_1,m_2}\,\frac{\lambda}{\varepsilon^{[\mathrm{f}]}}\,f^{[\mathrm{f},+]}_{1,m_1,m_2}\,(\mathit{ffH}^{[+]}_{\mathrm{s},m_1,m_2}[x_1^{[0]}]+\mathit{ffH}^{[-]}_{\mathrm{s},m_1,m_2}[x_1^{[0]}])=\\
&\quad\hat{s}'_{m_1,m_2}\,(\mathit{ffE}^{[+]}_{\mathrm{s},m_1,m_2}[x_1^{[1]}]+\mathit{ffE}^{[-]}_{\mathrm{s},m_1,m_2}[x_1^{[1]}])+\hat{q}'^{[+]}_{m_1,m_2}\,\frac{\lambda}{\varepsilon^{[\mathrm{f}]}}\,f^{[\mathrm{f},+]}_{1,m_1,m_2}\,(\mathit{ffH}^{[+]}_{\mathrm{s},m_1,m_2}[x_1^{[1]}]+\mathit{ffH}^{[-]}_{\mathrm{s},m_1,m_2}[x_1^{[1]}]),\\
&\hat{s}_{m_1,m_2}\,(\mathit{ffH}^{[+]}_{\mathrm{s},m_1,m_2}[x_1^{[0]}]-\mathit{ffH}^{[-]}_{\mathrm{s},m_1,m_2}[x_1^{[0]}])-\hat{q}^{[+]}_{m_1,m_2}\,\lambda\,f^{[\mathrm{f},+]}_{1,m_1,m_2}\,(\mathit{ffE}^{[+]}_{\mathrm{s},m_1,m_2}[x_1^{[0]}]-\mathit{ffE}^{[-]}_{\mathrm{s},m_1,m_2}[x_1^{[0]}])=\\
&\quad\hat{s}'_{m_1,m_2}\,(\mathit{ffH}^{[+]}_{\mathrm{s},m_1,m_2}[x_1^{[1]}]-\mathit{ffH}^{[-]}_{\mathrm{s},m_1,m_2}[x_1^{[1]}])-\hat{q}'^{[+]}_{m_1,m_2}\,\lambda\,f^{[\mathrm{f},+]}_{1,m_1,m_2}\,(\mathit{ffE}^{[+]}_{\mathrm{s},m_1,m_2}[x_1^{[1]}]-\mathit{ffE}^{[-]}_{\mathrm{s},m_1,m_2}[x_1^{[1]}])
\end{aligned}
\tag{15.3}
$$

(These equations assert continuity of the grating-tangential projections of $\mathit{ff}\vec{E}_{m_1,m_2}[x_1]$ and $\mathit{ff}\vec{H}_{m_1,m_2}[x_1]$ between $x_1^{[0]}$ and $x_1^{[1]}$.) The $f^{[\mathrm{f},+]}_{1,m_1,m_2}$ term is defined by Eq's. 6.37 and 15.2,

$$
f^{[\mathrm{f},+]}_{1,m_1,m_2}=\frac{\sqrt{\varepsilon^{[\mathrm{f}]}}}{\lambda}
\tag{15.4}
$$

The $\hat{s}$ and $\hat{q}^{[+]}$ basis vectors, and similarly $\hat{s}'$ and $\hat{q}'^{[+]}$, are orthonormal (from Eq's. 6.40, 6.41, and 6.43),

$$
\begin{aligned}
&\hat{s}_{m_1,m_2}=\hat{e}_2\,s_{2,m_1,m_2}+\hat{e}_3\,s_{3,m_1,m_2},\quad \hat{q}^{[+]}_{m_1,m_2}=\hat{e}_2\,s_{3,m_1,m_2}-\hat{e}_3\,s_{2,m_1,m_2},\quad (s_{2,m_1,m_2})^2+(s_{3,m_1,m_2})^2=1,\\
&\hat{s}'_{m_1,m_2}=\hat{e}_2\,s'_{2,m_1,m_2}+\hat{e}_3\,s'_{3,m_1,m_2},\quad \hat{q}'^{[+]}_{m_1,m_2}=\hat{e}_2\,s'_{3,m_1,m_2}-\hat{e}_3\,s'_{2,m_1,m_2},\quad (s'_{2,m_1,m_2})^2+(s'_{3,m_1,m_2})^2=1
\end{aligned}
\tag{15.5}
$$

Making these substitutions, Eq's. 15.3 are restated as

$$
\begin{gathered}
\text{With } (m_1,m_2)=(m_1^{[\perp]},m_2^{[\perp]}), \\
\begin{pmatrix}
-s'_{2,m_1,m_2} & -s'_{3,m_1,m_2} & s_{2,m_1,m_2} & s_{3,m_1,m_2} \\
-s'_{2,m_1,m_2} & -s'_{3,m_1,m_2} & -s_{2,m_1,m_2} & -s_{3,m_1,m_2} \\
-s'_{3,m_1,m_2} & s'_{2,m_1,m_2} & s_{3,m_1,m_2} & -s_{2,m_1,m_2} \\
s'_{3,m_1,m_2} & -s'_{2,m_1,m_2} & s_{3,m_1,m_2} & -s_{2,m_1,m_2}
\end{pmatrix}
\begin{pmatrix}
ffE_{\mathrm{s},m_1,m_2}^{[+]}[x_1^{[1]}] \\
ffH_{\mathrm{s},m_1,m_2}^{[+]}[x_1^{[1]}]/\sqrt{\varepsilon^{[\mathrm{f}]}} \\
ffE_{\mathrm{s},m_1,m_2}^{[-]}[x_1^{[0]}] \\
ffH_{\mathrm{s},m_1,m_2}^{[-]}[x_1^{[0]}]/\sqrt{\varepsilon^{[\mathrm{f}]}}
\end{pmatrix}
= \\
\begin{pmatrix}
-s_{2,m_1,m_2} & -s_{3,m_1,m_2} & s'_{2,m_1,m_2} & s'_{3,m_1,m_2} \\
-s_{2,m_1,m_2} & -s_{3,m_1,m_2} & -s'_{2,m_1,m_2} & -s'_{3,m_1,m_2} \\
-s_{3,m_1,m_2} & s_{2,m_1,m_2} & s'_{3,m_1,m_2} & -s'_{2,m_1,m_2} \\
s_{3,m_1,m_2} & -s_{2,m_1,m_2} & s'_{3,m_1,m_2} & -s'_{2,m_1,m_2}
\end{pmatrix}
\begin{pmatrix}
ffE_{\mathrm{s},m_1,m_2}^{[+]}[x_1^{[0]}] \\
ffH_{\mathrm{s},m_1,m_2}^{[+]}[x_1^{[0]}]/\sqrt{\varepsilon^{[\mathrm{f}]}} \\
ffE_{\mathrm{s},m_1,m_2}^{[-]}[x_1^{[1]}] \\
ffH_{\mathrm{s},m_1,m_2}^{[-]}[x_1^{[1]}]/\sqrt{\varepsilon^{[\mathrm{f}]}}
\end{pmatrix}
\end{gathered}
\tag{15.6}
$$

This simplifies to

$$
\begin{gathered}
\begin{pmatrix}
s_{3,m_1,m_2} & -s_{2,m_1,m_2} \\
s_{2,m_1,m_2} & s_{3,m_1,m_2}
\end{pmatrix}
\begin{pmatrix}
ffE_{\mathrm{s},m_1,m_2}^{[\pm]}[x_1^{[0]}] \\
ffH_{\mathrm{s},m_1,m_2}^{[\pm]}[x_1^{[0]}]/\sqrt{\varepsilon^{[\mathrm{f}]}}
\end{pmatrix}
= \\
\begin{pmatrix}
s'_{3,m_1,m_2} & -s'_{2,m_1,m_2} \\
s'_{2,m_1,m_2} & s'_{3,m_1,m_2}
\end{pmatrix}
\begin{pmatrix}
ffE_{\mathrm{s},m_1,m_2}^{[\pm]}[x_1^{[1]}] \\
ffH_{\mathrm{s},m_1,m_2}^{[\pm]}[x_1^{[1]}]/\sqrt{\varepsilon^{[\mathrm{f}]}}
\end{pmatrix}
\end{gathered}
\tag{15.7}
$$

Eq. 15.7 is solved for the outgoing fields,

$$
\begin{gathered}
\text{With } (m_1,m_2)=(m_1^{[\perp]},m_2^{[\perp]}), \\
\begin{pmatrix}
ffE_{\mathrm{s},m_1,m_2}^{[+]}[x_1^{[1]}] \\
ffH_{\mathrm{s},m_1,m_2}^{[+]}[x_1^{[1]}]/\sqrt{\varepsilon^{[\mathrm{f}]}} \\
ffE_{\mathrm{s},m_1,m_2}^{[-]}[x_1^{[0]}] \\
ffH_{\mathrm{s},m_1,m_2}^{[-]}[x_1^{[0]}]/\sqrt{\varepsilon^{[\mathrm{f}]}}
\end{pmatrix}
= \\
\begin{pmatrix}
\hat{s}_{m_1,m_2}\bullet\hat{s}'_{m_1,m_2} & -\hat{s}_{m_1,m_2}\bullet\hat{q}'^{[+]}_{m_1,m_2} & 0 & 0 \\
\hat{s}_{m_1,m_2}\bullet\hat{q}'^{[+]}_{m_1,m_2} & \hat{s}_{m_1,m_2}\bullet\hat{s}'_{m_1,m_2} & 0 & 0 \\
0 & 0 & \hat{s}_{m_1,m_2}\bullet\hat{s}'_{m_1,m_2} & \hat{s}_{m_1,m_2}\bullet\hat{q}'^{[+]}_{m_1,m_2} \\
0 & 0 & -\hat{s}_{m_1,m_2}\bullet\hat{q}'^{[+]}_{m_1,m_2} & \hat{s}_{m_1,m_2}\bullet\hat{s}'_{m_1,m_2}
\end{pmatrix}
\begin{pmatrix}
ffE_{\mathrm{s},m_1,m_2}^{[+]}[x_1^{[0]}] \\
ffH_{\mathrm{s},m_1,m_2}^{[+]}[x_1^{[0]}]/\sqrt{\varepsilon^{[\mathrm{f}]}} \\
ffE_{\mathrm{s},m_1,m_2}^{[-]}[x_1^{[1]}] \\
ffH_{\mathrm{s},m_1,m_2}^{[-]}[x_1^{[1]}]/\sqrt{\varepsilon^{[\mathrm{f}]}}
\end{pmatrix}
\end{gathered}
\tag{15.8}
$$

With $F_{(m_1,m_2,P)}^{[\pm]}[x_1]$ defined by Eq. 9.2, the nonzero S-matrix elements in Eq. 9.3 are defined by

With $(m_1, m_2) = (m_1^{[\perp]}, m_2^{[\perp]})$,

$$\begin{pmatrix} S^{[++]}_{(m_1,m_2,\mathrm{E}),(m_1,m_2,\mathrm{E})} & S^{[++]}_{(m_1,m_2,\mathrm{E}),(m_1,m_2,\mathrm{H})} \\ S^{[++]}_{(m_1,m_2,\mathrm{H}),(m_1,m_2,\mathrm{E})} & S^{[++]}_{(m_1,m_2,\mathrm{H}),(m_1,m_2,\mathrm{H})} \end{pmatrix} = \begin{pmatrix} \hat{s}_{m_1,m_2} \bullet \hat{s}'_{m_1,m_2} & -\hat{s}_{m_1,m_2} \bullet \hat{q}'^{[+]}_{m_1,m_2} / \sqrt{\varepsilon^{[\mathrm{f}]}} \\ \hat{s}_{m_1,m_2} \bullet \hat{q}'^{[+]}_{m_1,m_2} \sqrt{\varepsilon^{[\mathrm{f}]}} & \hat{s}_{m_1,m_2} \bullet \hat{s}'_{m_1,m_2} \end{pmatrix} \tag{15.9}$$

$$\begin{pmatrix} S^{[--]}_{(m_1,m_2,\mathrm{E}),(m_1,m_2,\mathrm{E})} & S^{[--]}_{(m_1,m_2,\mathrm{E}),(m_1,m_2,\mathrm{H})} \\ S^{[--]}_{(m_1,m_2,\mathrm{H}),(m_1,m_2,\mathrm{E})} & S^{[--]}_{(m_1,m_2,\mathrm{H}),(m_1,m_2,\mathrm{H})} \end{pmatrix} = \begin{pmatrix} \hat{s}_{m_1,m_2} \bullet \hat{s}'_{m_1,m_2} & \hat{s}_{m_1,m_2} \bullet \hat{q}'^{[+]}_{m_1,m_2} / \sqrt{\varepsilon^{[\mathrm{f}]}} \\ -\hat{s}_{m_1,m_2} \bullet \hat{q}'^{[+]}_{m_1,m_2} \sqrt{\varepsilon^{[\mathrm{f}]}} & \hat{s}_{m_1,m_2} \bullet \hat{s}'_{m_1,m_2} \end{pmatrix}$$

With $(m_1, m_2) \neq (m_1^{[\perp]}, m_2^{[\perp]})$,

$$\begin{pmatrix} S^{[++]}_{(m_1,m_2,\mathrm{E}),(m_1,m_2,\mathrm{E})} & S^{[++]}_{(m_1,m_2,\mathrm{E}),(m_1,m_2,\mathrm{H})} \\ S^{[++]}_{(m_1,m_2,\mathrm{H}),(m_1,m_2,\mathrm{E})} & S^{[++]}_{(m_1,m_2,\mathrm{H}),(m_1,m_2,\mathrm{H})} \end{pmatrix} = \begin{pmatrix} S^{[--]}_{(m_1,m_2,\mathrm{E}),(m_1,m_2,\mathrm{E})} & S^{[--]}_{(m_1,m_2,\mathrm{E}),(m_1,m_2,\mathrm{H})} \\ S^{[--]}_{(m_1,m_2,\mathrm{H}),(m_1,m_2,\mathrm{E})} & S^{[--]}_{(m_1,m_2,\mathrm{H}),(m_1,m_2,\mathrm{H})} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{15.10}$$

The inverse S matrix transformation (converting from the $\hat{s}'$ basis back to $\hat{s}$) has the same form as Eq's. 15.9 and 15.10, but with the primed and unprimed basis vectors interchanged, or equivalently, with $S^{[++]}$ and $S^{[--]}$ swapped (because $\hat{s}'_{m_1,m_2} \bullet \hat{q}^{[+]}_{m_1,m_2} = -\hat{s}_{m_1,m_2} \bullet \hat{q}'^{[+]}_{m_1,m_2}$). In implementing the grating stacking operations with TE and TM polarizations decoupled, the S matrix defined above must be applied to convert from the $\hat{s}$ basis defined by Eq. 13.78 (or 6.41) to that of Eq. 15.1; then the uniperiodic stratum's S matrix (polarization-decoupled form, Eq. 14.23) is applied; and then the inverse of the above S matrix is applied to revert back to the $\hat{s}$ basis of Eq. 13.78. (The basis change is only required if Eq. 15.2 holds.)

For a uniperiodic stratum, if $f_3^{[\mathrm{Inc},j]} = 0$ then $f_{3,n_1,0}^{[j]} = 0$ (Eq. 14.10) and Eq. 15.1 reduces to

$$f_3^{[\mathrm{Inc},j]} = 0 \quad \to \quad \left(s_{2,n_1,n_2}^{[j]}, \quad s_{3,n_1,n_2}^{[j]} \right) = \begin{cases} \left(0, \quad \mathrm{sign}[f_{2,n_1,n_2}^{[j]}]\right) & \text{if } f_{2,n_1,n_2}^{[j]} \neq 0 \\ \left(0, \quad 1\right) & \text{if } f_{2,n_1,n_2}^{[j]} = 0 \end{cases} \tag{15.11}$$

In this case $ds_2^{[j]} = \mathbf{0}$ in Eq. 13.102, and Eq's. 13.98-13.102 simplify to Eq's. 14.12-14.16.

16. The S matrix for a homogeneous stratum (with surfaces)

A homogeneous stratum is a special case of a periodic stratum in which the ranges of n_1 and n_2 in Eq. 13.1 are both limited to $\{0\}$. Denoting the stratum permittivity as $\varepsilon^{[\mathrm{c}]}$, Eq. 13.1 reduces to

$$\varepsilon[\vec{x}] = \varepsilon 1^{[l_1]}[x_2, x_3] = ff\, \varepsilon 1_{0,0}^{[l_1]} = \varepsilon^{[\mathrm{c}]} \tag{16.1}$$

In this case there is no diffractive coupling between the field's Fourier orders, so each decoupled index set is associated with a single Fourier order. Furthermore, there is no polarization coupling, so the S-matrix quadrants $S^{[\pm\pm',j]}$ are diagonal.

The matrices $rtt\varepsilon 1^{[l_1,j]}$, $rtrt\varepsilon 1^{[l_1,j]}$, and $trtr\varepsilon 1^{[l_1,j]}$ that appear in Eq's. 13.101 and 13.102 (and which are defined in Eq's. 13.60, 13.70, and 13.71) simplify to scalars,

$$rtt\varepsilon 1^{[l_1,j]} = 1/\varepsilon^{[\mathrm{c}]} \tag{16.2}$$

$$rtrt\varepsilon 1^{[l_1,j]} = \varepsilon^{[\mathrm{c}]} \tag{16.3}$$

$$trtr\varepsilon 1^{[l_1,j]} = \varepsilon^{[\mathrm{c}]} \tag{16.4}$$

The matrices $DEH^{[j]}$ and $DHE^{[j]}$ (Eq's. 13.101 and 13.102) are 2-by-2 anti-diagonal matrices having the same form as Eq. 14.11, with

$$DEH^{[\mathrm{TE},j]} = -\frac{2\pi}{\lambda} \tag{16.5}$$

$$DEH^{[\mathrm{TM},j]} = 2\pi\left(\frac{1}{\lambda} - \frac{\lambda}{\varepsilon^{[\mathrm{c}]}}\left((df_2^{[j]})^2 + (df_3^{[j]})^2\right)\right) = \frac{2\pi\,\lambda}{\varepsilon^{[\mathrm{c}]}}(f_1^{[\mathrm{c},+,j]})^2 \tag{16.6}$$

$$DHE^{[\mathrm{TM},j]} = \frac{-2\pi\,\varepsilon^{[\mathrm{c}]}}{\lambda} \tag{16.7}$$

$$DHE^{[\mathrm{TE},j]} = 2\pi\left(\frac{\varepsilon^{[\mathrm{c}]}}{\lambda} - \lambda\left((df_2^{[j]})^2 + (df_3^{[j]})^2\right)\right) = 2\pi\,\lambda\,(f_1^{[\mathrm{c},+,j]})^2 \tag{16.8}$$

$f_1^{[\mathrm{c},+,j]}$ is defined as

$$f_1^{[\mathrm{c},+,j]} = \sqrt{\frac{\varepsilon^{[\mathrm{c}]}}{\lambda^2} - (f_2^{[j]})^2 - (f_3^{[j]})^2} \tag{16.9}$$

(cf. Eq. 6.37).

Eq. 13.98 separates into decoupled TE and TM fields as in Eq. 14.16,

$$\partial_1 \begin{pmatrix} F^{[\mu,\mathrm{E},j]}[x_1] \\ F^{[\mu,\mathrm{H},j]}[x_1] \end{pmatrix} = \begin{pmatrix} \mathbf{0} & DEH^{[\mu,j]} \\ DHE^{[\mu,j]} & \mathbf{0} \end{pmatrix} \begin{pmatrix} F^{[\mu,\mathrm{E},j]}[x_1] \\ F^{[\mu,\mathrm{H},j]}[x_1] \end{pmatrix}, \quad \mu = \text{TE or TM} \tag{16.10}$$

where

$$\begin{pmatrix} F^{[\mathrm{TE,E},j]}[x_1] \\ F^{[\mathrm{TE,H},j]}[x_1] \end{pmatrix} = \begin{pmatrix} ffE_{\mathrm{s}}^{[j]}[x_1] \\ i\, ffH_{\mathrm{q}}^{[j]}[x_1] \end{pmatrix}, \quad \begin{pmatrix} F^{[\mathrm{TM,E},j]}[x_1] \\ F^{[\mathrm{TM,H},j]}[x_1] \end{pmatrix} = \begin{pmatrix} ffE_{\mathrm{q}}^{[j]}[x_1] \\ i\, ffH_{\mathrm{s}}^{[j]}[x_1] \end{pmatrix} \tag{16.11}$$

Solutions to Eq's. 16.10 are of the form

$$\begin{pmatrix} F^{[\mu,\mathrm{E},j]}[x_1^{[0]}+\Delta x_1] \\ F^{[\mu,\mathrm{H},j]}[x_1^{[0]}+\Delta x_1] \end{pmatrix} = \begin{pmatrix} \Phi^{[\mu,\mathrm{E},\mathrm{E},j]} & \Phi^{[\mu,\mathrm{E},\mathrm{H},j]} \\ \Phi^{[\mu,\mathrm{H},\mathrm{E},j]} & \Phi^{[\mu,\mathrm{H},\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} F^{[\mu,\mathrm{E},\mathrm{H},j]}[x_1^{[0]}] \\ F^{[\mu,\mathrm{H},j]}[x_1^{[0]}] \end{pmatrix} \tag{16.12}$$

where

$$\begin{pmatrix} \Phi^{[\mu,\mathrm{E},\mathrm{E},j]} & \Phi^{[\mu,\mathrm{E},\mathrm{H},j]} \\ \Phi^{[\mu,\mathrm{H},\mathrm{E},j]} & \Phi^{[\mu,\mathrm{H},\mathrm{H},j]} \end{pmatrix} = \exp\left[\begin{pmatrix} \mathbf{0} & DEH^{[\mu,j]} \\ DHE^{[\mu,j]} & \mathbf{0} \end{pmatrix} \Delta x_1 \right] \tag{16.13}$$

$$\begin{gathered} \begin{pmatrix} \Phi^{[\mathrm{TE},\mathrm{E},\mathrm{E},j]} & \Phi^{[\mathrm{TE},\mathrm{E},\mathrm{H},j]} \\ \Phi^{[\mathrm{TE},\mathrm{H},\mathrm{E},j]} & \Phi^{[\mathrm{TE},\mathrm{H},\mathrm{H},j]} \end{pmatrix} = \\ \begin{pmatrix} \cos[2\pi\, f_1^{[\mathrm{c},+,j]}\,\Delta x_1] & \dfrac{-1}{\lambda\, f_1^{[\mathrm{c},+,j]}} \sin[2\pi\, f_1^{[\mathrm{c},+,j]}\,\Delta x_1] \\ \lambda\, f_1^{[\mathrm{c},+,j]} \sin[2\pi\, f_1^{[\mathrm{c},+,j]}\,\Delta x_1] & \cos[2\pi\, f_1^{[\mathrm{c},+,j]}\,\Delta x_1] \end{pmatrix} \end{gathered} \tag{16.14}$$

$$\begin{gathered} \begin{pmatrix} \Phi^{[\mathrm{TM},\mathrm{E},\mathrm{E},j]} & \Phi^{[\mathrm{TM},\mathrm{E},\mathrm{H},j]} \\ \Phi^{[\mathrm{TM},\mathrm{H},\mathrm{E},j]} & \Phi^{[\mathrm{TM},\mathrm{H},\mathrm{H},j]} \end{pmatrix} = \\ \begin{pmatrix} \cos[2\pi\, f_1^{[\mathrm{c},+,j]}\,\Delta x_1] & \dfrac{\lambda\, f_1^{[\mathrm{c},+,j]}}{\varepsilon^{[\mathrm{c}]}} \sin[2\pi\, f_1^{[\mathrm{c},+,j]}\,\Delta x_1] \\ \dfrac{-\varepsilon^{[\mathrm{c}]}}{\lambda\, f_1^{[\mathrm{c},+,j]}} \sin[2\pi\, f_1^{[\mathrm{c},+,j]}\,\Delta x_1] & \cos[2\pi\, f_1^{[\mathrm{c},+,j]}\,\Delta x_1] \end{pmatrix} \end{gathered} \tag{16.15}$$

Eq. 16.12 has a form similar to Eq. 14.18, but with the Padé approximation replaced by an exact exponential matrix. The reciprocal of Eq. 16.13 is obtained by applying a similarity transformation,

$$\begin{aligned} \begin{pmatrix} \Phi^{[\mu,\mathrm{E},\mathrm{E},j]} & \Phi^{[\mu,\mathrm{E},\mathrm{H},j]} \\ \Phi^{[\mu,\mathrm{H},\mathrm{E},j]} & \Phi^{[\mu,\mathrm{H},\mathrm{H},j]} \end{pmatrix}^{-1} &= \exp\left[\begin{pmatrix} \mathbf{0} & -DEH^{[\mu,j]} \\ -DHE^{[\mu,j]} & \mathbf{0} \end{pmatrix} \Delta x_1 \right] \\ &= \exp\left[\begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -\mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{0} & DEH^{[\mu,j]} \\ DHE^{[\mu,j]} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -\mathbf{I} \end{pmatrix} \Delta x_1 \right] \\ &= \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -\mathbf{I} \end{pmatrix} \exp\left[\begin{pmatrix} \mathbf{0} & DEH^{[\mu,j]} \\ DHE^{[\mu,j]} & \mathbf{0} \end{pmatrix} \Delta x_1 \right] \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -\mathbf{I} \end{pmatrix} \\ &= \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -\mathbf{I} \end{pmatrix} \begin{pmatrix} \Phi^{[\mu,\mathrm{E},\mathrm{E},j]} & \Phi^{[\mu,\mathrm{E},\mathrm{H},j]} \\ \Phi^{[\mu,\mathrm{H},\mathrm{E},j]} & \Phi^{[\mu,\mathrm{H},\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -\mathbf{I} \end{pmatrix} = \begin{pmatrix} \Phi^{[\mu,\mathrm{E},\mathrm{E},j]} & -\Phi^{[\mu,\mathrm{E},\mathrm{H},j]} \\ -\Phi^{[\mu,\mathrm{H},\mathrm{E},j]} & \Phi^{[\mu,\mathrm{H},\mathrm{H},j]} \end{pmatrix} \end{aligned} \tag{16.16}$$

The field is separated into up/down waves in the bounding fictitious medium as in Eq. 14.19,

$$\begin{pmatrix} F^{[\mu,\mathrm{E},j]}[x_1] \\ F^{[\mu,\mathrm{H},j]}[x_1] \end{pmatrix} = \begin{pmatrix} \Gamma^{[\mu,\mathrm{E},j]} & \Gamma^{[\mu,\mathrm{E},j]} \\ \Gamma^{[\mu,\mathrm{H},j]} & -\Gamma^{[\mu,\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} F^{[\mu,+,j]}[x_1] \\ F^{[\mu,-,j]}[x_1] \end{pmatrix} \tag{16.17}$$

where

$$\Gamma^{[\mathrm{TE},\mathrm{E},j]} = 1, \quad \Gamma^{[\mathrm{TE},\mathrm{H},j]} = -i\,\lambda\, f_1^{[\mathrm{f},+,j]} \tag{16.18}$$

$$\Gamma^{[\mathrm{TM},\mathrm{E},j]} = (\lambda / \varepsilon^{[\mathrm{f}]})\, f_1^{[\mathrm{f},+,j]}, \quad \Gamma^{[\mathrm{TM},\mathrm{H},j]} = i \tag{16.19}$$

$$F^{[\mathrm{TE},\pm,j]}[x_1] = f\!f E_{\mathrm{s}}^{[\pm,j]}[x_1], \quad F^{[\mathrm{TM},\pm,j]}[x_1] = f\!f H_{\mathrm{s}}^{[\pm,j]}[x_1] \tag{16.20}$$

$f_1^{[\mathrm{f},+,j]}$ is defined by Eq. 13.76,

$$f_1^{[\mathrm{f},+,j]} = \pm\sqrt{\frac{\varepsilon^{[\mathrm{f}]}}{\lambda^2} - (f_2^{[j]})^2 - (f_3^{[j]})^2} \tag{16.21}$$

16.17 is substituted into Eq. 16.12,

$$\begin{pmatrix} F^{[\mu,+,j]}[x_1^{[0]} + \Delta x_1] \\ F^{[\mu,-,j]}[x_1^{[0]} + \Delta x_1] \end{pmatrix} = \begin{pmatrix} \Phi^{[\mu,++,j]} & \Phi^{[\mu,+-,j]} \\ \Phi^{[\mu,-+,j]} & \Phi^{[\mu,--,j]} \end{pmatrix} \begin{pmatrix} F^{[\mu,+,j]}[x_1^{[0]}] \\ F^{[\mu,-,j]}[x_1^{[0]}] \end{pmatrix} \tag{16.22}$$

where

$$\begin{gathered} \begin{pmatrix} \Phi^{[\mu,++,j]} & \Phi^{[\mu,+-,j]} \\ \Phi^{[\mu,-+,j]} & \Phi^{[\mu,--,j]} \end{pmatrix} = \\ \tfrac{1}{2} \begin{pmatrix} \left(\Gamma^{[\mu,\mathrm{E},j]}\right)^{-1} & \left(\Gamma^{[\mu,\mathrm{H},j]}\right)^{-1} \\ \left(\Gamma^{[\mu,\mathrm{E},j]}\right)^{-1} & -\left(\Gamma^{[\mu,\mathrm{H},j]}\right)^{-1} \end{pmatrix} \begin{pmatrix} \Phi^{[\mu,\mathrm{E},\mathrm{E},j]} & \Phi^{[\mu,\mathrm{E},\mathrm{H},j]} \\ \Phi^{[\mu,\mathrm{H},\mathrm{E},j]} & \Phi^{[\mu,\mathrm{H},\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} \Gamma^{[\mu,\mathrm{E},j]} & \Gamma^{[\mu,\mathrm{E},j]} \\ \Gamma^{[\mu,\mathrm{H},j]} & -\Gamma^{[\mu,\mathrm{H},j]} \end{pmatrix} \end{gathered} \tag{16.23}$$

Eq's. 16.14, 16.15, 16.18, and 16.19 are substituted in Eq. 16.23,

$$\Phi^{[\mathrm{TE},\pm\pm',j]} = \frac{1}{2} \left(\begin{gathered} \left(\cos[2\pi\, f_1^{[\mathrm{c},+,j]}\,\Delta x_1] \pm' i\,\frac{f_1^{[\mathrm{f},+,j]}}{f_1^{[\mathrm{c},+,j]}} \sin[2\pi\, f_1^{[\mathrm{c},+,j]}\,\Delta x_1] \right) \\ \pm \left(i\,\frac{f_1^{[\mathrm{c},+,j]}}{f_1^{[\mathrm{f},+,j]}} \sin[2\pi\, f_1^{[\mathrm{c},+,j]}\,\Delta x_1] \pm' \cos[2\pi\, f_1^{[\mathrm{c},+,j]}\,\Delta x_1] \right) \end{gathered} \right) \tag{16.24}$$

$$\Phi^{[\mathrm{TM},\pm\pm',j]} = \frac{1}{2}\begin{pmatrix} \left(\cos[2\pi\, f_1^{[\mathrm{c},+,j]}\,\Delta x_1] \pm' i\,\dfrac{\varepsilon^{[\mathrm{f}]}\, f_1^{[\mathrm{c},+,j]}}{\varepsilon^{[\mathrm{c}]}\, f_1^{[\mathrm{f},+,j]}} \sin[2\pi\, f_1^{[\mathrm{c},+,j]}\,\Delta x_1] \right) \\ \pm\left(i\,\dfrac{\varepsilon^{[\mathrm{c}]}\, f_1^{[\mathrm{f},+,j]}}{\varepsilon^{[\mathrm{f}]}\, f_1^{[\mathrm{c},+,j]}} \sin[2\pi\, f_1^{[\mathrm{c},+,j]}\,\Delta x_1] \pm' \cos[2\pi\, f_1^{[\mathrm{c},+,j]}\,\Delta x_1] \right) \end{pmatrix} \tag{16.25}$$

(The $\pm$ and $\pm'$ signs are uncorrelated.) The reciprocal of Eq. 16.23 is obtained from Eq. 16.16,

$$\begin{aligned}
&\begin{pmatrix} \Phi^{[\mu,++,j]} & \Phi^{[\mu,+-,j]} \\ \Phi^{[\mu,-+,j]} & \Phi^{[\mu,--,j]} \end{pmatrix}^{-1} \\
&= \tfrac{1}{2}\begin{pmatrix} \left(\Gamma^{[\mu,\mathrm{E},j]}\right)^{-1} & \left(\Gamma^{[\mu,\mathrm{H},j]}\right)^{-1} \\ \left(\Gamma^{[\mu,\mathrm{E},j]}\right)^{-1} & -\left(\Gamma^{[\mu,\mathrm{H},j]}\right)^{-1} \end{pmatrix} \begin{pmatrix} \Phi^{[\mu,\mathrm{E},\mathrm{E},j]} & \Phi^{[\mu,\mathrm{E},\mathrm{H},j]} \\ \Phi^{[\mu,\mathrm{H},\mathrm{E},j]} & \Phi^{[\mu,\mathrm{H},\mathrm{H},j]} \end{pmatrix}^{-1} \begin{pmatrix} \Gamma^{[\mu,\mathrm{E},j]} & \Gamma^{[\mu,\mathrm{E},j]} \\ \Gamma^{[\mu,\mathrm{H},j]} & -\Gamma^{[\mu,\mathrm{H},j]} \end{pmatrix} \\
&= \tfrac{1}{2}\begin{pmatrix} \left(\Gamma^{[\mu,\mathrm{E},j]}\right)^{-1} & \left(\Gamma^{[\mu,\mathrm{H},j]}\right)^{-1} \\ \left(\Gamma^{[\mu,\mathrm{E},j]}\right)^{-1} & -\left(\Gamma^{[\mu,\mathrm{H},j]}\right)^{-1} \end{pmatrix} \begin{pmatrix} \Phi^{[\mu,\mathrm{E},\mathrm{E},j]} & -\Phi^{[\mu,\mathrm{E},\mathrm{H},j]} \\ -\Phi^{[\mu,\mathrm{H},\mathrm{E},j]} & \Phi^{[\mu,\mathrm{H},\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} \Gamma^{[\mu,\mathrm{E},j]} & \Gamma^{[\mu,\mathrm{E},j]} \\ \Gamma^{[\mu,\mathrm{H},j]} & -\Gamma^{[\mu,\mathrm{H},j]} \end{pmatrix} \\
&= \tfrac{1}{2}\begin{pmatrix} \left(\Gamma^{[\mu,\mathrm{E},j]}\right)^{-1} & -\left(\Gamma^{[\mu,\mathrm{H},j]}\right)^{-1} \\ \left(\Gamma^{[\mu,\mathrm{E},j]}\right)^{-1} & \left(\Gamma^{[\mu,\mathrm{H},j]}\right)^{-1} \end{pmatrix} \begin{pmatrix} \Phi^{[\mu,\mathrm{E},\mathrm{E},j]} & \Phi^{[\mu,\mathrm{E},\mathrm{H},j]} \\ \Phi^{[\mu,\mathrm{H},\mathrm{E},j]} & \Phi^{[\mu,\mathrm{H},\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} \Gamma^{[\mu,\mathrm{E},j]} & \Gamma^{[\mu,\mathrm{E},j]} \\ -\Gamma^{[\mu,\mathrm{H},j]} & \Gamma^{[\mu,\mathrm{H},j]} \end{pmatrix} \\
&= \tfrac{1}{2}\begin{pmatrix} \mathbf{0} & \mathbf{I} \\ \mathbf{I} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \left(\Gamma^{[\mu,\mathrm{E},j]}\right)^{-1} & \left(\Gamma^{[\mu,\mathrm{H},j]}\right)^{-1} \\ \left(\Gamma^{[\mu,\mathrm{E},j]}\right)^{-1} & -\left(\Gamma^{[\mu,\mathrm{H},j]}\right)^{-1} \end{pmatrix} \begin{pmatrix} \Phi^{[\mu,\mathrm{E},\mathrm{E},j]} & \Phi^{[\mu,\mathrm{E},\mathrm{H},j]} \\ \Phi^{[\mu,\mathrm{H},\mathrm{E},j]} & \Phi^{[\mu,\mathrm{H},\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} \Gamma^{[\mu,\mathrm{E},j]} & \Gamma^{[\mu,\mathrm{E},j]} \\ \Gamma^{[\mu,\mathrm{H},j]} & -\Gamma^{[\mu,\mathrm{H},j]} \end{pmatrix} \begin{pmatrix} \mathbf{0} & \mathbf{I} \\ \mathbf{I} & \mathbf{0} \end{pmatrix} \\
&= \begin{pmatrix} \mathbf{0} & \mathbf{I} \\ \mathbf{I} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \Phi^{[\mu,++,j]} & \Phi^{[\mu,+-,j]} \\ \Phi^{[\mu,-+,j]} & \Phi^{[\mu,--,j]} \end{pmatrix} \begin{pmatrix} \mathbf{0} & \mathbf{I} \\ \mathbf{I} & \mathbf{0} \end{pmatrix} = \begin{pmatrix} \Phi^{[\mu,--,j]} & \Phi^{[\mu,-+,j]} \\ \Phi^{[\mu,+-,j]} & \Phi^{[\mu,++,j]} \end{pmatrix}
\end{aligned} \tag{16.26}$$

The outgoing waves are represented as linear functions of the incoming waves as in Eq. 14.23,

$$\begin{pmatrix} F^{[\mu,+,j]}[x_1^{[0]} + \Delta x_1] \\ F^{[\mu,-,j]}[x_1^{[0]}] \end{pmatrix} = \begin{pmatrix} S^{[\mu,++,j]} & S^{[\mu,+-,j]} \\ S^{[\mu,-+,j]} & S^{[\mu,--,j]} \end{pmatrix} \begin{pmatrix} F^{[\mu,+,j]}[x_1^{[0]}] \\ F^{[\mu,-,j]}[x_1^{[0]} + \Delta x_1] \end{pmatrix} \tag{16.27}$$

Eq. 16.27 is substituted into Eq. 16.22,

$$\begin{aligned}
&\begin{pmatrix} S^{[\mu,++,j]} & S^{[\mu,+-,j]} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \begin{pmatrix} F^{[\mu,+,j]}[x_1^{[0]}] \\ F^{[\mu,-,j]}[x_1^{[0]} + \Delta x_1] \end{pmatrix} = \\
&\quad \begin{pmatrix} \Phi^{[\mu,++,j]} & \Phi^{[\mu,+-,j]} \\ \Phi^{[\mu,-+,j]} & \Phi^{[\mu,--,j]} \end{pmatrix} \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ S^{[\mu,-+,j]} & S^{[\mu,--,j]} \end{pmatrix} \begin{pmatrix} F^{[\mu,+,j]}[x_1^{[0]}] \\ F^{[\mu,-,j]}[x_1^{[0]} + \Delta x_1] \end{pmatrix}
\end{aligned} \tag{16.28}$$

This holds for any right-hand factor; hence

$$\begin{pmatrix} S^{[\mu,++,j]} & S^{[\mu,+-,j]} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} = \begin{pmatrix} \Phi^{[\mu,++,j]} & \Phi^{[\mu,+-,j]} \\ \Phi^{[\mu,-+,j]} & \Phi^{[\mu,--,j]} \end{pmatrix} \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ S^{[\mu,-+,j]} & S^{[\mu,--,j]} \end{pmatrix} \tag{16.29}$$

With application of Eq. 16.26, the following equivalent condition is obtained,

$$\begin{pmatrix} \Phi^{[\mu,--,j]} & \Phi^{[\mu,-+,j]} \\ \Phi^{[\mu,+-,j]} & \Phi^{[\mu,++,j]} \end{pmatrix} \begin{pmatrix} S^{[\mu,++,j]} & S^{[\mu,+-,j]} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} = \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ S^{[\mu,-+,j]} & S^{[\mu,--,j]} \end{pmatrix} \tag{16.30}$$

The following results are obtained from the second block column of Eq. 16.29 and the first block column of Eq. 16.30,

$$\left. \begin{array}{l} S^{[\mu,++,j]} = S^{[\mu,--,j]} = \left(\Phi^{[\mu,--,j]}\right)^{-1} \\ S^{[\mu,-+,j]} = S^{[\mu,+-,j]} = \Phi^{[\mu,+-,j]} \, S^{[\mu,--,j]} \end{array} \right\} \tag{16.31}$$

The denominator $f_1^{[\mathrm{c},+,j]}$ in Eq’s. 16.24 and 16.25 can be zero, but the ratio $\sin[2\pi\, f_1^{[\mathrm{c},+,j]}\, \Delta x_1] / f_1^{[\mathrm{c},+,j]}$ reduces to $2\pi\, \Delta x_1$ when $f_1^{[\mathrm{c},+,j]}$ approaches zero[4]. (The denominator $f_1^{[\mathrm{f},+,j]}$ is not zero because $\varepsilon^{[\mathrm{f}]}$ is defined to have a positive imaginary part.)

$f_1^{[\mathrm{c},+,j]}$ can have a large, positive imaginary part for high diffraction orders including evanescent waves (Eq. 16.9), leading to exponential overflow in the cosine and sine functions in Eq’s. 16.24 and 16.25. This problem is overcome by calculating $\Phi^{[P,\pm\pm',j]}$ ratioed to the cosine factor,

$$(\Phi^{[\mathrm{TE},\pm\pm',j]} / \cos[2\pi\, f_1^{[\mathrm{c},+,j]}\, \Delta x_1]) = \tfrac{1}{2} \begin{pmatrix} 1 \pm' i \dfrac{f_1^{[\mathrm{f}+,j]}}{f_1^{[\mathrm{c},+,j]}} \tan[2\pi\, f_1^{[\mathrm{c},+,j]}\, \Delta x_1] \\ \pm\left(i \dfrac{f_1^{[\mathrm{c},+,j]}}{f_1^{[\mathrm{f}+,j]}} \tan[2\pi\, f_1^{[\mathrm{c},+,j]}\, \Delta x_1] \pm' 1 \right) \end{pmatrix} \tag{16.32}$$

$$(\Phi^{[\mathrm{TM},\pm\pm',j]} / \cos[2\pi\, f_1^{[\mathrm{c},+,j]}\, \Delta x_1]) = \tfrac{1}{2} \begin{pmatrix} 1 \pm' i \dfrac{\varepsilon^{[\mathrm{f}]}}{\varepsilon^{[\mathrm{c}]}} \dfrac{f_1^{[\mathrm{c},+,j]}}{f_1^{[\mathrm{f}+,j]}} \tan[2\pi\, f_1^{[\mathrm{c},+,j]}\, \Delta x_1] \\ \pm\left(i \dfrac{\varepsilon^{[\mathrm{c}]}}{\varepsilon^{[f]}} \dfrac{f_1^{[\mathrm{f}+,j]}}{f_1^{[\mathrm{c},+,j]}} \tan[2\pi\, f_1^{[\mathrm{c},+,j]}\, \Delta x_1] \pm' 1 \right) \end{pmatrix} \tag{16.33}$$

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[4] For numerical applications, the ratio $\sin[2\pi\, f_1^{[\mathrm{c},+,j]}\, \Delta x_1] / f_1^{[\mathrm{c},+,j]}$ should be replaced by $2\pi\, \Delta x_1$ when $\left|2\pi\, f_1^{[\mathrm{c},+,j]}\, \Delta x_1\right|^2 < 6\delta$, where δ is the numeric precision (i.e., the smallest value such that 1 and $1+\delta$ are numerically distinguishable, $\delta = 2^{-52}$ for double-precision).

As $f_1^{[c,+,j]}$ approaches $+i\infty$ the sine and cosine terms become infinite but the tangent approaches i and the ratio $\Phi^{[P,\pm\pm',j]}/\cos[\ldots]$ remains finite. Eq's. 16.31 are modified to use the cosine-normalized Φ factors,

$$\left.\begin{array}{l} S^{[\mu,++,j]} = S^{[\mu,--,j]} = (\Phi^{[\mu,--,j]}/\cos[\ldots])^{-1}/\cos[\ldots], \\ S^{[\mu,-+,j]} = S^{[\mu,+-,j]} = (\Phi^{[\mu,+-,j]}/\cos[\ldots])(\Phi^{[P,--,j]}/\cos[\ldots])^{-1} \end{array}\right\} \tag{16.34}$$

The cosine normalization in Eq's. 16.32 and 16.33 should only be used when the cosine factor is significantly larger than 1 in magnitude. The normalization should not be used in all cases because the cosine term can be zero.

17. The reflection and transmission matrices

Taking the S matrix in Eq. 9.3 to represent the cumulative S-matrix for the entire grating stack, the only non-zero terms on the right side of the equation are those corresponding to the incident field, $F^{[-]}_{(0,0,P')}[x_1^{[1]}]$,

$$\begin{pmatrix} F^{[+]}_{(m_1,m_2,P)}[x_1^{[1]}] \\ F^{[-]}_{(m_1,m_2,P)}[x_1^{[0]}] \end{pmatrix} = \sum_{P'\in\{\mathrm{E},\mathrm{H}\}} \begin{pmatrix} S^{[+-]}_{(m_1,m_2,P),(0,0,P')} \\ S^{[--]}_{(m_1,m_2,P),(0,0,P')} \end{pmatrix} F^{[-]}_{(0_1,0,P')}[x_1^{[1]}] \quad \text{for } (m_1,m_2)\in\boldsymbol{\mathcal{M}},\ P\in\{\mathrm{E},\mathrm{H}\} \tag{17.1}$$

The $x_1^{[0]}$ and $x_1^{[1]}$ values in this equation represent the x_1 coordinate below and above the grating, respectively,

$$x_1^{[0]} = b_1^{[0]} - 0 \tag{17.2}$$

$$x_1^{[1]} = b_1^{[L_1]} + 0 \tag{17.3}$$

(cf. Eq's. 3.2 and 3.3). The S-matrix includes the transitions between the fictitious medium and the external (superstrate or substrate) media.

With substitution from Eq. 9.2, Eq. 17.1 translates to the following two equations for the cases $P=$'E' and $P=$'H',

$$\begin{pmatrix} f\!f E^{[+]}_{\mathrm{s},m_1,m_2}[x_1^{[1]}] \\ f\!f E^{[-]}_{\mathrm{s},m_1,m_2}[x_1^{[0]}] \end{pmatrix} = \begin{pmatrix} S^{[+-]}_{(m_1,m_2,\mathrm{E}),(0,0,\mathrm{E})} \\ S^{[--]}_{(m_1,m_2,\mathrm{E}),(0,0,\mathrm{E})} \end{pmatrix} f\!f E^{[-]}_{\mathrm{s},0,0}[x_1^{[1]}] + \begin{pmatrix} S^{[+-]}_{(m_1,m_2,\mathrm{E}),(0,0,\mathrm{H})} \\ S^{[--]}_{(m_1,m_2,\mathrm{E}),(0,0,\mathrm{H})} \end{pmatrix} f\!f H^{[-]}_{\mathrm{s},0,0}[x_1^{[1]}] \tag{17.4}$$

$$\begin{pmatrix} f\!f H^{[+]}_{\mathrm{s},m_1,m_2}[x_1^{[1]}] \\ f\!f H^{[-]}_{\mathrm{s},m_1,m_2}[x_1^{[0]}] \end{pmatrix} = \begin{pmatrix} S^{[+-]}_{(m_1,m_2,\mathrm{H}),(0,0,\mathrm{E})} \\ S^{[--]}_{(m_1,m_2,\mathrm{H}),(0,0,\mathrm{E})} \end{pmatrix} f\!f E^{[-]}_{\mathrm{s},0,0}[x_1^{[1]}] + \begin{pmatrix} S^{[+-]}_{(m_1,m_2,\mathrm{H}),(0,0,\mathrm{H})} \\ S^{[--]}_{(m_1,m_2,\mathrm{H}),(0,0,\mathrm{H})} \end{pmatrix} f\!f H^{[-]}_{\mathrm{s},0,0}[x_1^{[1]}] \tag{17.5}$$

The H-field amplitudes $\mathit{ffH}^{[\pm]}_{\mathrm{s},m_1,m_2}$ are related to the E-field amplitudes $\mathit{ffE}^{[\pm]}_{\mathrm{p},m_1,m_2}$ by Eq. 6.50 (with $\varepsilon^{[\mathrm{c}]} = \varepsilon^{[\mathrm{sup}]}$ or $\varepsilon^{[\mathrm{c}]} = \varepsilon^{[\mathrm{sub}]}$ for the superstrate or substrate, respectively, Eq's. 3.11, 3.12),

$$\mathit{ffH}^{[-]}_{\mathrm{s},0,0}[x_1^{[1]}] = \sqrt{\varepsilon^{[\mathrm{sup}]}}\,\mathit{ffE}^{[-]}_{\mathrm{p},0,0}[x_1^{[1]}] \tag{17.6}$$

$$\mathit{ffH}^{[-]}_{\mathrm{s},m_1,m_2}[x_1^{[0]}] = \sqrt{\varepsilon^{[\mathrm{sub}]}}\,\mathit{ffE}^{[-]}_{\mathrm{p},m_1,m_2}[x_1^{[0]}] \tag{17.7}$$

$$\mathit{ffH}^{[+]}_{\mathrm{s},m_1,m_2}[x_1^{[1]}] = \sqrt{\varepsilon^{[\mathrm{sup}]}}\,\mathit{ffE}^{[+]}_{\mathrm{p},m_1,m_2}[x_1^{[1]}] \tag{17.8}$$

The incident, reflected, and transmitted field amplitudes are designated as follows in Eq's. 4.34 and 4.35,

$$E^{[\mathrm{Inc}]}_{\mathrm{s}}[\hat{e}_1\,x_1^{[1]}] = \mathit{ffE}^{[-]}_{\mathrm{s},0,0}[x_1^{[1]}] \tag{17.9}$$

$$E^{[\mathrm{Inc}]}_{\mathrm{p}}[\hat{e}_1\,x_1^{[1]}] = \mathit{ffE}^{[-]}_{\mathrm{p},0,0}[x_1^{[1]}] \tag{17.10}$$

$$\mathit{ffE}^{[\mathrm{R}]}_{\mathrm{s},m_1,m_2}[\hat{e}_1\,x_1^{[1]}] = \mathit{ffE}^{[+]}_{\mathrm{s},m_1,m_2}[x_1^{[1]}] \tag{17.11}$$

$$\mathit{ffE}^{[\mathrm{R}]}_{\mathrm{p},m_1,m_2}[\hat{e}_1\,x_1^{[1]}] = \mathit{ffE}^{[+]}_{\mathrm{p},m_1,m_2}[x_1^{[1]}] \tag{17.12}$$

$$\mathit{ffE}^{[\mathrm{T}]}_{\mathrm{s},m_1,m_2}[\hat{e}_1\,x_1^{[0]}] = \mathit{ffE}^{[-]}_{\mathrm{s},m_1,m_2}[x_1^{[0]}] \tag{17.13}$$

$$\mathit{ffE}^{[\mathrm{T}]}_{\mathrm{p},m_1,m_2}[\hat{e}_1\,x_1^{[0]}] = \mathit{ffE}^{[-]}_{\mathrm{p},m_1,m_2}[x_1^{[0]}] \tag{17.14}$$

Making these substitutions in Eq's. 17.4 and 17.5, and comparing with Eq's. 4.34 and 4.35, the following results are obtained,

$$\begin{aligned}
&\begin{pmatrix} \mathit{ffE}^{[\mathrm{R}]}_{\mathrm{s},m_1,m_2}[\hat{e}_1\,x_1^{[1]}] \\ \mathit{ffE}^{[\mathrm{T}]}_{\mathrm{s},m_1,m_2}[\hat{e}_1\,x_1^{[0]}] \end{pmatrix} \\
&= \begin{pmatrix} S^{[+-]}_{(m_1,m_2,\mathrm{E}),(0,0,\mathrm{E})} \\ S^{[--]}_{(m_1,m_2,\mathrm{E}),(0,0,\mathrm{E})} \end{pmatrix} E^{[\mathrm{Inc}]}_{\mathrm{s}}[\hat{e}_1\,x_1^{[1]}] + \begin{pmatrix} S^{[+-]}_{(m_1,m_2,\mathrm{E}),(0,0,\mathrm{H})} \\ S^{[--]}_{(m_1,m_2,\mathrm{E}),(0,0,\mathrm{H})} \end{pmatrix} \sqrt{\varepsilon^{[\mathrm{sup}]}}\, E^{[\mathrm{Inc}]}_{\mathrm{p}}[\hat{e}_1\,x_1^{[1]}] \\
&= \begin{pmatrix} R_{\mathrm{s},\mathrm{s},m_1,m_2} & R_{\mathrm{s},\mathrm{p},m_1,m_2} \\ T_{\mathrm{s},\mathrm{s},m_1,m_2} & T_{\mathrm{s},\mathrm{p},m_1,m_2} \end{pmatrix} \begin{pmatrix} E^{[\mathrm{Inc}]}_{\mathrm{s}}[\hat{e}_1\,x_1^{[1]}] \\ E^{[\mathrm{Inc}]}_{\mathrm{p}}[\hat{e}_1\,x_1^{[1]}] \end{pmatrix}
\end{aligned} \tag{17.15}$$

$$\begin{pmatrix} ffE^{[\mathrm{R}]}_{\mathrm{p},m_1,m_2}[\hat{e}_1\, x_1^{[1]}] \\ ffE^{[\mathrm{T}]}_{\mathrm{p},m_1,m_2}[\hat{e}_1\, x_1^{[0]}] \end{pmatrix}$$

$$= \begin{pmatrix} (1/\sqrt{\varepsilon^{[\mathrm{sup}]}})\, S^{[+-]}_{(m_1,m_2,\mathrm{H}),(0,0,\mathrm{E})} \\ (1/\sqrt{\varepsilon^{[\mathrm{sub}]}})\, S^{[--]}_{(m_1,m_2,\mathrm{H}),(0,0,\mathrm{E})} \end{pmatrix} E^{[\mathrm{Inc}]}_{\mathrm{s}}[\hat{e}_1\, x_1^{[1]}] + \begin{pmatrix} S^{[+-]}_{(m_1,m_2,\mathrm{H}),(0,0,\mathrm{H})} \\ \sqrt{\varepsilon^{[\mathrm{sup}]}/\varepsilon^{[\mathrm{sub}]}}\, S^{[--]}_{(m_1,m_2,\mathrm{H}),(0,0,\mathrm{H})} \end{pmatrix} E^{[\mathrm{Inc}]}_{\mathrm{p}}[\hat{e}_1\, x_1^{[1]}] \quad (17.16)$$

$$= \begin{pmatrix} R_{\mathrm{p,s},m_1,m_2} & R_{\mathrm{p,p},m_1,m_2} \\ T_{\mathrm{p,s},m_1,m_2} & T_{\mathrm{p,p},m_1,m_2} \end{pmatrix} \begin{pmatrix} E^{[\mathrm{Inc}]}_{\mathrm{s}}[\hat{e}_1\, x_1^{[1]}] \\ E^{[\mathrm{Inc}]}_{\mathrm{p}}[\hat{e}_1\, x_1^{[1]}] \end{pmatrix}$$

Hence, the reflection and transmission matrices are defined as follows,

$$\begin{pmatrix} R_{\mathrm{s,s},m_1,m_2} & R_{\mathrm{s,p},m_1,m_2} \\ R_{\mathrm{p,s},m_1,m_2} & R_{\mathrm{p,p},m_1,m_2} \end{pmatrix} = \begin{pmatrix} S^{[+-]}_{(m_1,m_2,\mathrm{E}),(0,0,\mathrm{E})} & \sqrt{\varepsilon^{[\mathrm{sup}]}}\, S^{[+-]}_{(m_1,m_2,\mathrm{E}),(0,0,\mathrm{H})} \\ (1/\sqrt{\varepsilon^{[\mathrm{sup}]}})\, S^{[+-]}_{(m_1,m_2,\mathrm{H}),(0,0,\mathrm{E})} & S^{[+-]}_{(m_1,m_2,\mathrm{H}),(0,0,\mathrm{H})} \end{pmatrix} \quad (17.17)$$

$$\begin{pmatrix} T_{\mathrm{s,s},m_1,m_2} & T_{\mathrm{s,p},m_1,m_2} \\ T_{\mathrm{p,s},m_1,m_2} & T_{\mathrm{p,p},m_1,m_2} \end{pmatrix} = \begin{pmatrix} S^{[--]}_{(m_1,m_2,\mathrm{E}),(0,0,\mathrm{E})} & \sqrt{\varepsilon^{[\mathrm{sup}]}}\, S^{[--]}_{(m_1,m_2,\mathrm{E}),(0,0,\mathrm{H})} \\ (1/\sqrt{\varepsilon^{[\mathrm{sub}]}})\, S^{[--]}_{(m_1,m_2,\mathrm{H}),(0,0,\mathrm{E})} & \sqrt{\varepsilon^{[\mathrm{sup}]}/\varepsilon^{[\mathrm{sub}]}}\, S^{[--]}_{(m_1,m_2,\mathrm{H}),(0,0,\mathrm{H})} \end{pmatrix} \quad (17.18)$$

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Appendix A. Power Flux and Diffraction Efficiency

The physical electric and magnetic fields, as functions of position $\vec{x}$ and time t, are

$$\vec{E}^{[\text{physical}]}[\vec{x},t] = \operatorname{Re}\left[\vec{E}[\vec{x}]\exp[-i\,2\pi\,c\,t\,/\,\lambda]\right] \tag{A.1}$$

$$\vec{H}^{[\text{physical}]}[\vec{x},t] = \operatorname{Re}\left[\vec{H}[\vec{x}]\exp[-i\,2\pi\,c\,t\,/\,\lambda]\right] \tag{A.2}$$

where $\vec{E}[\vec{x}]$ and $\vec{H}[\vec{x}]$ have the Fourier expansions in Eq's. 5.7 and 5.12. The directional power flux in the electromagnetic field is represented by the Poynting vector,

$$\begin{aligned}\vec{S} &= \vec{E}^{[\text{physical}]}[\vec{x},t]\times\vec{H}^{[\text{physical}]}[\vec{x},t]\\ &= \tfrac{1}{2}\operatorname{Re}\left[\vec{E}[\vec{x}]\times\vec{H}[\vec{x}]^{*}+\vec{E}[\vec{x}]\times\vec{H}[\vec{x}]\exp[-i\,4\pi\,c\,t\,/\,\lambda]\right]\end{aligned} \tag{A.3}$$

Denoting the time-average as $\langle\ldots\rangle_t$, the time-average Poynting vector is

$$\langle \vec{S} \rangle_t = \tfrac{1}{2}\,\mathrm{Re}\big[\vec{E}[\vec{x}] \times \vec{H}[\vec{x}]^* \big] \tag{A.4}$$

The power flux in the $\hat{e}_1$ direction (i.e., per unit area on a surface parallel to the grating substrate) is

$$\langle S_1 \rangle_t = \hat{e}_1 \bullet \langle \vec{S} \rangle_t = \tfrac{1}{2}\,\mathrm{Re}\big[E_2[\vec{x}]\, H_3[\vec{x}]^* - E_3[\vec{x}]\, H_2[\vec{x}]^* \big] \tag{A.5}$$

With substitution from Eq's. 5.7 and 5.12,

$$\langle S_1 \rangle_t = \tfrac{1}{2} \sum_{m_1, m_2, m'_1, m'_2} \mathrm{Re}\left[\begin{array}{l} \left(\mathit{ffE}_{2,m_1,m_2}[x_1]\, \mathit{ffH}_{3,m'_1,m'_2}[x_1]^* - \mathit{ffE}_{3,m_1,m_2}[x_1]\, \mathit{ffH}_{2,m'_1,m'_2}[x_1]^* \right) \\ \exp[i\, 2\pi\, (\vec{f}^{[||]}_{m_1,m_2} - \vec{f}^{[||]}_{m'_1,m'_2}) \bullet \vec{x}] \end{array} \right] \tag{A.6}$$

where $\vec{f}^{[||]}_{m_1,m_2}$ is the tangential spatial frequency vector defined by Eq. 5.8. The exponential factor in Eq. A.6 averages to zero over x_2 and x_3 except when $(m'_1, m'_2) = (m_1, m_2)$; thus,

$$\langle S_1 \rangle_{t,x_2,x_3} = \tfrac{1}{2} \sum_{m_1, m_2} \mathrm{Re}\Big[\mathit{ffE}_{2,m_1,m_2}[x_1]\, \mathit{ffH}_{3,m_1,m_2}[x_1]^* - \mathit{ffE}_{3,m_1,m_2}[x_1]\, \mathit{ffH}_{2,m_1,m_2}[x_1]^* \Big] \tag{A.7}$$

where $\langle \ldots \rangle_{t,x_2,x_3}$ denotes the average over t, x_2, and x_3. The power flux is additively separable between diffraction orders, with the flux in order (m_1, m_2) equal to

$$\langle S_{1,m_1,m_2} \rangle_{t,x_2,x_3} = \tfrac{1}{2}\,\mathrm{Re}\Big[\mathit{ffE}_{2,m_1,m_2}[x_1]\, \mathit{ffH}_{3,m_1,m_2}[x_1]^* - \mathit{ffE}_{3,m_1,m_2}[x_1]\, \mathit{ffH}_{2,m_1,m_2}[x_1]^* \Big] \tag{A.8}$$

The field's Fourier orders in the substrate and superstrate are separated into up and down waves, Eq's. 6.44-6.51, where $\varepsilon^{[\mathrm{c}]}$ is the medium permittivity ($\varepsilon^{[\mathrm{sub}]}$ for the substrate or $\varepsilon^{[\mathrm{sup}]}$ for the superstrate, Eq's. 3.11, 3.12). Eq. A.8 is simplified by making substitutions from Eq's. 6.44, 6.45, 6.48, 6.49, 6.40, and 6.42, the relation ${s_{2,m_1,m_2}}^2 + {s_{3,m_1,m_2}}^2 = 1$ (from Eq. 6.14), and Eq's. 6.50 and 6.51:

$$\left\langle S_{1,m_1,m_2}\right\rangle_{t,x_2,x_3} = \sum_{\pm,\pm'} \tfrac{1}{2}\operatorname{Re}\Big[ffE_{2,m_1,m_2}^{[\pm]}[x_1]\, ffH_{3,m_1,m_2}^{[\pm']}[x_1]^* - ffE_{3,m_1,m_2}^{[\pm]}[x_1]\, ffH_{2,m_1,m_2}^{[\pm']}[x_1]^* \Big]$$

$$= \sum_{\pm,\pm'} \pm' \tfrac{1}{2}\operatorname{Re}\left[\begin{array}{l} \left(s_{2,m_1,m_2}\, ffE_{\mathrm{s},m_1,m_2}^{[\pm]}[x_1] + p_{2,m_1,m_2}^{[\pm]}\, ffE_{\mathrm{p},m_1,m_2}^{[\pm]}[x_1]\right)\left(s_{3,m_1,m_2}\, ffH_{\mathrm{s},m_1,m_2}^{[\pm']}[x_1] + p_{3,m_1,m_2}^{[\pm']}\, ffH_{\mathrm{p},m_1,m_2}^{[\pm']}[x_1]\right)^* \\ -\left(s_{3,m_1,m_2}\, ffE_{\mathrm{s},m_1,m_2}^{[\pm]}[x_1] + p_{3,m_1,m_2}^{[\pm]}\, ffE_{\mathrm{p},m_1,m_2}^{[\pm]}[x_1]\right)\left(s_{2,m_1,m_2}\, ffH_{\mathrm{s},m_1,m_2}^{[\pm']}[x_1] + p_{2,m_1,m_2}^{[\pm']}\, ffH_{\mathrm{p},m_1,m_2}^{[\pm']}[x_1]\right)^* \end{array}\right]$$

$$= \sum_{\pm,\pm'} \pm' \tfrac{1}{2}\operatorname{Re}\left[\begin{array}{l} \left(s_{2,m_1,m_2}\, ffE_{\mathrm{s},m_1,m_2}^{[\pm]}[x_1] + s_{3,m_1,m_2}\dfrac{\lambda}{\sqrt{\varepsilon^{[\mathrm{c}]}}} f_{1,m_1,m_2}^{[+]}\, ffE_{\mathrm{p},m_1,m_2}^{[\pm]}[x_1]\right)\cdot \\ \quad \left(s_{3,m_1,m_2}\, ffH_{\mathrm{s},m_1,m_2}^{[\pm']}[x_1] - s_{2,m_1,m_2}\dfrac{\lambda}{\sqrt{\varepsilon^{[\mathrm{c}]}}} f_{1,m_1,m_2}^{[+]}\, ffH_{\mathrm{p},m_1,m_2}^{[\pm']}[x_1]\right)^* \\ -\left(s_{3,m_1,m_2}\, ffE_{\mathrm{s},m_1,m_2}^{[\pm]}[x_1] - s_{2,m_1,m_2}\dfrac{\lambda}{\sqrt{\varepsilon^{[\mathrm{c}]}}} f_{1,m_1,m_2}^{[+]}\, ffE_{\mathrm{p},m_1,m_2}^{[\pm]}[x_1]\right)\cdot \\ \quad \left(s_{2,m_1,m_2}\, ffH_{\mathrm{s},m_1,m_2}^{[\pm']}[x_1] + s_{3,m_1,m_2}\dfrac{\lambda}{\sqrt{\varepsilon^{[\mathrm{c}]}}} f_{1,m_1,m_2}^{[+]}\, ffH_{\mathrm{p},m_1,m_2}^{[\pm']}[x_1]\right)^* \end{array}\right]$$

$$= \sum_{\pm,\pm'} \pm' \tfrac{1}{2}\operatorname{Re}\left[-ffE_{\mathrm{s},m_1,m_2}^{[\pm]}[x_1]\frac{\lambda}{\sqrt{\varepsilon^{[\mathrm{c}]}}^*} f_{1,m_1,m_2}^{[+]}{}^*\, ffH_{\mathrm{p},m_1,m_2}^{[\pm']}[x_1]^* + \frac{\lambda}{\sqrt{\varepsilon^{[\mathrm{c}]}}} f_{1,m_1,m_2}^{[+]}\, ffE_{\mathrm{p},m_1,m_2}^{[\pm]}[x_1]\, ffH_{\mathrm{s},m_1,m_2}^{[\pm']}[x_1]^* \right]$$

$$= \sum_{\pm,\pm'} \pm' \tfrac{1}{2}\lambda\operatorname{Re}\left[f_{1,m_1,m_2}^{[+]}{}^*\, ffE_{\mathrm{s},m_1,m_2}^{[\pm]}[x_1]\, ffE_{\mathrm{s},m_1,m_2}^{[\pm']}[x_1]^* + \frac{\varepsilon^{[\mathrm{c}]*}}{\left|\varepsilon^{[\mathrm{c}]}\right|} f_{1,m_1,m_2}^{[+]}\, ffE_{\mathrm{p},m_1,m_2}^{[\pm]}[x_1]\, ffE_{\mathrm{p},m_1,m_2}^{[\pm']}[x_1]^* \right]$$

$$= \tfrac{1}{2}\lambda\left(\begin{array}{l} \operatorname{Re}\Big[f_{1,m_1,m_2}^{[+]}\Big]\left(\left|ffE_{\mathrm{s},m_1,m_2}^{[+]}[x_1]\right|^2 - \left|ffE_{\mathrm{s},m_1,m_2}^{[-]}[x_1]\right|^2\right) + \operatorname{Re}\left[\dfrac{\varepsilon^{[\mathrm{c}]*}}{\left|\varepsilon^{[\mathrm{c}]}\right|} f_{1,m_1,m_2}^{[+]}\right]\left(\left|ffE_{\mathrm{p},m_1,m_2}^{[+]}[x_1]\right|^2 - \left|ffE_{\mathrm{p},m_1,m_2}^{[-]}[x_1]\right|^2\right) \\ -2\operatorname{Im}\Big[f_{1,m_1,m_2}^{[+]}\Big]\operatorname{Im}\Big[ffE_{\mathrm{s},m_1,m_2}^{[+]}[x_1]\, ffE_{\mathrm{s},m_1,m_2}^{[-]}[x_1]^*\Big] - 2\operatorname{Im}\left[\dfrac{\varepsilon^{[\mathrm{c}]}}{\left|\varepsilon^{[\mathrm{c}]}\right|} f_{1,m_1,m_2}^{[+]}\right]\operatorname{Im}\Big[ffE_{\mathrm{p},m_1,m_2}^{[+]}[x_1]\, ffE_{\mathrm{p},m_1,m_2}^{[-]}[x_1]^*\Big] \end{array}\right) \tag{A.9}$$

In the substrate, there are no up waves and Eq. A.9 simplifies to

$$\begin{aligned} &\text{In the substrate } (\varepsilon^{[\mathrm{c}]} = \varepsilon^{[\mathrm{sub}]})\text{: } ffE_{\mathrm{s},m_1,m_2}^{[+]}[x_1] = 0,\ \ ffE_{\mathrm{p},m_1,m_2}^{[+]}[x_1], \\ &\left\langle S_{1,m_1,m_2}\right\rangle_{t,x_2,x_3} = -\tfrac{1}{2}\lambda\left(\operatorname{Re}\Big[f_{1,m_1,m_2}^{[+]}\Big]\left|ffE_{\mathrm{s},m_1,m_2}^{[-]}[x_1]\right|^2 + \operatorname{Re}\left[\frac{\varepsilon^{[\mathrm{sub}]*}}{\left|\varepsilon^{[\mathrm{sub}]}\right|} f_{1,m_1,m_2}^{[+]}\right]\left|ffE_{\mathrm{p},m_1,m_2}^{[-]}[x_1]\right|^2 \right) \end{aligned} \tag{A.10}$$

(The minus sign indicates that the power is directed downward, away from the grating.) In the superstrate the power flux in Fourier order (m_1, m_2) is additively separable between up and down waves under the condition that either the down wave (incident beam) is zero-amplitude (the usual case for $(m_1, m_2) \neq (0,0)$), or $f_{1,m_1,m_2}^{[+]}$ is real-valued (implying that $\varepsilon^{[\mathrm{sup}]}$ is also real-valued, Eq. 6.37 with $\varepsilon^{[\mathrm{c}]} = \varepsilon^{[\mathrm{sup}]}$), In the superstrate ($\varepsilon^{[\mathrm{c}]} = \varepsilon^{[\mathrm{sup}]}$):

If either $ffE^{[-]}_{\mathrm{s},m_1,m_2}[x_1] = 0$ and $ffE^{[-]}_{\mathrm{p},m_1,m_2}[x_1] = 0$, or $\mathrm{Im}\left[f^{[+]}_{1,m_1,m_2} \right] = 0$, then (A.11)

$$\left\langle S_{1,m_1,m_2} \right\rangle_{t,x_2,x_3} = \tfrac{1}{2}\lambda \left(\begin{array}{l} \mathrm{Re}\left[f^{[+]}_{1,m_1,m_2} \right]\left(\left| ffE^{[+]}_{\mathrm{s},m_1,m_2}[x_1] \right|^2 - \left| ffE^{[-]}_{\mathrm{s},m_1,m_2}[x_1] \right|^2 \right) \\ \quad + \mathrm{Re}\left[\dfrac{\varepsilon^{[\mathrm{sup}]*}}{\left|\varepsilon^{[\mathrm{sup}]}\right|} f^{[+]}_{1,m_1,m_2} \right]\left(\left| ffE^{[+]}_{\mathrm{p},m_1,m_2}[x_1] \right|^2 - \left| ffE^{[-]}_{\mathrm{p},m_1,m_2}[x_1] \right|^2 \right) \end{array} \right)$$

(If the premise of Eq. A.11 does not hold, then the cross terms between $ffE^{[+]}$ and $ffE^{[-]}$ in Eq. A.9 are nonzero and the power flux is not separable into up and down components.)

Diffraction efficiency formulas are obtained from Eq's. A.10 and A.11 under the premise that there is one incident order $(m_1, m_2) = (m_1^{[\mathrm{Inc}]}, m_2^{[\mathrm{Inc}]})$ (not necessarily the $(0,0)$ order) and that $f^{[+]}_{1,m_1,m_2}$ is real-valued for the incident order (implying that $\varepsilon^{[\mathrm{sup}]}$ is real-valued).

In the superstrate:

For $(m_1, m_2) \neq (m_1^{[\mathrm{Inc}]}, m_2^{[\mathrm{Inc}]})$, $ffE^{[-]}_{\mathrm{s},m_1,m_2}[x_1] = 0$ and $ffE^{[-]}_{\mathrm{p},m_1,m_2}[x_1] = 0$ (A.12)

$$f_1^{[\mathrm{Inc}]} = -f^{[+]}_{1,m_1^{[\mathrm{Inc}]},m_2^{[\mathrm{Inc}]}} = -\sqrt{\frac{\varepsilon^{[\mathrm{sup}]}}{\lambda^2} - \left(f_{2,m_1^{[\mathrm{Inc}]},m_2^{[\mathrm{Inc}]}} \right)^2 - \left(f_{3,m_1^{[\mathrm{Inc}]},m_2^{[\mathrm{Inc}]}} \right)^2},$$
$$\mathrm{Im}\left[f_1^{[\mathrm{Inc}]} \right] = 0, \quad \mathrm{Im}[\varepsilon^{[\mathrm{sup}]}] = 0 \tag{A.13}$$

(cf. Eq. 6.37). The power flux $P^{[\mathrm{Inc}]}$ in the incident order, at $x_1 = b_1^{[L1]}+$ (Eq. 3.1), is obtained from Eq. A.11 (with the factor of $\frac{1}{2}$ omitted),

$$P^{[\mathrm{Inc}]} = -\lambda\, f_1^{[\mathrm{Inc}]} \left(|A|^2 + |B|^2 \right) \tag{A.14}$$

where

$$A = ffE^{[-]}_{\mathrm{s},m_1^{[\mathrm{Inc}]},m_2^{[\mathrm{Inc}]}}[b_1^{[L1]}+], \quad B = ffE^{[-]}_{\mathrm{p},m_1^{[\mathrm{Inc}]},m_2^{[\mathrm{Inc}]}}[b_1^{[L1]}+] \tag{A.15}$$

The reflected power $P^{[\mathrm{R}]}_{m_1,m_2}$ in order (m_1, m_2) (including the case $(m_1, m_2) = (m_1^{[\mathrm{Inc}]}, m_2^{[\mathrm{Inc}]})$) is also obtained from Eq. A.11,

$$P^{[\mathrm{R}]}_{m_1,m_2} = \mathrm{Re}\left[\lambda\, f^{[\mathrm{R}]}_{1,m_1,m_2} \right]\left(\left| ffE^{[+]}_{\mathrm{s},m_1,m_2}[b_1^{[L1]}+] \right|^2 + \left| ffE^{[+]}_{\mathrm{p},m_1,m_2}[b_1^{[L1]}+] \right|^2 \right) \tag{A.16}$$

where

$$f_{1,m_1,m_2}^{[\mathrm{R}]} = \sqrt{\frac{\varepsilon^{[\mathrm{sup}]}}{\lambda^2} - \left(f_{2,m_1,m_2}\right)^2 - \left(f_{3,m_1,m_2}\right)^2} \tag{A.17}$$

The transmitted power $P_{m_1,m_2}^{[\mathrm{T}]}$ in order (m_1, m_2), at $x_1 = b_1^{[0]}-$ (Eq. 3.1), is obtained from Eq. A.10,

$$P_{m_1,m_2}^{[\mathrm{T}]} = -\mathrm{Re}\left[\lambda\, f_{1,m_1,m_2}^{[\mathrm{T}]}\right]\left(\left|f\!fE_{\mathrm{s},m_1,m_2}^{[-]}[b_1^{[0]}-]\right|^2 + \left|f\!fE_{\mathrm{p},m_1,m_2}^{[-]}[b_1^{[0]}-]\right|^2\right) \tag{A.18}$$

where

$$f_{1,m_1,m_2}^{[\mathrm{T}]} = -\sqrt{\frac{\varepsilon^{[\mathrm{sub}]}}{\lambda^2} - \left(f_{2,m_1,m_2}\right)^2 - \left(f_{3,m_1,m_2}\right)^2} \tag{A.19}$$

The field amplitudes in Eq's. A.15, A.16, and A.18 have the following form (cf. Eq's. 4.1, 4.4, 4.6, 5.7, 5.12, 6.44-6.49),

$$A = E_{\mathrm{s}}^{[\mathrm{Inc}]}[\hat{e}_1\, b_1^{[L_1]}], \quad B = E_{\mathrm{p}}^{[\mathrm{Inc}]}[\hat{e}_1\, b_1^{[L_1]}] \tag{A.20}$$

$$f\!fE_{\mathrm{s},m_1,m_2}^{[+]}[b_1^{[L1]}+] = f\!fE_{\mathrm{s},m_1,m_2}^{[\mathrm{R}]}[\hat{e}_1\, b_1^{[L_1]}], \quad f\!fE_{\mathrm{p},m_1,m_2}^{[+]}[b_1^{[L1]}+] = f\!fE_{\mathrm{p},m_1,m_2}^{[\mathrm{R}]}[\hat{e}_1\, b_1^{[L_1]}] \tag{A.21}$$

$$f\!fE_{\mathrm{s},m_1,m_2}^{[-]}[b_1^{[0]}-] = f\!fE_{\mathrm{s},m_1,m_2}^{[\mathrm{T}]}[\hat{e}_1\, b_1^{[0]}], \quad f\!fE_{\mathrm{p},m_1,m_2}^{[-]}[b_1^{[0]}-] = f\!fE_{\mathrm{p},m_1,m_2}^{[\mathrm{T}]}[\hat{e}_1\, b_1^{[0]}] \tag{A.22}$$

The diffracted wave amplitudes are linear functions of A and B (Eq's. 4.34, 4.35)

$$\begin{pmatrix} f\!fE_{\mathrm{s},m_1,m_2}^{[+]}[b_1^{[L1]}+] \\ f\!fE_{\mathrm{p},m_1,m_2}^{[+]}[b_1^{[L1]}+] \end{pmatrix} = \begin{pmatrix} R_{\mathrm{s,s},m_1,m_2} & R_{\mathrm{s,p},m_1,m_2} \\ R_{\mathrm{p,s},m_1,m_2} & R_{\mathrm{p,p},m_1,m_2} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} \tag{A.23}$$

$$\begin{pmatrix} f\!fE_{\mathrm{s},m_1,m_2}^{[-]}[b_1^{[0]}-] \\ f\!fE_{\mathrm{p},m_1,m_2}^{[-]}[b_1^{[0]}-] \end{pmatrix} = \begin{pmatrix} T_{\mathrm{s,s},m_1,m_2} & T_{\mathrm{s,p},m_1,m_2} \\ T_{\mathrm{p,s},m_1,m_2} & T_{\mathrm{p,p},m_1,m_2} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} \tag{A.24}$$

The diffraction efficiencies $\eta_{m_1,m_2}^{[\mathrm{R}]}$ for reflected orders and $\eta_{m_1,m_2}^{[\mathrm{T}]}$ for transmitted orders (i.e., the ratio of diffracted to incident power) are obtained from Eq's. A.14, A.16, A.18, A.23, and A.24.

$$\eta_{m_1,m_2}^{[\mathrm{R}]} = \frac{P_{m_1,m_2}^{[\mathrm{R}]}}{P^{[\mathrm{Inc}]}} = -\frac{\mathrm{Re}\left[f_{1,m_1,m_2}^{[\mathrm{R}]}\right]}{f_1^{[\mathrm{Inc}]}} \left(\frac{\left|R_{\mathrm{s,s},m_1,m_2}\, A + R_{\mathrm{s,p},m_1,m_2}\, B\right|^2 + \left|R_{\mathrm{p,s},m_1,m_2}\, A + R_{\mathrm{p,p},m_1,m_2}\, B\right|^2}{|A|^2 + |B|^2}\right) \tag{A.25}$$

$$\eta_{m_1,m_2}^{[\mathrm{T}]} = \frac{P_{m_1,m_2}^{[\mathrm{T}]}}{P^{[\mathrm{Inc}]}} = \frac{\mathrm{Re}\left[f_{1,m_1,m_2}^{[\mathrm{T}]}\right]}{f_1^{[\mathrm{Inc}]}} \left(\frac{\left|T_{\mathrm{s,s},m_1,m_2}\, A + T_{\mathrm{s,p},m_1,m_2}\, B\right|^2 + \left|T_{\mathrm{p,s},m_1,m_2}\, A + T_{\mathrm{p,p},m_1,m_2}\, B\right|^2}{|A|^2 + |B|^2}\right) \tag{A.26}$$

The diffraction efficiency for an arbitrary incident polarization state can be determined from four basic polarization states, with corresponding efficiencies denoted as $\eta 1$, $\eta 2$, $\eta 3$, and $\eta 4$:

$$\left.\begin{aligned}
&\eta 1^{[\mathrm{R}]}_{m_1,m_2} = \eta^{[\mathrm{R}]}_{m_1,m_2}\Big|_{A=1,B=0} = -\frac{\mathrm{Re}\left[f^{[\mathrm{R}]}_{1,m_1,m_2}\right]}{f^{[\mathrm{Inc}]}_1}\left(\left|R_{\mathrm{s,s},m_1,m_2}\right|^2+\left|R_{\mathrm{p,s},m_1,m_2}\right|^2\right)\\
&\eta 2^{[\mathrm{R}]}_{m_1,m_2} = \eta^{[\mathrm{R}]}_{m_1,m_2}\Big|_{A=0,B=1} = -\frac{\mathrm{Re}\left[f^{[\mathrm{R}]}_{1,m_1,m_2}\right]}{f^{[\mathrm{Inc}]}_1}\left(\left|R_{\mathrm{s,p},m_1,m_2}\right|^2+\left|R_{\mathrm{p,p},m_1,m_2}\right|^2\right)\\
&\eta 3^{[\mathrm{R}]}_{m_1,m_2} = \eta^{[\mathrm{R}]}_{m_1,m_2}\Big|_{A=B=1/\sqrt{2}} =\\
&\quad \tfrac{1}{2}\left(\eta 1^{[\mathrm{R}]}_{m_1,m_2}+\eta 2^{[\mathrm{R}]}_{m_1,m_2}\right) - \frac{\mathrm{Re}\left[f^{[\mathrm{R}]}_{1,m_1,m_2}\right]}{f^{[\mathrm{Inc}]}_1}\mathrm{Re}\left[R_{\mathrm{s,s},m_1,m_2}\,R_{\mathrm{s,p},m_1,m_2}{}^{*}+R_{\mathrm{p,s},m_1,m_2}\,R_{\mathrm{p,p},m_1,m_2}{}^{*}\right]\\
&\eta 4^{[\mathrm{R}]}_{m_1,m_2} = \eta^{[\mathrm{R}]}_{m_1,m_2}\Big|_{A=1/\sqrt{2},B=-i/\sqrt{2}} =\\
&\quad \tfrac{1}{2}\left(\eta 1^{[\mathrm{R}]}_{m_1,m_2}+\eta 2^{[\mathrm{R}]}_{m_1,m_2}\right) + \frac{\mathrm{Re}\left[f^{[\mathrm{R}]}_{1,m_1,m_2}\right]}{f^{[\mathrm{Inc}]}_1}\mathrm{Im}\left[R_{\mathrm{s,s},m_1,m_2}\,R_{\mathrm{s,p},m_1,m_2}{}^{*}+R_{\mathrm{p,s},m_1,m_2}\,R_{\mathrm{p,p},m_1,m_2}{}^{*}\right]
\end{aligned}\right\} \tag{A.27}$$

$$\eta^{[\mathrm{R}]}_{m_1,m_2} = \frac{1}{|A|^2+|B|^2}\begin{pmatrix}
\eta 1^{[\mathrm{R}]}_{m_1,m_2}\,|A|^2\\
+\eta 2^{[\mathrm{R}]}_{m_1,m_2}\,|B|^2\\
+\left(2\,\eta 3^{[\mathrm{R}]}_{m_1,m_2}-\eta 1^{[\mathrm{R}]}_{m_1,m_2}-\eta 2^{[\mathrm{R}]}_{m_1,m_2}\right)\mathrm{Re}\left[A\,B^{*}\right]\\
+\left(2\,\eta 4^{[\mathrm{R}]}_{m_1,m_2}-\eta 1^{[\mathrm{R}]}_{m_1,m_2}-\eta 2^{[\mathrm{R}]}_{m_1,m_2}\right)\mathrm{Im}\left[A\,B^{*}\right]
\end{pmatrix} \tag{A.28}$$

$$\left.\begin{aligned}
&\eta 1^{[\mathrm{T}]}_{m_1,m_2} = \eta^{[\mathrm{T}]}_{m_1,m_2}\Big|_{A=1,B=0} = \frac{\mathrm{Re}\left[f^{[\mathrm{T}]}_{1,m_1,m_2}\right]}{f^{[\mathrm{Inc}]}_1}\left(\left|T_{\mathrm{s,s},m_1,m_2}\right|^2+\left|T_{\mathrm{p,s},m_1,m_2}\right|^2\right)\\
&\eta 2^{[\mathrm{T}]}_{m_1,m_2} = \eta^{[\mathrm{T}]}_{m_1,m_2}\Big|_{A=0,B=1} = \frac{\mathrm{Re}\left[f^{[\mathrm{T}]}_{1,m_1,m_2}\right]}{f^{[\mathrm{Inc}]}_1}\left(\left|T_{\mathrm{s,p},m_1,m_2}\right|^2+\left|T_{\mathrm{p,p},m_1,m_2}\right|^2\right)\\
&\eta 3^{[\mathrm{T}]}_{m_1,m_2} = \eta^{[\mathrm{T}]}_{m_1,m_2}\Big|_{A=B=1/\sqrt{2}} =\\
&\quad \tfrac{1}{2}\left(\eta 1^{[\mathrm{T}]}_{m_1,m_2}+\eta 2^{[\mathrm{T}]}_{m_1,m_2}\right) + \frac{\mathrm{Re}\left[f^{[\mathrm{T}]}_{1,m_1,m_2}\right]}{f^{[\mathrm{Inc}]}_1}\mathrm{Re}\left[T_{\mathrm{s,s},m_1,m_2}\,T_{\mathrm{s,p},m_1,m_2}{}^{*}+T_{\mathrm{p,s},m_1,m_2}\,T_{\mathrm{p,p},m_1,m_2}{}^{*}\right]\\
&\eta 4^{[\mathrm{T}]}_{m_1,m_2} = \eta^{[\mathrm{T}]}_{m_1,m_2}\Big|_{A=1/\sqrt{2},B=-i/\sqrt{2}} =\\
&\quad \tfrac{1}{2}\left(\eta 1^{[\mathrm{T}]}_{m_1,m_2}+\eta 2^{[\mathrm{T}]}_{m_1,m_2}\right) - \frac{\mathrm{Re}\left[f^{[\mathrm{T}]}_{1,m_1,m_2}\right]}{f^{[\mathrm{Inc}]}_1}\mathrm{Im}\left[T_{\mathrm{s,s},m_1,m_2}\,T_{\mathrm{s,p},m_1,m_2}{}^{*}+T_{\mathrm{p,s},m_1,m_2}\,T_{\mathrm{p,p},m_1,m_2}{}^{*}\right]
\end{aligned}\right\} \tag{A.29}$$

$$\eta_{m_1,m_2}^{[\mathrm{T}]} = \frac{1}{|A|^2 + |B|^2} \begin{pmatrix} \eta 1_{m_1,m_2}^{[\mathrm{T}]} |A|^2 \\ +\eta 2_{m_1,m_2}^{[\mathrm{T}]} |B|^2 \\ +2\left(\eta 3_{m_1,m_2}^{[\mathrm{T}]} - \frac{1}{2}\left(\eta 1_{m_1,m_2}^{[\mathrm{T}]} + \eta 2_{m_1,m_2}^{[\mathrm{T}]}\right)\right) \mathrm{Re}\left[A B^*\right] \\ +2\left(\eta 4_{m_1,m_2}^{[\mathrm{T}]} - \frac{1}{2}\left(\eta 1_{m_1,m_2}^{[\mathrm{T}]} + \eta 2_{m_1,m_2}^{[\mathrm{T}]}\right)\right) \mathrm{Im}\left[A B^*\right] \end{pmatrix} \tag{A.30}$$

The incident field corresponding to amplitudes A and B at $\vec{x} = \hat{e}_1 b_1^{[L_1]}$ is

$$\vec{E}^{[\mathrm{Inc}]}[\hat{e}_1 b_1^{[L_1]}] = A\,\hat{s}^{[\mathrm{Inc}]} + B\,\hat{p}^{[\mathrm{Inc}]} \tag{A.31}$$

(from Eq's. 4.21 and A.20). The time-dependent, physical incident field at $\vec{x} = \hat{e}_1 b_1^{[L_1]}$ is

$$\begin{aligned} &\vec{E}^{[\text{physical, Inc}]}[\hat{e}_1 b_1^{[L_1]}, t] = \mathrm{Re}\left[\vec{E}^{[\mathrm{Inc}]}[\hat{e}_1 b_1^{[L_1]}] \exp[-i\,2\pi\,c\,t/\lambda]\right] \\ &= \mathrm{Re}\left[(A\,\hat{s}^{[\mathrm{Inc}]} + B\,\hat{p}^{[\mathrm{Inc}]}) \exp[-i\,2\pi\,c\,t/\lambda]\right] \\ &= (\mathrm{Re}[A]\,\hat{s}^{[\mathrm{Inc}]} + \mathrm{Re}[B]\,\hat{p}^{[\mathrm{Inc}]}) \cos[2\pi\,c\,t/\lambda] + (\mathrm{Im}[A]\,\hat{s}^{[\mathrm{Inc}]} + \mathrm{Im}[B]\,\hat{p}^{[\mathrm{Inc}]}) \sin[2\pi\,c\,t/\lambda] \end{aligned} \tag{A.32}$$

(cf. Eq. A.1). For example, with $A = 1/\sqrt{2}$, $B = -i/\sqrt{2}$ (the case for the $\eta 4$ efficiencies in Eq's. A.27 and A.29), the incident field is $\left(\hat{s}^{[\mathrm{Inc}]} \cos[2\pi\,c\,t/\lambda] - \hat{p}^{[\mathrm{Inc}]} \sin[2\pi\,c\,t/\lambda]\right)/\sqrt{2}$. The field transitions from $\hat{s}^{[\mathrm{Inc}]}/\sqrt{2}$ at $t = 0$, to $-\hat{p}^{[\mathrm{Inc}]}/\sqrt{2}$ after a quarter-period time delay. The vector triplet $\left(\vec{f}^{[\mathrm{Inc}]}\,\lambda/\sqrt{\varepsilon^{[\sup]}} \quad \hat{s}^{[\mathrm{Inc}]} \quad \hat{p}^{[\mathrm{Inc}]}\right)$ forms a right-handed coordinate basis set (Eq. 4.20), so the $\eta 4$ efficiencies correspond to left-handed circular polarization.

Appendix B. Computation of the field inside the grating

The electromagnetic field inside the grating is determined by applying Eq's. 8.1 and 8.2 where $x_1^{[0]}$ and $x_1^{[2]}$ are the x_1 coordinates at the bottom and top of the grating ($x_1^{[0]} = b_1^{[0]} - 0$, $x_1^{[2]} = b_1^{[L_1]} + 0$, Eq's. 3.1-3.3). $x_1^{[1]}$ is the x_1 level at which the field is to be determined, and Sa and Sb are the cumulative S matrices for the portions of the grating below and above $x_1^{[1]}$, respectively.

The incident field below the grating ($F^{[+]}[x_1^{[0]}]$) is zero, so Eq. 8.1 reduces to

$$\begin{pmatrix} F^{[+]}[x_1^{[1]}] \\ F^{[-]}[x_1^{[0]}] \end{pmatrix} = \begin{pmatrix} Sa^{[+-]} \\ Sa^{[--]} \end{pmatrix} F^{[-]}[x_1^{[1]}] \quad \left(F^{[+]}[x_1^{[0]}] = 0\right) \tag{B.1}$$

In principle, the transmitted field ($F^{[-]}[x_1^{[0]}]$) could be computed and used in Eq. B.1 to determine the internal field at $x_1^{[1]}$ ($F^{[-]}[x_1^{[1]}] = (Sa^{[--]})^{-1}\,F^{[-]}[x_1^{[0]}]$, $F^{[+]}[x_1^{[1]}] = Sa^{[+-]}\,F^{[-]}[x_1^{[1]}]$). However, this process is numerically unstable if, for example, the lower portion of the grating is opaque so that $Sa^{[--]}$ and $F^{[-]}[x_1^{[0]}]$ are both zero. This difficulty is avoided by determining $F^{[-]}[x_1^{[1]}]$ from Eq. 8.2,

$$F^{[-]}[x_1^{[1]}] = Sb^{[-+]}\,F^{[+]}[x_1^{[1]}] + Sb^{[--]}\,F^{[-]}[x_1^{[2]}] \tag{B.2}$$

The $F^{[-]}[x_1^{[2]}]$ term in Eq. B.2 represents the incident field, and the $F^{[+]}[x_1^{[1]}]$ term is determined by substituting Eq. B.2 in the first block row of Eq. B.1,

$$F^{[+]}[x_1^{[1]}] = (\mathbf{I} - Sa^{[+-]}\,Sb^{[-+]})^{-1}\,Sa^{[+-]}\,Sb^{[--]}\,F^{[-]}[x_1^{[2]}] \tag{B.3}$$

Thus, the internal field has the following form,

$$\begin{pmatrix} F^{[+]}[x_1^{[1]}] \\ F^{[-]}[x_1^{[1]}] \end{pmatrix} = \begin{pmatrix} S^{[+-]} \\ S^{[--]} \end{pmatrix} F^{[-]}[x_1^{[2]}] \tag{B.4}$$

where

$$S^{[+-]} = (\mathbf{I} - Sa^{[+-]}\,Sb^{[-+]})^{-1}\,Sa^{[+-]}\,Sb^{[--]} \tag{B.5}$$

$$S^{[--]} = Sb^{[-+]}\,S^{[+-]} + Sb^{[--]} \tag{B.6}$$

The computation procedure defined by Eq's. B.5 and B.6 depends only on $Sa^{[+-]}$, $Sb^{[-+]}$, and $Sb^{[--]}$. $Sa^{[+-]}$ is computed efficiently from Eq. 8.8 using bottom-up stacking from $x_1^{[0]}$ to $x_1^{[1]}$. In the context of Eq. 8.8 Sa represents the S matrix of a multilayer grating stack, Sb is the S matrix of an individual layer added to the top of the stack, and the cumulative S matrix S on the left side of the equation corresponds to Sa in Eq. B.5. The S matrix quadrant $S^{[+-]}$ in Eq. 8.8 ($Sa^{[+-]}$ in Eq. B.5) only depends on the $Sa^{[+-]}$ quadrant of Sa on the right side of the equation, so only this quadrant need be computed for the internal field calculation. However, $S^{[--]}$ is also needed for the transmitted field calculation (Eq. 7.3), so Eq. 8.8 is typically applied to calculate both $S^{[+-]}$ and $S^{[--]}$. These quadrants depend only on the Sa quadrants $Sa^{[+-]}$ and $Sa^{[--]}$, and they share the common subexpression $(\boldsymbol{I} - Sb^{[-+]}\,Sa^{[+-]})^{-1}\,Sb^{[--]}$ in Eq. 8.8.

The $Sb^{[-+]}$ and $Sb^{[--]}$ matrices in Eq's. B.5 and B.6 are computed efficiently from Eq. 8.11 using top-down stacking from $x_1^{[2]}$ to $x_1^{[1]}$. In the context of Eq. 8.11 Sb represents the S matrix of a multilayer grating stack, Sa is the S matrix of an individual layer added to the bottom of the stack, and the cumulative matrix S on the left side of the equation corresponds to Sb in Eq's. B.5 and B.6. The cumulative S matrix quadrants $S^{[-+]}$ and $S^{[--]}$ in Eq. 8.11 ($Sb^{[-+]}$ and $Sb^{[--]}$ in Eq's. B.5 and B.6) depend only on the $Sb^{[-+]}$ and $Sb^{[--]}$ quadrants of Sb, and they contain a common subexpression $Sa^{[--]}\,(\boldsymbol{I} - Sb^{[-+]}\,Sa^{[+-]})^{-1}$.

After determining $F^{[+]}[x_1^{[1]}]$ and $F^{[-]}[x_1^{[1]}]$, the grating-tangential electromagnetic fields (up/down $\hat{s}$ projections) are determined from Eq. 9.2. If the grating is homogeneous at $x_1 = x_1^{[1]}$, the total tangential electromagnetic field is then determined by applying Eq's. 6.52-6.55, and the grating-normal fields are obtained from Eq's. 6.44, 6.45, 6.56, and 6.57. If the grating is inhomogeneous at $x_1 = x_1^{[1]}$, then $F^{[+]}[x_1^{[1]}]$ and $F^{[-]}[x_1^{[1]}]$ represent up/down fields in the fictitious medium and the derivations in Section 13 apply. Eq's. 13.80-13.83, which are equivalent to Eq's. 6.52-6.55, determine the tangential field projections. (These equations are applied in the fictitious medium, but the total field's tangential projections are continuous across the fictitious layer boundaries.) The grating-normal field projections ($ffH_1^{[j]}$ and $ffE_1^{[j]}$) are determined by Eq's. 13.62 and 13.68. ($ffH_1^{[j]}$ is continuous across boundary surfaces, and Eq. 13.68 defines $ffE_1^{[j]}$ in the optical medium defined by Eq. 13.1 – not in the fictitious medium.) This procedure yields the Fourier components of the total internal electromagnetic field, including both incident and scattered fields. (The incident field in the superstrate must be subtracted from the total field to get only the reflected field.)

Appendix C. Fourier expansion of the permittivity

The following description of the permittivity distribution in stratum l_1 uses a coordinate orientation with $\hat{e}_2$ parallel to $\vec{f}_1^{[s,l_1]}$ (Eq's. 13.18). The stratum stripes for a biperiodic stratum are parallel to the period vector $\vec{d}_2^{[s,l_1]}$ (e.g., see Figure 3), and $\vec{d}_2^{[s,l_1]}$ is orthogonal to $\vec{f}_1^{[s,l_1]}$ (Eq. 3.32), so the stripes are parallel to $\hat{e}_3$,

$$d_{2,2}^{[s,l_1]} = 0; \quad \vec{d}_2^{[s,l_1]} = \hat{e}_3\, d_{3,2}^{[s,l_1]} \quad \text{(biperiodic)} \tag{C.1}$$

Figure 10 illustrates the relationship between the stratum's period vectors ($\vec{d}_1^{[s,l_1]}$, $\vec{d}_2^{[s,l_1]}$), its basis frequency vectors ($\vec{f}_1^{[s,l_1]}$, $\vec{f}_2^{[s,l_1]}$), and the coordinate bases $\hat{e}_2$ and $\hat{e}_3$. The period and frequency vectors are biorthogonal: $\vec{f}_1^{[s,l_1]}\bullet\vec{d}_1^{[s,l_1]} = 1$, $\vec{f}_1^{[s,l_1]}\bullet\vec{d}_2^{[s,l_1]} = 0$, $\vec{f}_2^{[s,l_1]}\bullet\vec{d}_1^{[s,l_1]} = 0$, $\vec{f}_2^{[s,l_1]}\bullet\vec{d}_2^{[s,l_1]} = 1$ (cf. Eq's. 3.15-3.16, 3.30-3.32).

For a uniperiodic stratum $\vec{f}_1^{[s,l_1]}$ is parallel to $\vec{d}_1^{[s,l_1]}$ (Eq. 3.25), and $\vec{f}_1^{[s,l_1]}$ is also parallel to $\hat{e}_2$ (Eq's. 13.18); hence $\vec{d}_1^{[s,l_1]}$ is parallel to $\hat{e}_2$,

$$d_{3,1}^{[s,l_1]} = 0; \quad \vec{d}_1^{[s,l_1]} = \hat{e}_2\, d_{2,1}^{[s,l_1]} \quad \text{(uniperiodic)} \tag{C.2}$$

In this case, $\vec{d}_1^{[s,l_1]}$ is orthogonal to the stripe orientation, so the stripes are also parallel to $\hat{e}_3$ for the uniperiodic case.

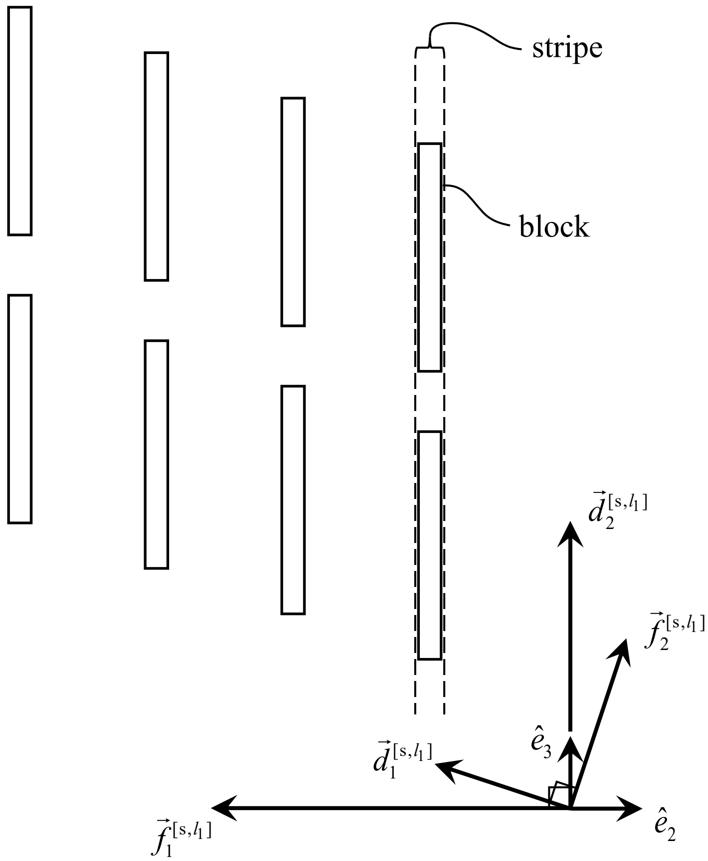

Figure 10. Stratum period vectors, basis frequency vectors, and coordinate bases.

Within stratum l_1 the grating permittivity is independent of x_1, and in the case of a homogeneous stratum is constant; hence the permittivity has the functional form

$$\varepsilon[\vec{x}] = \begin{cases} \varepsilon 1^{[l_1]}[x_2, x_3] & \text{(periodic stratum)} \\ \varepsilon 1^{[l_1]} & \text{(homogeneous stratum)} \end{cases} \quad \text{for } b_1^{[l_1-1]} < x_1 < b_1^{[l_1]}, l_1 = 1, \ldots L_1 \tag{C.3}$$

The stratum boundaries are at $x_1 = b_1^{[0]}, b_1^{[1]}, \ldots, b_1^{[L_1]}$, where L_1 is the number of strata (Eq's. 3.1 and 3.10).

A periodic stratum is partitioned into stripes. The permittivity within each stripe is independent of x_2, and in the case of a uniperiodic stratum is constant,

$$\varepsilon 1^{[l_1]}[x_2, x_3] = \begin{cases} \varepsilon 2^{[l_1,l_2]}[x_3] & \text{(biperiodic stratum)} \\ \varepsilon 2^{[l_1,l_2]} & \text{(uniperiodic stratum)} \end{cases} \quad \text{for } x_2 \text{ between } b_2^{[l_1,l_2-1]} \text{ and } b_2^{[l_1,l_2]} \tag{C.4}$$

The stripe boundaries are at $x_2 = \ldots, b_2^{[l_1,0]}, b_2^{[l_1,1]}, \ldots$. (The boundary positions $b_2^{[l_1,0]}, b_2^{[l_1,1]}, \ldots$ may be sorted in either increasing or decreasing order.)

Each stripe of a biperiodic stratum is partitioned into homogeneous blocks,

$$\varepsilon 2^{[l_1,l_2]}[x_3] = \varepsilon 3^{[l_1,l_2,l_3]} \quad \text{for } x_3 \text{ between } b_3^{[l_1,l_2,l_3-1]} \text{ and } b_3^{[l_1,l_2,l_3]} \tag{C.5}$$

The block boundaries are at $x_3 = \ldots, b_3^{[l_1,l_2,0]}, b_3^{[l_1,l_2,1]}, \ldots$ (cf. Eq. 3.34).

The number of stripes per period in stratum l_1 is $L_2[l_1]$, and the stripe boundaries $b_2^{[l_1,l_2]}$ are defined in terms of the dimensionless parameters $c_1^{[l_1,l_2]}$, which satisfy relations 3.35 and 3.36:

$$b_2^{[l_1,l_2]} = c_1^{[l_1,l_2]}\, d_{2,1}^{[\mathrm{s},l_1]}, \quad l_2 = 1,\ldots,L_2[l_1] \tag{C.6}$$

$$b_2^{[l_1,l_2+L_2[l_1]]} = b_2^{[l_1,l_2]} + d_{2,1}^{[\mathrm{s},l_1]} \tag{C.7}$$

The number of blocks per period in stripe l_2 of stratum l_1 is $L_3[l_1,l_2]$, and the block boundaries $b_3^{[l_1,l_2,l_3]}$ within each inhomogeneous stripe are defined in terms of the dimensionless parameters $c_2^{[l_1,l_2,l_3]}$, which satisfy relations 3.37-3.39:

$$b_3^{[l_1,l_2,l_3]} = c_1^{[l_1,l_2]}\, d_{3,1}^{[\mathrm{s},l_1]} + c_2^{[l_1,l_2,l_3]}\, d_{3,2}^{[\mathrm{s},l_1]}, \quad l_2 = 1,\ldots,L_2[l_1], \quad l_3 = 1,\ldots,L_3[l_1,l_2] \tag{C.8}$$

$$b_3^{[l_1,l_2+L_2[l_1],l_3]} = b_3^{[l_1,l_2,l_3]} + d_{3,1}^{[\mathrm{s},l_1]} \tag{C.9}$$

$$b_3^{[l_1,l_2,l_3+L_3[l_1,l_2]]} = b_3^{[l_1,l_2,l_3]} + d_{3,2}^{[\mathrm{s},l_1]} \tag{C.10}$$

A biperiodic stratum is periodic in x_3,

$$\varepsilon 1^{[l_1]}[x_2, x_3 + d_{3,2}^{[\mathrm{s},l_1]}] = \varepsilon 1^{[l_1]}[x_2, x_3] \tag{C.11}$$

(from Eq's. 3.18 and C.1); hence the permittivity has a Fourier expansion of the form in Eq. 13.19,

$$\varepsilon 1^{[l_1]}[x_2, x_3] = \sum_{n_2} f\varepsilon 1_{n_2}^{[l_1]}[x_2] \exp[i\, 2\pi\, n_2\, f_{3,2}^{[\mathrm{s},l_1]}\, x_3] \tag{C.12}$$

where

$$f_{3,2}^{[\mathrm{s},l_1]} = 1 / d_{3,2}^{[\mathrm{s},l_1]} \tag{C.13}$$

(Eq's. 3.32, C.1). Eq. C.4 implies that $f\varepsilon 1_{n_2}^{[l_1]}[x_2]$ is of the form

$$f\varepsilon 1_{n_2}^{[l_1]}[x_2] = f\varepsilon 2_{n_2}^{[l_1,l_2]} \quad \text{for } x_2 \text{ between } b_2^{[l_1,l_2-1]} \text{ and } b_2^{[l_1,l_2]} \tag{C.14}$$

where

$$\varepsilon 2^{[l_1,l_2]}[x_3] = \sum_{n_2} f\varepsilon 2_{n_2}^{[l_1,l_2]} \exp[i\,2\pi\, n_2\, f_{3,2}^{[\mathrm{s},l_1]}\, x_3] \tag{C.15}$$

Eq. C.5 is substituted on the left side of Eq. C.15, and the Fourier inversion formula is applied to determine the Fourier coefficients $f\varepsilon 2_{n_2}^{[l_1,l_2]}$,

$$\begin{aligned} f\varepsilon 2_{n_2}^{[l_1,l_2]} &= f_{3,2}^{[\mathrm{s},l_1]} \int_{b_3^{[l_1,l_2,0]}}^{b_3^{[l_1,l_2,L_3[l_1,l_2]]}} \varepsilon 2^{[l_1,l_2]}[x_3] \exp[-i\,2\pi\, n_2\, f_{3,2}^{[\mathrm{s},l_1]}\, x_3]\, dx_3 \\ &= \sum_{l_3=1}^{L_3[l_1,l_2]} \left(\begin{array}{l} \varepsilon 3^{[l_1,l_2,l_3]}\, f_{3,2}^{[\mathrm{s},l_1]}\, (b_3^{[l_1,l_2,l_3]} - b_3^{[l_1,l_2,l_3-1]}) \cdot \\ \quad \mathrm{sinc}[\pi\, n_2\, f_{3,2}^{[\mathrm{s},l_1]}\, (b_3^{[l_1,l_2,l_3]} - b_3^{[l_1,l_2,l_3-1]})] \cdot \\ \quad \exp[-i\,\pi\, n_2\, f_{3,2}^{[\mathrm{s},l_1]}\, (b_3^{[l_1,l_2,l_3]} + b_3^{[l_1,l_2,l_3-1]})] \end{array} \right) \end{aligned} \tag{C.16}$$

where the sinc function is defined as[5]

$$\mathrm{sinc}[x] = \begin{cases} \sin[x]/x & \text{if } x \neq 0 \\ 1 & \text{if } x = 0 \end{cases} \tag{C.17}$$

For a uniperiodic stratum $\varepsilon 2^{[l_1,l_2]}[x_3]$ is constant (Eq. C.4) and Eq. C.15 is simply

$$\varepsilon 2^{[l_1,l_2]}[x_3] = f\varepsilon 2_0^{[l_1,l_2]} \quad \text{(uniperiodic)} \tag{C.18}$$

Eq. C.16 is recast in a form that is independent of the $\hat{e}_2$, $\hat{e}_3$ coordinate orientation by using the following identity (from Eq's. C.8, C.1, and 3.32),

[5] For numerical applications the sinc function is implemented as follows to avoid excessive round-off errors for small x:

$$\mathrm{sinc}[x] = \begin{cases} \sin[x]/x & \text{if } x^2 \geq 6\,\delta \\ 1 & \text{if } x^2 < 6\,\delta \end{cases}$$

where δ is the numeric precision (i.e., the smallest value such that 1 and $1+\delta$ are numerically distinguishable, $\delta = 2^{-52}$ for double-precision).

$$
\begin{aligned}
f_{3,2}^{[s,l_1]}\, b_3^{[l_1,l_2,l_3]} &= (\vec{f}_2^{[s,l_1]} \bullet \hat{e}_3)\,((c_1^{[l_1,l_2]}\, \vec{d}_1^{[s,l_1]} + c_2^{[l_1,l_2,l_3]}\, \vec{d}_2^{[s,l_1]}) \bullet \hat{e}_3) \\
&= \frac{(\vec{f}_2^{[s,l_1]} \bullet \vec{d}_2^{[s,l_1]})\,((c_1^{[l_1,l_2]}\, \vec{d}_1^{[s,l_1]} + c_2^{[l_1,l_2,l_3]}\, \vec{d}_2^{[s,l_1]}) \bullet \vec{d}_2^{[s,l_1]})}{\vec{d}_2^{[s,l_1]} \bullet \vec{d}_2^{[s,l_1]}} \\
&= c_1^{[l_1,l_2]}\, \frac{\vec{d}_1^{[s,l_1]} \bullet \vec{d}_2^{[s,l_1]}}{\vec{d}_2^{[s,l_1]} \bullet \vec{d}_2^{[s,l_1]}} + c_2^{[l_1,l_2,l_3]}
\end{aligned}
\tag{C.19}
$$

Define

$$
\gamma^{[l_1]} = \frac{\vec{d}_1^{[s,l_1]} \bullet \vec{d}_2^{[s,l_1]}}{\vec{d}_2^{[s,l_1]} \bullet \vec{d}_2^{[s,l_1]}}
\tag{C.20}
$$

(For a uniperiodic stratum $\vec{d}_2^{[s,l_1]}$ is implicitly of infinite magnitude and perpendicular to $\vec{d}_1^{[s,l_1]}$, so $\gamma^{[l_1]}$ is zero.) Eq. C.16 simplifies to

$$
f\varepsilon 2_{n_2}^{[l_1,l_2]} = \sum_{l_3=1}^{L_3[l_1,l_2]} \left(\begin{array}{l} \varepsilon 3^{[l_1,l_2,l_3]}\,(c_2^{[l_1,l_2,l_3]} - c_2^{[l_1,l_2,l_3-1]}) \cdot \\ \quad \operatorname{sinc}[\pi\, n_2\, (c_2^{[l_1,l_2,l_3]} - c_2^{[l_1,l_2,l_3-1]})] \cdot \\ \quad \exp[-i\,\pi\, n_2\, (c_2^{[l_1,l_2,l_3]} + c_2^{[l_1,l_2,l_3-1]} + 2\, c_1^{[l_1,l_2]}\, \gamma^{[l_1]})] \end{array} \right)
\tag{C.21}
$$

The periodicity condition, Eq. 3.17, or equivalently Eq. 13.45, is applied to Eq. C.12 to obtain the x_2-periodicity condition, Eq. 13.47, for $f\varepsilon 1$,

$$
\begin{aligned}
& f\varepsilon 1_{n_2}^{[l_1]}[x_2 + 1/f_{2,1}^{[s,l_1]}] \exp[-i\,2\pi\, n_2\, f_{2,2}^{[s,l_1]}\,(x_2 + 1/f_{2,1}^{[s,l_1]})] = \\
& \quad f\varepsilon 1_{n_2}^{[l_1]}[x_2] \exp[-i\,2\pi\, n_2\, f_{2,2}^{[s,l_1]}\, x_2]
\end{aligned}
\tag{C.22}
$$

where

$$
f_{2,1}^{[s,l_1]} = 1/d_{2,1}^{[s,l_1]}
\tag{C.23}
$$

$$
f_{2,2}^{[s,l_1]} = -d_{3,1}^{[s,l_1]} / (d_{2,1}^{[s,l_1]}\, d_{3,2}^{[s,l_1]})
\tag{C.24}
$$

(from Eq's. 13.18 and 3.32). Figure 10 illustrates the geometric relationships defined by Eq's. 13.18, C.1, C.13, C.23, and C.24. The Fourier expansion for $f\varepsilon 1$, Eq. 13.20, is obtained from Eq. C.22,

$$
f\varepsilon 1_{n_2}^{[l_1]}[x_2] = \sum_{n_1} ff\varepsilon 1_{n_1,n_2}^{[l_1]} \exp[i\,2\pi\,(n_1\, f_{2,1}^{[s,l_1]} + n_2\, f_{2,2}^{[s,l_1]})\, x_2]
\tag{C.25}
$$

Substituting from Eq. C.14, the Fourier coefficients $ff\varepsilon1_{n_1,n_2}^{[l_1]}$ are obtained via the Fourier inversion formula,

$$\begin{aligned} ff\varepsilon1_{n_1,n_2}^{[l_1]} &= f_{2,1}^{[s,l_1]} \int_{b_2^{[l_1,0]}}^{b_2^{[l_1,L_2[l_1]]}} f\varepsilon1_{n_2}^{[l_1]}[x_2]\exp[-i\,2\pi\,(n_1\, f_{2,1}^{[s,l_1]} + n_2\, f_{2,2}^{[s,l_1]})\,x_2]\,dx_2 \\ &= \sum_{l_2=1}^{L_2[l_1]} \left(\begin{array}{l} f\varepsilon2_{n_2}^{[l_1,l_2]}\, f_{2,1}^{[s,l_1]}\,(b_2^{[l_1,l_2]} - b_2^{[l_1,l_2-1]}) \cdot \\ \quad \mathrm{sinc}[\pi\,(n_1\, f_{2,1}^{[s,l_1]} + n_2\, f_{2,2}^{[s,l_1]})\,(b_2^{[l_1,l_2]} - b_2^{[l_1,l_2-1]})] \cdot \\ \quad \exp[-i\,\pi\,(n_1\, f_{2,1}^{[s,l_1]} + n_2\, f_{2,2}^{[s,l_1]})\,(b_2^{[l_1,l_2]} + b_2^{[l_1,l_2-1]})] \end{array} \right) \end{aligned} \tag{C.26}$$

Eq. C.26 is recast in a form that is independent of the $\hat{e}_2$, $\hat{e}_3$ coordinate orientation by using the following identities,

$$f_{2,1}^{[s,l_1]}\, b_2^{[l_1,l_2]} = (\vec{f}_1^{[s,l_1]} \bullet \hat{e}_2)\,(c_1^{[l_1,l_2]}\, \vec{d}_1^{[s,l_1]} \bullet \hat{e}_2) = c_1^{[l_1,l_2]}\, \vec{d}_1^{[s,l_1]} \bullet \vec{f}_1^{[s,l_1]} = c_1^{[l_1,l_2]} \tag{C.27}$$

$$\begin{aligned} f_{2,2}^{[s,l_1]}\, b_2^{[l_1,l_2]} &= (\vec{f}_2^{[s,l_1]} \bullet \hat{e}_2)\,(c_1^{[l_1,l_2]}\, \vec{d}_1^{[s,l_1]} \bullet \hat{e}_2) = \frac{(\vec{f}_2^{[s,l_1]} \bullet \vec{f}_1^{[s,l_1]})\,(c_1^{[l_1,l_2]}\, \vec{d}_1^{[s,l_1]} \bullet \vec{f}_1^{[s,l_1]})}{\vec{f}_1^{[s,l_1]} \bullet \vec{f}_1^{[s,l_1]}} \\ &= c_1^{[l_1,l_2]}\, \frac{\vec{f}_2^{[s,l_1]} \bullet \vec{f}_1^{[s,l_1]}}{\vec{f}_1^{[s,l_1]} \bullet \vec{f}_1^{[s,l_1]}} = -c_1^{[l_1,l_2]}\, \frac{\vec{d}_1^{[s,l_1]} \bullet \vec{d}_2^{[s,l_1]}}{\vec{d}_2^{[s,l_1]} \bullet \vec{d}_2^{[s,l_1]}} = -c_1^{[l_1,l_2]}\, \gamma^{[l_1]} \end{aligned} \tag{C.28}$$

(from Eq's. C.6, 13.18, 3.32, and C.20). With these substitutions, Eq. C.26 simplifies to

$$ff\varepsilon1_{n_1,n_2}^{[l_1]} = \sum_{l_2=1}^{L_2[l_1]} \left(\begin{array}{l} f\varepsilon2_{n_2}^{[l_1,l_2]}\,(c_1^{[l_1,l_2]} - c_1^{[l_1,l_2-1]}) \cdot \\ \quad \mathrm{sinc}[\pi\,(n_1 - n_2\,\gamma^{[l_1]})\,(c_1^{[l_1,l_2]} - c_1^{[l_1,l_2-1]})] \cdot \\ \quad \exp[-i\,\pi\,(n_1 - n_2\,\gamma^{[l_1]})\,(c_1^{[l_1,l_2]} + c_1^{[l_1,l_2-1]})] \end{array} \right) \tag{C.29}$$

The Toeplitz matrix in Eq. 13.58 evaluates to

$$\begin{aligned} &tt\varepsilon1_{(n_1,n_2),(n_1',n_2')}^{[l_1,j]} = \sum_{l_2=1}^{L_2[l_1]} \left(\begin{array}{l} f\varepsilon2_{n_2-n_2'}^{[l_1,l_2]}\,(c_1^{[l_1,l_2]} - c_1^{[l_1,l_2-1]}) \cdot \\ \quad \mathrm{sinc}[\pi\,(n_1 - n_1' - (n_2 - n_2')\,\gamma^{[l_1]})\,(c_1^{[l_1,l_2]} - c_1^{[l_1,l_2-1]})] \cdot \\ \quad \exp[-i\,\pi\,(n_1 - n_1' - (n_2 - n_2')\,\gamma^{[l_1]})\,(c_1^{[l_1,l_2]} + c_1^{[l_1,l_2-1]})] \end{array} \right), \\ &\quad (n_1,n_2),\,(n_1',n_2') \in \mathcal{N}^{[j]} \end{aligned} \tag{C.30}$$

The Toeplitz matrix $t\varepsilon1$ (Eq. 13.39) has the following form (from Eq. C.14),

$$t\varepsilon1_{n_2,n_2'}^{[l_1]}[x_2] = f\varepsilon1_{n_2-n_2'}^{[l_1]}[x_2] = t\varepsilon2_{n_2,n_2'}^{[l_1,l_2]} \quad \text{for } x_2 \text{ between } b_2^{[l_1,l_2-1]} \text{ and } b_2^{[l_1,l_2]} \tag{C.31}$$

where

$$t\varepsilon 2^{[l_1,l_2]}_{n_2,n'_2} = f\varepsilon 2^{[l_1,l_2]}_{n_2-n'_2} \tag{C.32}$$

The truncated $t\varepsilon 1^{[l_1]}$ and $t\varepsilon 2^{[l_1,l_2]}$ matrices, limited to $n_2, n'_2 \in \boldsymbol{\mathcal{N}}_2^{[j]}$, are denoted as $t\varepsilon 1^{[l_1,j]}$ and $t\varepsilon 2^{[l_1,l_2,j]}$. The reciprocal of $t\varepsilon 1^{[l_1,j]}$, denoted as $rt\varepsilon 1^{[l_1,j]}$ (Eq. 13.41), has the following form,

$$rt\varepsilon 1^{[l_1,j]}_{n_2,n'_2}[x_2] = rt\varepsilon 2^{[l_1,l_2,j]}_{n_2,n'_2} \quad \text{for } x_2 \text{ between } b_2^{[l_1,l_2-1]} \text{ and } b_2^{[l_1,l_2]} \tag{C.33}$$

where

$$rt\varepsilon 2^{[l_1,l_2,j]} = (t\varepsilon 2^{[l_1,l_2,j]})^{-1} \tag{C.34}$$

$rt\varepsilon 1^{[l_1,j]}$ is represented by Fourier expansion 13.50,

$$rt\varepsilon 1^{[l_1,j]}_{n_2,n'_2}[x_2] = \sum_{n_1} frt\varepsilon 1^{[l_1,j]}_{n_1,n_2,n'_2} \exp[i\,2\pi\,(n_1\, f_{2,1}^{[\mathrm{s},l_1]} + (n_2 - n'_2)\, f_{2,2}^{[\mathrm{s},l_1]})\, x_2] \tag{C.35}$$

where the Fourier coefficients are determined from Eq. C.33 via the Fourier inversion formula,

$$\begin{aligned} frt\varepsilon 1^{[l_1,j]}_{n_1,n_2,n'_2} &= f_{2,1}^{[\mathrm{s},l_1]} \int_{b_2^{[l_1,0]}}^{b_2^{[l_1,L_2[l_1]]}} rt\varepsilon 1^{[l_1,j]}_{n_2,n'_2}[x_2] \exp[-i\,2\pi\,(n_1\, f_{2,1}^{[\mathrm{s},l_1]} + (n_2 - n'_2)\, f_{2,2}^{[\mathrm{s},l_1]})\, x_2]\, dx_2 \\ &= \sum_{l_2=1}^{L_2[l_1]} \left(\begin{aligned} & rt\varepsilon 2^{[l_1,l_2,j]}_{n_2,n'_2}\, f_{2,1}^{[\mathrm{s},l_1]}\, (b_2^{[l_1,l_2]} - b_2^{[l_1,l_2-1]}) \cdot \\ & \quad \mathrm{sinc}[\pi\,(n_1\, f_{2,1}^{[\mathrm{s},l_1]} + (n_2 - n'_2)\, f_{2,2}^{[\mathrm{s},l_1]})\,(b_2^{[l_1,l_2]} - b_2^{[l_1,l_2-1]})] \cdot \\ & \quad \exp[-i\,\pi\,(n_1\, f_{2,1}^{[\mathrm{s},l_1]} + (n_2 - n'_2)\, f_{2,2}^{[\mathrm{s},l_1]})\,(b_2^{[l_1,l_2]} + b_2^{[l_1,l_2-1]})] \end{aligned} \right) \end{aligned} \tag{C.36}$$

With substitution from Eq's. C.27 and C.28, this simplifies to

$$frt\varepsilon 1^{[l_1,j]}_{n_1,n_2,n'_2} = \sum_{l_2=1}^{L_2[l_1]} \left(\begin{aligned} & rt\varepsilon 2^{[l_1,l_2,j]}_{n_2,n'_2}\, (c_1^{[l_1,l_2]} - c_1^{[l_1,l_2-1]}) \cdot \\ & \quad \mathrm{sinc}[\pi\,(n_1 - (n_2 - n'_2)\,\gamma^{[l_1]})\,(c_1^{[l_1,l_2]} - c_1^{[l_1,l_2-1]})] \cdot \\ & \quad \exp[-i\,\pi\,(n_1 - (n_2 - n'_2)\,\gamma^{[l_1]})\,(c_1^{[l_1,l_2]} + c_1^{[l_1,l_2-1]})] \end{aligned} \right) \tag{C.37}$$

Eq. 13.59 evaluates to

$$trt\varepsilon 1^{[l_1,j]}_{(n_1,n_2),(n'_1,n'_2)} = \sum_{l_2=1}^{L_2[l_1]} \left(\begin{aligned} & rt\varepsilon 2^{[l_1,l_2,j]}_{n_2,n'_2}\, (c_1^{[l_1,l_2]} - c_1^{[l_1,l_2-1]}) \cdot \\ & \quad \mathrm{sinc}[\pi\,(n_1 - n'_1 - (n_2 - n'_2)\,\gamma^{[l_1]})\,(c_1^{[l_1,l_2]} - c_1^{[l_1,l_2-1]})] \cdot \\ & \quad \exp[-i\,\pi\,(n_1 - n'_1 - (n_2 - n'_2)\,\gamma^{[l_1]})\,(c_1^{[l_1,l_2]} + c_1^{[l_1,l_2-1]})] \end{aligned} \right) \tag{C.38}$$

The reciprocal permittivity is denoted as "$r\varepsilon$",

$$r\varepsilon[\vec{x}] = \frac{1}{\varepsilon[\vec{x}]} \tag{C.39}$$

Most of the above equations involving ε (Eq's. C.3-C.5, C.11, C.12, C.14-C.16, C.18, C.21, C.22, C.31-C.38) also apply with the symbolic substitution of "$r\varepsilon$" for "ε" (cf. Eq's. 13.32 and 13.51).

Appendix D. Padé approximation to coupled-wave equations

Eq. 13.104 is an approximate solution of the coupled wave equations represented by Eq. 13.98, based on a Padé approximation to the exponential matrix (Ref. [6]). The exact solution of Eq. 13.98 is

$$F[x_1^{[0]} + \Delta x_1] = \exp\left[\Delta x_1\, D\right] F[x_1^{[0]}] \tag{D.1}$$

where

$$D = \begin{pmatrix} \mathbf{0} & DEH \\ DHE & \mathbf{0} \end{pmatrix} \tag{D.2}$$

$$F[x_1] = \begin{pmatrix} F^{[\mathrm{E}]}[x_1] \\ F^{[\mathrm{H}]}[x_1] \end{pmatrix} \tag{D.3}$$

(The "j" labels on $DEH^{[j]}$, $DHE^{[j]}$, $F^{[\mathrm{E},j]}[x_1]$, and $F^{[\mathrm{H},j]}[x_1]$ in Eq. 13.98 are omitted here for brevity.) Eq. 14.16 (the polarization-decoupled form of Eq. 13.98) has a similar solution.

The Padé approximation is

$$\exp[2\,h\,D] \cong \Phi[2\,h\,D] = P[-h\,D]^{-1}\, P[h\,D] \tag{D.4}$$

where

$$h = \tfrac{1}{2}\Delta x_1 \tag{D.5}$$

(from Eq. 14 in Ref. 6). P is a polynomial function,

$$P[X] = \sum_{j=0}^{n} c_j\, X^j \tag{D.6}$$

where n is the Padé order and

$$c_j = \frac{n!(2n-j)!2^j}{(2n)!\,j!(n-j)!} = \frac{1}{j!}\prod_{k=0}^{j-1}\left(1-\frac{k}{2n-k}\right) \tag{D.7}$$

Denoting the P function for order n as P_n, the polynomial coefficients c_j for P_n can be calculated from the recursion formula,

$$\left.\begin{array}{l} P_0[X] = \mathbf{I}, \\ P_1[X] = \mathbf{I} + X, \\ P_{n+1}[X] = P_n[X] + \dfrac{X^2}{4n^2-1} P_{n-1}[X] \end{array}\right\} \tag{D.8}$$

(from Eq's. 11 and 12 in Ref. 6; $\mathbf{I}$ is an identity matrix).

Eq. D.6 can be efficiently implemented by taking advantage of the block-anti-diagonal structure of matrix D. The D powers have the form

$$D^{2j+1} = \begin{pmatrix} \mathbf{0} & DD^j\ DEH \\ DHE\ DD^j & \mathbf{0} \end{pmatrix}, \quad D^{2j+2} = \begin{pmatrix} DD^{j+1} & \mathbf{0} \\ \mathbf{0} & DHE\ DD^j\ DEH \end{pmatrix} \tag{D.9}$$

where

$$DD = DEH\ DHE \tag{D.10}$$

$P[h\,D]$ has the form

$$P[h\,D] = \begin{pmatrix} P^{[\mathrm{E,E}]}[h\,D] & P^{[\mathrm{E,H}]}[h\,D] \\ P^{[\mathrm{H,E}]}[h\,D] & P^{[\mathrm{H,H}]}[h\,D] \end{pmatrix} = \begin{pmatrix} \mathbf{I} + h^2\ DD\,U[h^2\ DD] & h\,V[h^2\ DD]\,DEH \\ h\,DHE\ V[h^2\ DD] & \mathbf{I} + h^2\ DHE\ U[h^2\ DD]\,DEH \end{pmatrix} \tag{D.11}$$

where

$$U[X] = \sum_{j=0}^{\mathrm{floor}[n/2]-1} c_{2j+2}\,X^j, \quad V[X] = \sum_{j=0}^{\mathrm{floor}[(n-1)/2]} c_{2j+1}\,X^j \tag{D.12}$$

An alternative, equivalent formulation of Eq's. D.9 and D.11 is

$$D^{2j+1} = \begin{pmatrix} \mathbf{0} & DEH\ DD'^j \\ DD'^j\ DHE & \mathbf{0} \end{pmatrix}, \quad D^{2j+2} = \begin{pmatrix} DEH\ DD'^j\ DHE & \mathbf{0} \\ \mathbf{0} & DD'^{j+1} \end{pmatrix} \tag{D.13}$$

$$P[h\,D] = \begin{pmatrix} P^{[\mathrm{E,E}]}[h\,D] & P^{[\mathrm{E,H}]}[h\,D] \\ P^{[\mathrm{H,E}]}[h\,D] & P^{[\mathrm{H,H}]}[h\,D] \end{pmatrix} = \begin{pmatrix} \mathbf{I} + h^2\,DEH\,U[h^2\,DD']\,DHE & h\,DEH\,V[h^2\,DD'] \\ h\,V[h^2\,DD']\,DHE & \mathbf{I} + h^2\,DD'\,U[h^2\,DD'] \end{pmatrix} \tag{D.14}$$

where

$$DD' = DHE\,DEH \tag{D.15}$$

The Padé order n is restricted to being even because an odd order could be incremented without increasing the number of powers X^j in Eq's. D.12,

$$n = 2\,m > 0 \tag{D.16}$$

$$U[X] = \sum_{j=0}^{m-1} c_{2\,j+2}\,X^j\,, \quad V[X] = \sum_{j=0}^{m-1} c_{2\,j+1}\,X^j \tag{D.17}$$

For $m > 1$ the number of matrix multiplies needed to calculate $P[h\,D]$ is $m+4$ (including the one multiply for DD in Eq. D.10, plus $m-2$ multiplies to calculate the powers DD^j in Eq's. D.17, and 5 multiplies in Eq. D.11).

Eq. D.11 implies the following identity,

$$P[-h\,D] = \begin{pmatrix} P^{[\mathrm{E,E}]}[-h\,D] & P^{[\mathrm{E,H}]}[-h\,D] \\ P^{[\mathrm{H,E}]}[-h\,D] & P^{[\mathrm{H,H}]}[-h\,D] \end{pmatrix} = \begin{pmatrix} P^{[\mathrm{E,E}]}[h\,D] & -P^{[\mathrm{E,H}]}[h\,D] \\ -P^{[\mathrm{H,E}]}[h\,D] & P^{[\mathrm{H,H}]}[h\,D] \end{pmatrix} \tag{D.18}$$

It follows from Eq's. D.1-D.5 and D.18 that

$$\begin{gathered} \begin{pmatrix} P^{[\mathrm{E,E}]}[\tfrac{1}{2}\,\Delta x_1\,D] & -P^{[\mathrm{E,H}]}[\tfrac{1}{2}\,\Delta x_1\,D] \\ -P^{[\mathrm{H,E}]}[\tfrac{1}{2}\,\Delta x_1\,D] & P^{[\mathrm{H,H}]}[\tfrac{1}{2}\,\Delta x_1\,D] \end{pmatrix} \begin{pmatrix} F^{[\mathrm{E}]}[x_1^{[0]} + \Delta x_1] \\ F^{[\mathrm{H}]}[x_1^{[0]} + \Delta x_1] \end{pmatrix} = \\ \begin{pmatrix} P^{[\mathrm{E,E}]}[\tfrac{1}{2}\,\Delta x_1\,D] & P^{[\mathrm{E,H}]}[\tfrac{1}{2}\,\Delta x_1\,D] \\ P^{[\mathrm{H,E}]}[\tfrac{1}{2}\,\Delta x_1\,D] & P^{[\mathrm{H,H}]}[\tfrac{1}{2}\,\Delta x_1\,D] \end{pmatrix} \begin{pmatrix} F^{[\mathrm{E}]}[x_1^{[0]}] \\ F^{[\mathrm{H}]}[x_1^{[0]}] \end{pmatrix} \end{gathered} \tag{D.19}$$

Eq. 13.104 is based on Eq. D.19 with $P^{[u,v]}[\tfrac{1}{2}\,\Delta x_1\,D]$ renamed to $P^{[u,v,j]}$ and $F^{[v]}$ renamed to $F^{[v,j]}$ ($u, v =$ “E” or “H”).

The scaling power sp in Eq. 13.103 is determined by the same criteria used for the exponential matrix, as follows (adapted from Ref. 6). Eq. D.4 is an approximation to the following exact equation (from Eq. 13 in Ref. 6),

$$\frac{D^{2n+1}}{(2n)!}\int_{-h}^{h} \exp[(x+h)D](x^2-h^2)^n\,dx = P[-h\,D]\exp[2\,h\,D] - P[h\,D] \tag{D.20}$$

The Padé approximation to the exponential matrix (Eq. D.4) replaces the left side of Eq. D.20 with zero. Eq's. D.4, D.5, and 13.103 are applied to obtain the following approximation via the scale-and-square algorithm:

$$\exp[(x_1^{[1]} - x_1^{[0]})\,D] = \exp[2^{sp+1}\,h\,D] = \exp[2\,h\,D]^{2^{sp}} \cong \Phi[2\,h\,D]^{2^{sp}} \tag{D.21}$$

The relative error in the $\exp[2\,h\,D]$ approximation, denoted as $\delta^{[\mathrm{rel}]}[2\,h]$, is defined by

$$\Phi[2\,h\,D] = (\mathbf{I} + \delta^{[\mathrm{rel}]}[2\,h])\exp[2\,h\,D] \tag{D.22}$$

($\delta^{[\mathrm{rel}]}[2\,h]$ is a matrix.) The relative error in $\exp[2^{sp+1}\,h\,D]$ (i.e., $\exp[2\,h\,D]^{2^{sp}}$) is denoted as $\delta^{[\mathrm{rel}]}[2^{sp+1}\,h]$ and is similarly defined by

$$\Phi[2\,h\,D]^{2^{sp}} = (\mathbf{I} + \delta^{[\mathrm{rel}]}[2^{sp+1}\,h])\exp[2\,h\,D]^{2^{sp}} \tag{D.23}$$

The above definitions imply

$$\mathbf{I} + \delta^{[\mathrm{rel}]}[2^{sp+1}\,h] = (\mathbf{I} + \delta^{[\mathrm{rel}]}[2\,h])^{2^{sp}} \tag{D.24}$$

sp is sufficiently large (and h is sufficiently small) to satisfy the bounding condition,

$$\left\|\delta^{[\mathrm{rel}]}[2\,h]\right\| \le \kappa \tag{D.25}$$

where $\|\ldots\|$ is the Frobenius norm (the root-sum-square of the matrix elements). This implies the bound

$$\begin{aligned}\left\|\delta^{[\mathrm{rel}]}[2^{sp+1}\,h]\right\| &= \left\|(\mathbf{I} + \delta^{[\mathrm{rel}]}[2\,h])^{2^{sp}} - \mathbf{I}\right\| \le (1 + \left\|\delta^{[\mathrm{rel}]}[2\,h]\right\|)^{2^{sp}} - 1 \\ &\le (1+\kappa)^{2^{sp}} - 1 \le \exp[\kappa]^{2^{sp}} - 1 = \exp[2^{sp}\,\kappa] - 1\end{aligned} \tag{D.26}$$

κ is defined by[6]

$$\exp[2^{sp}\,\kappa] - 1 = \epsilon, \quad \kappa = 2^{-sp}\log[1+\epsilon] \tag{D.27}$$

where ϵ is a specified relative accuracy target. The approximation error in $F[x_1^{[1]}]$, denoted as $\delta F[x_1^{[1]}]$, has the bound

[6] The $\log[1+\epsilon]$ factor is accurately calculated using MATLAB's **`log1p`** function.

$$\begin{aligned}&\left|\delta F[x_1^{[1]}]\right| = \left|(\Phi\left[\Delta x_1\,D\right]^{2^{sp}} - \exp\left[\Delta x_1\,D\right]^{2^{sp}})\,F[x_1^{[0]}]\right| = \left|\delta^{[\mathrm{rel}]}[2^{sp+1}\,h]\exp[2\,h\,D]^{2^{sp}}\;F[x_1^{[0]}]\right|\\&= \left|\delta^{[\mathrm{rel}]}[2^{sp+1}\,h]\,F[x_1^{[1]}]\right| \le \left\|\delta^{[\mathrm{rel}]}[2^{sp+1}\,h]\right\|\cdot\left|F[x_1^{[1]}]\right| \le \epsilon\left|F[x_1^{[1]}]\right|\end{aligned} \tag{D.28}$$

(from Eq's. 13.103, D.1, D.4, D.5, D.23, D.26, and D.27).

A formula for the $\delta^{[\mathrm{rel}]}[2\,h]$ factor in Eq. D.25 is obtained by eliminating $P[h\,D]$ between Eq's. D.20 and D.4, and substituting Eq. D.22,

$$\delta^{[\mathrm{rel}]}[2\,h] = -P[-h\,D]^{-1}\exp[-h\,D]\,\Delta \tag{D.29}$$

where

$$\Delta = \frac{D^{2n+1}}{(2\,n)!}\int_{-h}^{h}\exp[x\,D](x^2-h^2)^n\,dx \tag{D.30}$$

The $\exp[x\,D]$ integrand factor in Eq. D.30 can be replaced with $\cosh[x\,D]$ due to the symmetric integration limits; hence Δ is an odd function of D and is therefore block-anti-diagonal,

$$\Delta = \begin{pmatrix} \mathbf{0} & \Delta^{[\mathrm{EH}]} \\ \Delta^{[\mathrm{HE}]} & \mathbf{0} \end{pmatrix} \tag{D.31}$$

where

$$\left.\begin{aligned}\Delta^{[\mathrm{EH}]} &= \left(\frac{DD^n}{(2\,n)!}\int_{-h}^{h}\cosh[x\sqrt{DD}](x^2-h^2)^n\,dx\right)DEH\\&= DEH\left(\frac{DD'^{\,n}}{(2\,n)!}\int_{-h}^{h}\cosh[x\sqrt{DD'}](x^2-h^2)^n\,dx\right)\\\Delta^{[\mathrm{HE}]} &= \left(\frac{DD'^{\,n}}{(2\,n)!}\int_{-h}^{h}\cosh[x\sqrt{DD'}](x^2-h^2)^n\,dx\right)DHE\\&= DHE\left(\frac{DD^n}{(2\,n)!}\int_{-h}^{h}\cosh[x\sqrt{DD}](x^2-h^2)^n\,dx\right)\end{aligned}\right\} \tag{D.32}$$

A bound on $\left\|\delta^{[\mathrm{rel}]}[2\,h]\right\|$ is determined by separating Eq. D.29 into three factors and establishing a separate bound for each factor,

$$\delta^{[\mathrm{rel}]}[2\,h] = -(P[h\,D]\,P[-h\,D])^{-1}\,(P[h\,D]\exp[-h\,D])\,\Delta \tag{D.33}$$

The divisor in Eq. D.33 has the following block-diagonal form (from Eq's. D.10, D.11, D.14, and D.15),

$$
\begin{aligned}
&P[h\,D]\,P[-h\,D] \\
&= \begin{pmatrix} P^{[\mathrm{E,E}]}[h\,D]^2 - P^{[\mathrm{E,H}]}[h\,D]\,P^{[\mathrm{H,E}]}[h\,D] & \mathbf{0} \\ \mathbf{0} & P^{[\mathrm{H,H}]}[h\,D]^2 - P^{[\mathrm{H,E}]}[h\,D]\,P^{[\mathrm{E,H}]}[h\,D] \end{pmatrix} \\
&= \begin{pmatrix} PP[h^2\,DD] & \mathbf{0} \\ \mathbf{0} & PP[h^2\,DD'] \end{pmatrix}
\end{aligned}
\tag{D.34}
$$

where

$$
PP[X] = (\mathbf{I} + X\,U[X])^2 - X\,V[X]^2 \tag{D.35}
$$

The reciprocal factor is similarly block-diagonal,

$$
(P[h\,D]\,P[-h\,D])^{-1} = \begin{pmatrix} PP[h^2\,DD]^{-1} & \mathbf{0} \\ \mathbf{0} & PP[h^2\,DD']^{-1} \end{pmatrix} \tag{D.36}
$$

The following bounding condition is applied to $PP[X]^{-1}$ with $X = h^2\,DD$ or $X = h^2\,DD'$, and with R representing right-hand factors in Eq. D.33:

$$
\left\| PP[X] - \mathbf{I} \right\| < 1 \;\rightarrow\; \left\| PP[X]^{-1}\,R \right\| \le (1 - \left\| PP[X] - \mathbf{I} \right\|)^{-1}\,\|R\| \tag{D.37}
$$

Eq. D.37 follows from the general relation $\left\| (\mathbf{I} + A)^{-1}\,R \right\| \le (1 - \|A\|)^{-1}\,\|R\|$ when $\|A\| < 1$, which can be derived from a Taylor series expansion of $(\mathbf{I} + A)^{-1}$:

$$
\left\| (\mathbf{I} + A)^{-1}\,R \right\| = \left\| R + \sum_{j=1}^{\infty} (-A)^j\,R \right\| \le \|R\| + \sum_{j=1}^{\infty} \|A\|^j\,\|R\| = (1 - \|A\|)^{-1}\,\|R\| \tag{D.38}
$$

Eq. D.34 has the following series representation (from Eq. 32 in Ref. 6),

$$
P[h\,D]\,P[-h\,D] = \sum_{j=0}^{2m} a_j\,h^{2j} \begin{pmatrix} DD^j & \mathbf{0} \\ \mathbf{0} & DD'^j \end{pmatrix}, \quad a_j = \frac{(-1)^j\,j!(4m - 2j)!}{(4m - j)!}\,c_j{}^2 \tag{D.39}
$$

Eq's. D.34 and D.39 are combined to obtain the following relation with $X = h^2\,DD$ or $X = h^2\,DD'$,

$$
PP[X] = \sum_{j=0}^{2m} a_j\,X^j \tag{D.40}
$$

Eq. D.40 is a polynomial equivalence, which holds generally for any argument X. A bound on $\left\| PP[X] - \mathbf{I} \right\|$ in Eq. D.37 is obtained from Eq. D.40,

$$\left\| PP[X]-\mathbf{I} \right\| \le \sum_{j=1}^{2m} |\, a_j \,| \|X\|^j = \sum_{j=1}^{2m} a_j \, (-\|X\|)^j = PP[-\|X\|]-1 \tag{D.41}$$

(Note: The identity matrix $\mathbf{I}$ in Eq. D.35 is size-matched to the argument X and is 1 when the argument is scalar, as in the right side of Eq. D.41.) Eq's. D.37 and D.41 are combined to obtain the following condition,

$$PP[-\|X\|] < 2 \;\rightarrow\; \left\| PP[X]^{-1}\, R \right\| \le (2-PP[-\|X\|])^{-1}\, \|R\| \tag{D.42}$$

In practice the "$\ldots < 2$" condition can be replaced by a somewhat tighter limit, e.g., $\ldots < 1.9$, to ensure that the right-hand reciprocal factor is not very large.

The second factor in Eq. D.33, $P[h\,D]\exp[-h\,D]$, is separated into even and odd functions,

$$\begin{aligned} &P[h\,D]\exp[-h\,D] = \\ &\quad \tfrac{1}{2}(P[h\,D]\exp[-h\,D] + P[-h\,D]\exp[h\,D]) + \\ &\quad \tfrac{1}{2}(P[h\,D]\exp[-h\,D] - P[-h\,D]\exp[h\,D]) \end{aligned} \tag{D.43}$$

The odd function equates to $-\frac{1}{2}\Delta$ (from Eq's. D.20, D.30)

$$\tfrac{1}{2}(P[h\,D]\exp[-h\,D] - P[-h\,D]\exp[h\,D]) = -\tfrac{1}{2}\Delta \tag{D.44}$$

The even function is reformulated with the differences $\exp[\pm h\,D] - P[\pm h\,D]$ separated out and then further separated into even and odd terms,

$$\begin{aligned} &P[h\,D]\exp[-h\,D] + P[-h\,D]\exp[h\,D] \\ &= \mathbf{I} + P[h\,D]\,P[-h\,D] - (\exp[h\,D]-P[h\,D])(\exp[-h\,D]-P[-h\,D]) \\ &= \mathbf{I} + P[h\,D]\,P[-h\,D] - (\cosh[h\,D]-P^{[\text{even}]}[h\,D])^2 + (\sinh[h\,D]-P^{[\text{odd}]}[h\,D])^2 \end{aligned} \tag{D.45}$$

where

$$P^{[\text{even}]}[X] = \tfrac{1}{2}(P[X]+P[-X]) = \begin{pmatrix} P^{[\text{E,E}]}[X] & \mathbf{0} \\ \mathbf{0} & P^{[\text{H,H}]}[X] \end{pmatrix} \tag{D.46}$$

$$P^{[\text{odd}]}[X] = \tfrac{1}{2}(P[X]-P[-X]) = \begin{pmatrix} \mathbf{0} & P^{[\text{E,H}]}[X] \\ P^{[\text{H,E}]}[X] & \mathbf{0} \end{pmatrix} \tag{D.47}$$

(cf. Eq. D.11; the right-hand equalities in Eq's. D.46 and D.47 apply when X is a multiple of D). The last two terms in Eq. D.45 are block-diagonal,

$$
\begin{aligned}
&(\cosh[h\,D]-P^{[\text{even}]}[h\,D])^2 = \\
&\quad\begin{pmatrix} (\cosh[h\sqrt{DD}]-P^{[\text{even}]}[h\sqrt{DD}])^2 & \mathbf{0} \\ \mathbf{0} & (\cosh[h\sqrt{DD'}]-P^{[\text{even}]}[h\sqrt{DD'}])^2 \end{pmatrix}
\end{aligned} \tag{D.48}
$$

$$
\begin{aligned}
&(\sinh[h\,D]-P^{[\text{odd}]}[h\,D])^2 = \\
&\quad\begin{pmatrix} (\sinh[h\sqrt{DD}]-P^{[\text{odd}]}[h\sqrt{DD}])^2 & \mathbf{0} \\ \mathbf{0} & (\sinh[h\sqrt{DD'}]-P^{[\text{odd}]}[h\sqrt{DD'}])^2 \end{pmatrix}
\end{aligned} \tag{D.49}
$$

The function $\exp[X]-P[X]$ has a Taylor expansion with non-negative coefficients,

$$
\exp[X]-P[X]=\sum_{j=2}^{n}\left(1-\prod_{k=1}^{j-1}\left(1-\frac{k}{2\,n-k}\right)\right)\frac{X^j}{j\,!}+\sum_{j=n+1}^{\infty}\frac{X^j}{j\,!} \tag{D.50}
$$

The even and odd parts of Eq. D.50, $\cosh[X]-P^{[\text{even}]}[X]$ and $\sinh[X]-P^{[\text{odd}]}[X]$, also have non-negative Taylor series coefficients, and so do the squares of the these functions. Furthermore, the squared terms are even functions of X; hence they have the bounds

$$
\left\|(\cosh[X]-P^{[\text{even}]}[X])^2\right\| \le (\cosh[\sqrt{\|X^2\|}]-P^{[\text{even}]}[\sqrt{\|X^2\|}])^2 \tag{D.51}
$$

$$
\left\|(\sinh[X]-P^{[\text{odd}]}[X])^2\right\| \le (\sinh[\sqrt{\|X^2\|}]-P^{[\text{odd}]}[\sqrt{\|X^2\|}])^2 \tag{D.52}
$$

These bounds apply to Eq’s. D.48 and D.49 with $X=h\sqrt{DD}$ or $X=h\sqrt{DD'}$.

Eq’s. D.43-D.45 are combined and substituted in Eq. D.33,

$$
\delta^{[\text{rel}]}[2\,h]=-\tfrac{1}{2}\left(\mathbf{I}+(P[h\,D]P[-h\,D])^{-1}\begin{pmatrix}\mathbf{I}-(\cosh[h\,D]-P^{[\text{even}]}[h\,D])^2 \\ +(\sinh[h\,D]-P^{[\text{odd}]}[h\,D])^2-\Delta\end{pmatrix}\right)\Delta \tag{D.53}
$$

With substitution from Eq’s. D.31, D.36, D.48, and D.49, this expands to

$$
\delta^{[\text{rel}]}[2\,h]=\begin{pmatrix}\delta^{[\text{rel, EE}]}[2\,h] & \delta^{[\text{rel, EH}]}[2\,h] \\ \delta^{[\text{rel, HE}]}[2\,h] & \delta^{[\text{rel, HH}]}[2\,h]\end{pmatrix} \tag{D.54}
$$

where

$$
\delta^{[\text{rel, EE}]}[2\,h]=\tfrac{1}{2}\,PP[h^2\,DD]^{-1}\,\Delta^{[\text{EH}]}\,\Delta^{[\text{HE}]}=\tfrac{1}{2}\Delta^{[\text{EH}]}\;PP[h^2\,DD']^{-1}\,\Delta^{[\text{HE}]} \tag{D.55}
$$

$$\delta^{[\mathrm{rel,\,EH}]}[2\,h] = -\tfrac{1}{2}\left(\mathbf{I} + PP[h^2\,DD]^{-1}\begin{pmatrix}\mathbf{I} - (\cosh[h\sqrt{DD}] - P^{[\mathrm{even}]}[h\sqrt{DD}])^2 \\ +(\sinh[h\sqrt{DD}] - P^{[\mathrm{odd}]}[h\sqrt{DD}])^2\end{pmatrix}\right)\Delta^{[\mathrm{EH}]}$$
$$= -\tfrac{1}{2}\,\Delta^{[\mathrm{EH}]}\left(\mathbf{I} + PP[h^2\,DD']^{-1}\begin{pmatrix}\mathbf{I} - (\cosh[h\sqrt{DD'}] - P^{[\mathrm{even}]}[h\sqrt{DD'}])^2 \\ +(\sinh[h\sqrt{DD'}] - P^{[\mathrm{odd}]}[h\sqrt{DD'}])^2\end{pmatrix}\right) \tag{D.56}$$

$$\delta^{[\mathrm{rel,\,HE}]}[2\,h] = -\tfrac{1}{2}\left(\mathbf{I} + PP[h^2\,DD']^{-1}\begin{pmatrix}\mathbf{I} - (\cosh[h\sqrt{DD'}] - P^{[\mathrm{even}]}[h\sqrt{DD'}])^2 \\ (\sinh[h\sqrt{DD'}] - P^{[\mathrm{odd}]}[h\sqrt{DD'}])^2\end{pmatrix}\right)\Delta^{[\mathrm{HE}]}$$
$$= -\tfrac{1}{2}\,\Delta^{[\mathrm{HE}]}\left(\mathbf{I} + PP[h^2\,DD]^{-1}\begin{pmatrix}\mathbf{I} - (\cosh[h\sqrt{DD}] - P^{[\mathrm{even}]}[h\sqrt{DD}])^2 \\ (\sinh[h\sqrt{DD}] - P^{[\mathrm{odd}]}[h\sqrt{DD}])^2\end{pmatrix}\right) \tag{D.57}$$

$$\delta^{[\mathrm{rel,\,HH}]}[2\,h] = \tfrac{1}{2}\,PP[h^2\,DD']^{-1}\,\Delta^{[\mathrm{HE}]}\,\Delta^{[\mathrm{EH}]} = \tfrac{1}{2}\,\Delta^{[\mathrm{HE}]}\,PP[h^2\,DD]^{-1}\,\Delta^{[\mathrm{EH}]} \tag{D.58}$$

(The last equalities in Eq's. D.55 and D.58 are obtained using Eq's D.32 and the relations $PP[h^2\,DD']^{-1}\,DHE = DHE\,PP[h^2\,DD]^{-1}$ and $DEH\,PP[h^2\,DD']^{-1} = PP[h^2\,DD]^{-1}\,DEH$.)

Eq's. D.55-D.58 have the following bounds (from Eq's. D.42, D.51, D.52),

$$PP[-h^2\,\|DD\|] < 2 \;\rightarrow\; \left\|\delta^{[\mathrm{rel,\,EE}]}[2\,h]\right\| \le \tfrac{1}{2}(2 - PP[-h^2\,\|DD\|])^{-1}\,\|\Delta^{[\mathrm{EH}]}\|\cdot\|\Delta^{[\mathrm{HE}]}\| \tag{D.59}$$

$$PP[-h^2\,\|DD\|] < 2 \;\rightarrow\; \left\|\delta^{[\mathrm{rel,\,EH}]}[2\,h]\right\| \le \tfrac{1}{2}\,A\left\|\Delta^{[\mathrm{EH}]}\right\| \tag{D.60}$$

$$PP[-h^2\,\|DD\|] < 2 \;\rightarrow\; \left\|\delta^{[\mathrm{rel,\,HE}]}[2\,h]\right\| \le \tfrac{1}{2}\,A\left\|\Delta^{[\mathrm{HE}]}\right\| \tag{D.61}$$

$$PP[-h^2\,\|DD\|] < 2 \;\rightarrow\; \left\|\delta^{[\mathrm{rel,\,HH}]}[2\,h]\right\| \le \tfrac{1}{2}(2 - PP[-h^2\,\|DD\|]])^{-1}\,\|\Delta^{[\mathrm{HE}]}\|\cdot\|\Delta^{[\mathrm{EH}]}\| \tag{D.62}$$

where

$$A = 1 + (2 - PP[-h^2\,\|DD\|])^{-1}\begin{pmatrix}1 + (\cosh[h\sqrt{\|DD\|}] - P^{[\mathrm{even}]}[h\sqrt{\|DD\|}])^2 \\ +(\sinh[h\sqrt{\|DD\|}] - P^{[\mathrm{odd}]}[h\sqrt{\|DD\|}])^2\end{pmatrix} \tag{D.63}$$

$\delta^{[\mathrm{rel}]}[2\,h]$ has the bound

$$PP[-h^2\,\|DD\|] < 2 \;\rightarrow$$
$$\left\|\delta^{[\mathrm{rel}]}[2\,h]\right\| = \sqrt{\left\|\delta^{[\mathrm{rel,\,EE}]}[2\,h]\right\|^2 + \left\|\delta^{[\mathrm{rel,\,EH}]}[2\,h]\right\|^2 + \left\|\delta^{[\mathrm{rel,\,HE}]}[2\,h]\right\|^2 + \left\|\delta^{[\mathrm{rel,\,HH}]}[2\,h]\right\|^2}$$
$$\le \tfrac{1}{2}\sqrt{A^2\left(\left\|\Delta^{[\mathrm{EH}]}\right\|^2 + \left\|\Delta^{[\mathrm{HE}]}\right\|^2\right) + 2\left((2 - PP[-h^2\,\|DD\|])^{-1}\,\|\Delta^{[\mathrm{EH}]}\|\cdot\|\Delta^{[\mathrm{HE}]}\|\right)^2} \tag{D.64}$$

(As noted after Eq. D.42, the "$\ldots < 2$" condition can be replaced by a somewhat tighter limit, e.g., $\ldots < 1.9$, to ensure that the reciprocal factor is not very large.)

Bounds on $\|\Delta^{[\mathrm{EH}]}\|$ and $\|\Delta^{[\mathrm{HE}]}\|$ are obtained from Eq's. D.32,

$$\|\Delta^{[\mathrm{EH}]}\| \le \frac{B\|DEH\|}{(2n)!\,h^{2n}} \int_{-|h|}^{|h|} (h^2 - x^2)^n \, dx \tag{D.65}$$

$$\|\Delta^{[\mathrm{HE}]}\| \le \frac{B\|DHE\|}{(2n)!\,h^{2n}} \int_{-|h|}^{|h|} (h^2 - x^2)^n \, dx \tag{D.66}$$

where

$$B = \|(h^2\, DD)^n\| \cosh[h\sqrt{\|DD\|}] \tag{D.67}$$

(DD can be replaced by DD' in Eq's. D.59-D.67. Typically, the norms of the DD and DD' powers are nearly identical, so it makes little difference which alternative is used.) The integral evaluates to the following expression (from Eq. 49 in Ref. 6),

$$\int_{-|h|}^{|h|} (h^2 - x^2)^n \, dx = \frac{2\,(2\,n)!!}{(2\,n+1)!!} |h|^{2n+1} \tag{D.68}$$

With this substitution Eq's. D.65 and D.66 simplify to

$$\|\Delta^{[\mathrm{EH}]}\| \le \frac{2\,B\|h\, DEH\|}{(2\,n+1)\,(2\,n-1)!!^2} \tag{D.69}$$

$$\|\Delta^{[\mathrm{HE}]}\| \le \frac{2\,B\|h\, DHE\|}{(2\,n+1)\,(2\,n-1)!!^2} \tag{D.70}$$

Eq's. D.69 and D.70 can be replaced by slightly looser bounds that do not require explicit calculation of $(h^2\, X)^n$ in Eq. D.67 (with $X = DD$). This factor has the bound

$$\|(h^2\, X)^n\| \le h^{2n} \|X^{j_1}\| \cdot \|X^{j_2}\| \cdot \ldots, \quad j_1 + j_2 + \ldots = n \tag{D.71}$$

The powers $X^{j_1}, X^{j_2}, \ldots$ are selected from the precomputed matrices for Eq's. D.17.

Note that in the context of Eq. 14.16, TE case, the DEH matrix ($DEH^{[\mathrm{TE},j]}$) is a scalar multiple of $\mathbf{I}$ ($DEH = s\,\mathbf{I}$ with $s = -2\pi/\lambda$, Eq. 14.12). In this case the $\|h\,DEH\|$ factor in Eq. D.69 can be replaced with $|h\,s|$ because $\|h\,DEH\;X\| = \|h\,s\,X\| \le |h\,s|\,\|X\|$.