Implicit handling of multilayered material substrates in full-wave SCUFF-EM calculations

Homer Reid

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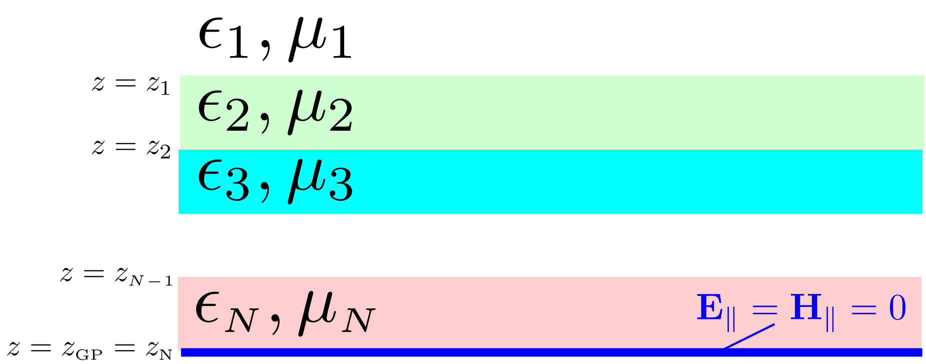

Figure 1: Geometry of the layered substrate. The nth layer has relative permittivity and permeability ϵ_n, μ_n, and its lower surface lies at $z = z_n$. The ground plane, if present, lies at $z = z_{\rm GP}$.

1 Overview

In a previous memo[1] I considered SCUFF-STATIC electrostatics calculations in the presence of a multilayered dielectric substrate. In this memo I extend that discussion to the case of *full-wave* (i.e. nonzero frequencies beyond the quasistatic regime) scattering calculations in the SCUFF-EM core library.

Substrate geometry

As shown in Figure 1, I consider a multilayered substrate consisting of N material layers possibly terminated by a perfectly-conducting ground plane. The uppermost layer (layer 1) is the infinite half-space above the substrate. The nth layer has relative permittivity and permeability ϵ_n, μ_n, and its lower surface lies at $z = z_n$. The ground plane, if present, lies at $z \equiv z_{\rm N} \equiv z_{\rm GP}$. If the ground plane is absent, layer N is an infinite half-space[2] ($z_{\rm N} = -\infty$).

Mechanics of implementation in SCUFF-EM

The mechanics of implementing support for multilayer substrates in SCUFF-EM boils down to a two-step process:

- Devise a numerical scheme for computing the substrate contribution $\boldsymbol{\mathcal{G}}^{\rm subs}$ to the full dyadic Green's function (DGF) $\boldsymbol{\mathcal{G}} \equiv \boldsymbol{\mathcal{G}}^0 + \boldsymbol{\mathcal{G}}^{\rm subs}$. The quantity $\boldsymbol{\mathcal{G}}(\mathbf{x}, \mathbf{x}')$ describes the fields at $\mathbf{x}$ due to point sources at $\mathbf{x}'$, including both the direct vacuum contributions ($\boldsymbol{\mathcal{G}}^0$) and the contributions due to scattering from the substrate ($\boldsymbol{\mathcal{G}}^{\rm subs}$).

[1] "Implicit handling of multilayered dielectric substrates in -wave SCUFF-STATIC"

[2] As in the electrostatic case, this means that a finite-thickness substrate consisting of N material layers is described as a stack of $N + 1$ layers in which the bottommost layer is an infinite vacuum half-space.

- Incorporate the substrate DGF correction $\boldsymbol{\mathcal{G}}^{\text{subs}}$ into the existing SCUFF-EM framework for evaluating 4-dimensional integrals of the form $\Big\langle \mathbf{b}_\alpha \Big| \boldsymbol{\mathcal{G}} \Big| \mathbf{b}_\beta \Big\rangle$ where $\mathbf{b}_{\alpha,\beta}$ are RWG basis functions. To achieve reasonable efficiency, this will require combining a variety of numerical computational techiques, including look-up tables, interpolation schemes, and asymptotic expansions.

In this memo I will discuss methods for attacking both of these challenges.

2 Evaluation of substrate Green's-function correction

My calculation of $\boldsymbol{\mathcal{G}}^{\text{subs}}$ proceeds in two stages:

- Obtain expressions for the 2D Fourier transform of the substrate GF correction, $\widetilde{\boldsymbol{\mathcal{G}}}^{\text{subs}}(\mathbf{q})$. I consider two separate ways of doing this:
  - By using surface-integral-equation methods to solve a scattering problem to determine effective surface-current densities induced on material interfaces by radiating point sources (Section 2.1).
  - By resolving the fields radiated by point sources into superpositions of plane waves, then considering the reflection of each individual plane wave from the multilayer substrate (Section 2.2).
- Evaluate the 2D integrals over the $\mathbf{q}$ variable to effect the inverse Fourier transform from momentum space to real space, $\widetilde{\boldsymbol{\mathcal{G}}}^{\text{subs}}(\mathbf{q}) \rightarrow \boldsymbol{\mathcal{G}}^{\text{subs}}(\boldsymbol{\rho})$. This calculation proceeds in two stages:
  - Use the known structure of $\widetilde{\boldsymbol{\mathcal{G}}}(\mathbf{q})$ to reduce 2D integrals over $\mathbf{q}$ to 1D integrals over q_z (Section 2.3).
  - Devise numerical quadrature methods for evaluating the q_z integrals, including efficient and accurate handling of integrable singularities and undamped oscillatory integrands (Section 2.4).

2.1 Derivation of momentum-space DGF, take 1: Effective surface-current picture

One way to account for the disturbance produced by the substrate is to consider the effective tangential electric and magnetic surface currents $\mathbf{K}$ and $\mathbf{N}$ induced on the interfacial layers by the external field sources (Figure 2). This is the direct extension to full-wave problems of the formalism I used in the electrostatic case, and it comports well with the spirit of surface-integral-equation methods.

More specifically, on the material interface layer at $z = z_n$ I have a four-vector surface-current density $\boldsymbol{\mathcal{S}}_n(\boldsymbol{\rho})$, where $\boldsymbol{\rho} = (x, y)$ and the components of $\boldsymbol{\mathcal{S}}$ are

$$\boldsymbol{\mathcal{S}}_n(\boldsymbol{\rho}) = \left(\begin{array}{c} K_x(\boldsymbol{\rho}) \\ K_y(\boldsymbol{\rho}) \\ N_x(\boldsymbol{\rho}) \\ N_y(\boldsymbol{\rho}) \end{array}\right). \tag{1}$$

Fields in layer interiors. I will adopt the convention that the lower (upper) bounding surface for each region is the positive (negative) bounding surface for that region in the usual sense of SCUFF-EM regions and surfaces (in which the sign of a (surface,region) pair $(\mathcal{S}, \mathcal{R})$ is the sign with which surface currents on

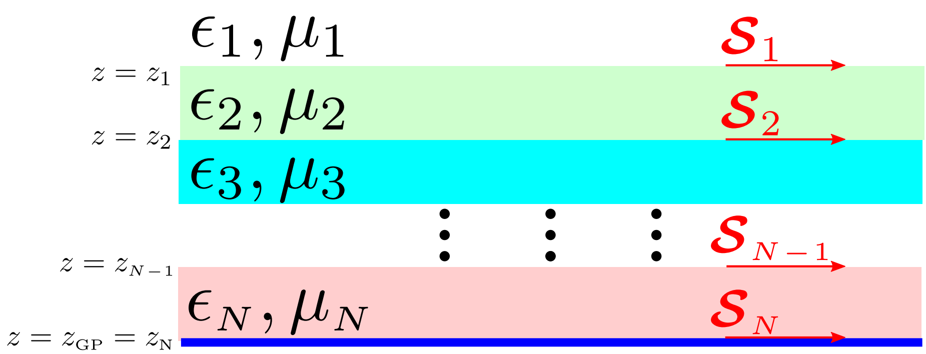

Figure 2: Effective surface-current approach to treatment of multilayer substrate. External field sources induce a distribution of electric and magnetic surface currents $\boldsymbol{\mathcal{S}}_n = \binom{\mathbf{K}_n}{\mathbf{N}_n}$ on the nth material interface, and the fields radiated by these effective currents account for the disturbance presented by the substrate.

$\mathcal{S}$ contribute to fields in $\mathcal{R}$. Thus, at a point $\mathbf{x} = (\boldsymbol{\rho}, z)$ in the interior of layer n $(z_{n-1} < z < z_n)$, the six-vector of total fields $\boldsymbol{\mathcal{F}} = \left(\begin{array}{c}\mathbf{E}\\ \mathbf{H}\end{array}\right)$ reads

$$\boldsymbol{\mathcal{F}}_n(\boldsymbol{\rho}, z) = -\boldsymbol{\mathcal{G}}_n(z_{n-1}) \star \boldsymbol{\mathcal{S}}_{n-1} + \boldsymbol{\mathcal{G}}_n(z_n) \star \boldsymbol{\mathcal{S}}_n + \boldsymbol{\mathcal{F}}_n^{\mathrm{ext}}(\boldsymbol{\rho}, z) \tag{2}$$

where $\boldsymbol{\mathcal{F}}_n^{\mathrm{ext}}$ are the externally-sourced (incident) fields due to sources in layer n, $\boldsymbol{\mathcal{G}}_n$ is the dyadic Green's function for material layer n, and $\star$ is shorthand for the convolution operation

$$\text{``}\boldsymbol{\mathcal{F}}(\boldsymbol{\rho}, z) \equiv \boldsymbol{\mathcal{G}}(z') \star \boldsymbol{\mathcal{S}}'' \quad \Longrightarrow \quad \boldsymbol{\mathcal{F}}(\boldsymbol{\rho}, z) = \int \boldsymbol{\mathcal{G}}(\boldsymbol{\rho} - \boldsymbol{\rho}', z - z') \cdot \boldsymbol{\mathcal{S}}(\boldsymbol{\rho}') d\boldsymbol{\rho}' \tag{3}$$

where the integral extends over the entire interfacial plane. I will evaluate convolutions of this form using the 2D Fourier representation[3] of $\boldsymbol{\mathcal{G}}$:

$$\boldsymbol{\mathcal{G}}_n(\boldsymbol{\rho}, z) = \int \frac{d^2\mathbf{q}}{(2\pi)^2} \widetilde{\boldsymbol{\mathcal{G}}_n}(\mathbf{q}, z) e^{i\mathbf{q}\cdot\boldsymbol{\rho}} \tag{4a}$$

$$\widetilde{\boldsymbol{\mathcal{G}}}_n(\mathbf{q}, z) = \frac{i}{2q_z} \left(\begin{array}{cc} ikZ_0Z_n\widetilde{\mathbf{G}}^{\pm} & ik\widetilde{\mathbf{C}}^{\pm} \\ -ik\widetilde{\mathbf{C}}^{\pm} & \frac{ik}{Z_0Z_n}\widetilde{\mathbf{G}}^{\pm} \end{array} \right) e^{iq_z|z|} \tag{4b}$$

$$\widetilde{\mathbf{G}}^{\pm}(k, \mathbf{q}) = \left(\begin{array}{ccc} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{array} \right) - \frac{1}{k^2} \left(\begin{array}{ccc} q_x^2 & q_xq_y & \pm q_xq_z \\ q_yq_x & q_y^2 & \pm q_yq_z \\ \pm q_zq_x & \pm q_zq_y & q_z^2 \end{array} \right) \tag{4c}$$

$$\widetilde{\mathbf{C}}^{\pm}(k, \mathbf{q}) = \frac{1}{k} \left(\begin{array}{ccc} 0 & \pm q_z & -q_y \\ \mp iq_z & 0 & q_x \\ q_y & -q_x & 0 \end{array} \right) \tag{4d}$$

$$q_z \equiv \sqrt{k^2 - |\mathbf{q}|^2}, \qquad \pm = \text{sign} z. \tag{4e}$$

With this representation, convolutions like (17) become products in Fourier space:

$$\boldsymbol{\mathcal{G}}(z') \star \boldsymbol{\mathcal{S}} = \boldsymbol{\mathcal{F}}(\boldsymbol{\rho}, z) = \int \frac{d^2\mathbf{q}}{(2\pi)^2} \widetilde{\boldsymbol{\mathcal{F}}}(\mathbf{q}, z) e^{i\mathbf{q}\cdot\boldsymbol{\rho}}, \quad \text{with} \quad \widetilde{\boldsymbol{\mathcal{F}}(\mathbf{q}, z)} = \widetilde{\boldsymbol{\mathcal{G}}}(\mathbf{q}, z - z')\widetilde{\boldsymbol{\mathcal{S}}}(\mathbf{q})$$

Matching tangential fields at layer boundaries The boundary condition at $z = z_n$ is that the tangential $\mathbf{E}, \mathbf{H}$ fields be continuous: in Fourier space, we have

$$\widetilde{\boldsymbol{\mathcal{F}}}_{\parallel}(\mathbf{q}, z = z_n^+) = \widetilde{\boldsymbol{\mathcal{F}}}_{\parallel}(\mathbf{q}, z = z_n^-) \tag{5}$$

The fields just **above** the interface ($z \to z_n^+$) receive contributions from three sources:

- Surface currents at $z = z_{n-1}$, which contribute with a minus sign and via the Green's function for region n;
- Surface currents at $z = z_n$, which contribute with a plus sign and via the Green's function for region n; and
- external field sources in region n.

The fields just **below** the interface ($z = z_n^-$) receive contributions from three sources:

[3] An equivalent alternative expression for $\widetilde{\boldsymbol{\mathcal{G}}}$ in equation(18b) is

$$\widetilde{\boldsymbol{\mathcal{G}}} = \frac{1}{2} \left(\begin{array}{cc} -\frac{\omega\mu}{q_z}\widetilde{\mathbf{G}} & \widetilde{\not{\mathrm{C}}} \\ -\widetilde{\not{\mathrm{C}}} & -\frac{\epsilon\mu}{q_z}\widetilde{\mathbf{G}} \end{array} \right), \qquad \not{\mathrm{C}}^{\pm} = \left(\begin{array}{ccc} 0 & \mp 1 & \sin\theta \\ \pm 1 & 0 & -\cos\theta \\ -\sin\theta & \cos\theta & 0 \end{array} \right), \qquad \sin\theta = \frac{q_y}{q_z}, \qquad \cos\theta = \frac{q_x}{q_z}.$$

.

- Surface currents at $z = z_n$, which contribute with a minus sign and via the Green's function for region $n+1$;
- Surface currents at $z = z_{n+1}$, which contribute with a plus sign and via the Green's function for region $n+1$; and
- external field sources in region $n+1$.

Then equation (5) reads

$$\begin{aligned}
&-\widetilde{\boldsymbol{\mathcal{G}}}_{n\|}(z_n - z_{n-1})\cdot\widetilde{\boldsymbol{\mathcal{S}}}_{n-1} + \widetilde{\boldsymbol{\mathcal{G}}}_{n\|}(0^+)\cdot\widetilde{\boldsymbol{\mathcal{S}}}_n + \widetilde{\boldsymbol{\mathcal{F}}}^{\text{ext}}_{n\|}(z_n)\\
&\qquad = -\widetilde{\boldsymbol{\mathcal{G}}}_{n+1\|}(0^-)\cdot\widetilde{\boldsymbol{\mathcal{S}}}_n + \widetilde{\boldsymbol{\mathcal{G}}}_{n+1\|}(z_n - z_{n+1})\cdot\widetilde{\boldsymbol{\mathcal{S}}}_{n+1} + \widetilde{\boldsymbol{\mathcal{F}}}^{\text{ext}}_{n+1\|}(z_n)
\end{aligned}$$

Writing down this equation for all N layers yields a $4N\times 4N$ system of linear equations (with triadiagonal 4×4 block form) relating the surface currents on all layers to the external fields due to sources in all regions ($z_{mn}\equiv z_m = z_n$):

$$\Big[\widetilde{\boldsymbol{\mathcal{G}}}_{0\|}(0^+) + \widetilde{\boldsymbol{\mathcal{G}}}_{1\|}(0^-)\Big]\widetilde{\boldsymbol{\mathcal{S}}}_1 - \widetilde{\boldsymbol{\mathcal{G}}}_{1\|}(z_{12})\widetilde{\boldsymbol{\mathcal{S}}}_2 = \widetilde{\boldsymbol{\mathcal{F}}}_{1\|}(z_1) - \widetilde{\boldsymbol{\mathcal{F}}}_{0\|}(z_1) \tag{6a}$$

$$-\widetilde{\boldsymbol{\mathcal{G}}}_{1\|}(-z_{12})\widetilde{\boldsymbol{\mathcal{S}}}_1 + \Big[\widetilde{\boldsymbol{\mathcal{G}}}_{1\|}(0^+) + \widetilde{\boldsymbol{\mathcal{G}}}_{2\|}(0^-)\Big]\widetilde{\boldsymbol{\mathcal{S}}}_2 - \widetilde{\boldsymbol{\mathcal{G}}}_{2\|}(z_{23})\widetilde{\boldsymbol{\mathcal{S}}}_3 = \widetilde{\boldsymbol{\mathcal{F}}}_{2\|}(z_2) - \widetilde{\boldsymbol{\mathcal{F}}}_{1\|}(z_2) \tag{6b}$$

$$\vdots \qquad\qquad \vdots \qquad\qquad \vdots$$

$$-\widetilde{\boldsymbol{\mathcal{G}}}_{n\|}(-z_{n-1,n})\widetilde{\boldsymbol{\mathcal{S}}}_n + \Big[\widetilde{\boldsymbol{\mathcal{G}}}_{n\|}(0^+) + \widetilde{\boldsymbol{\mathcal{G}}}_{n+1\|}(0^-)\Big]\widetilde{\boldsymbol{\mathcal{S}}}_n - \widetilde{\boldsymbol{\mathcal{G}}}_{n+1\|}(z_{n,n+1})\widetilde{\boldsymbol{\mathcal{S}}}_{n+1} = \widetilde{\boldsymbol{\mathcal{F}}}_{n\|}(z_n) - \widetilde{\boldsymbol{\mathcal{F}}}_{n-1,\|}(z_n) \tag{6c}$$

Here $\widetilde{\boldsymbol{\mathcal{F}}}_{\|r\to s}$ denotes the (Fourier-space representation of the) tangential components of the region-r-sourced external fields evaluated at $z = z_s$, and $\mathbf{M}_{s',s}$ describes the contributions of surface currents at $z = z_s$ to the tangential fields at $z = z'_s$; that is, $\mathbf{M}_{s',s}$ is a 4×4 matrix that operates on $\widetilde{\boldsymbol{\mathcal{S}}}_s$ to yield the (Fourier components of) the contribution of $\boldsymbol{\mathcal{S}}_s$ to the tangential fields at $z_{s'}$. This matrix has 2×2 block structure:

$$\mathbf{M}_{s\pm 1,s} = \frac{1}{2}\left(\begin{array}{cc} \frac{ik_r Z_0 Z_r}{q_{zr}}\mathbf{g}(\mathbf{q}) & \pm\mathbf{c} \\ \mp\mathbf{c} & \frac{ik_r}{Z_0 Z_r q_{zr}}\mathbf{g}(\mathbf{q})\end{array}\right), \qquad r = \min\{s\pm 1, s\} \tag{7}$$

$$\mathbf{M}_{ss} = \sum_{r\in\{s-1,s\}}\left(\begin{array}{cc} \frac{ik_r Z_0 Z_r}{q_{zr}}\mathbf{g}(\mathbf{q}) & 0 \\ 0 & \frac{ik_r}{Z_0 Z_r q_{zr}}\mathbf{g}(\mathbf{q})\end{array}\right) \tag{8}$$

where $\mathbf{g}$ and $\mathbf{c}$ denote 2×2 matrices:

$$\mathbf{g}(k;\mathbf{q}) = \mathbf{1} - \frac{\mathbf{q}\mathbf{q}^\dagger}{k^2}, \qquad \mathbf{c}^{\pm}(k;\mathbf{q}) = \frac{q_z(k;\mathbf{q})}{k}\left(\begin{array}{cc} 0 & \pm 1 \\ \mp 1 & 0\end{array}\right) \tag{9}$$

DGF for sources above single layer

The simplest case is that in which we have only a single material interface, i.e. the geometry consists of two semi-infinite half-spaces that meet at $z = z_1$. Then the first of Equation (6) decouples into separate 2×2 systems for $\widetilde{\mathbf{K}}$ and $\widetilde{\mathbf{N}}$:

$$\underbrace{\left[-\frac{k_{\rm A} Z_0 Z_{\rm A}}{2q_{z\rm A}}\mathbf{g}(k_{\rm A},\mathbf{q}) - \frac{k_1 Z_0 Z_{\rm 1}}{2q_{z1}}\mathbf{g}(k_{\rm 1},\mathbf{q})\right]}_{\mathbf{M}_{\rm K}}\widetilde{\mathbf{K}} = -\widetilde{\mathbf{E}}^{\rm ext}_{\parallel 0}(z_1)$$

$$\underbrace{\left[-\frac{k_{\rm A}}{2Z_0 Z_{\rm A} q_{z\rm A}}\mathbf{g}(k_{\rm A},\mathbf{q}) - \frac{k_1}{2Z_0 Z_{\rm 1} q_{z1}}\mathbf{g}(k_{\rm 1},\mathbf{q})\right]}_{\mathbf{M}_{\rm N}}\widetilde{\mathbf{N}} = -\widetilde{\mathbf{H}}^{\rm ext}_{\parallel 0}(z_1)$$

If the externally-sourced fields are produced by point electric and magnetic sources $\mathbf{p},\mathbf{m}$ at a point $\mathbf{x}_s = (\boldsymbol{\rho}_s, z_s)$ ("s" stands for "source") above the interface at z_1, we may insert equation 20 for the RHS here and solve for $\widetilde{\mathbf{K}},\widetilde{\mathbf{N}}$:

$$\widetilde{\mathbf{K}} = +\frac{e^{-i\mathbf{q}\cdot\boldsymbol{\rho}_s + iq_{zA}|z_1 - z_s|}}{2\omega q_z}\Big[ik_{\rm A} Z_0 Z_{\rm A}\mathbf{M}_{\rm K}^{-1}\widetilde{\mathbf{G}}^{-}_{\parallel}(\mathbf{k}_{\rm A},\mathbf{q})\cdot\mathbf{p} + ik_{\rm A}\mathbf{M}_{\rm K}^{-1}\widetilde{\mathbf{C}}^{-}_{\parallel}(\mathbf{k}_{\rm A},\mathbf{q})\cdot\mathbf{m}\Big]$$

$$\widetilde{\mathbf{N}} = +\frac{e^{-i\mathbf{q}\cdot\boldsymbol{\rho}_s + iq_{zA}|z_1 - z_s|}}{2\omega q_z}\Big[-ik_{\rm A}\mathbf{M}_{\rm N}^{-1}\widetilde{\mathbf{C}}^{-}_{\parallel}(\mathbf{k}_{\rm A},\mathbf{q})\cdot\mathbf{p} + \frac{ik_{\rm A}}{Z_0 Z_{\rm A}}\mathbf{M}_{\rm N}^{-1}\widetilde{\mathbf{G}}^{-}_{\parallel}(\mathbf{k}_{\rm A},\mathbf{q})\cdot\mathbf{m}\Big]$$

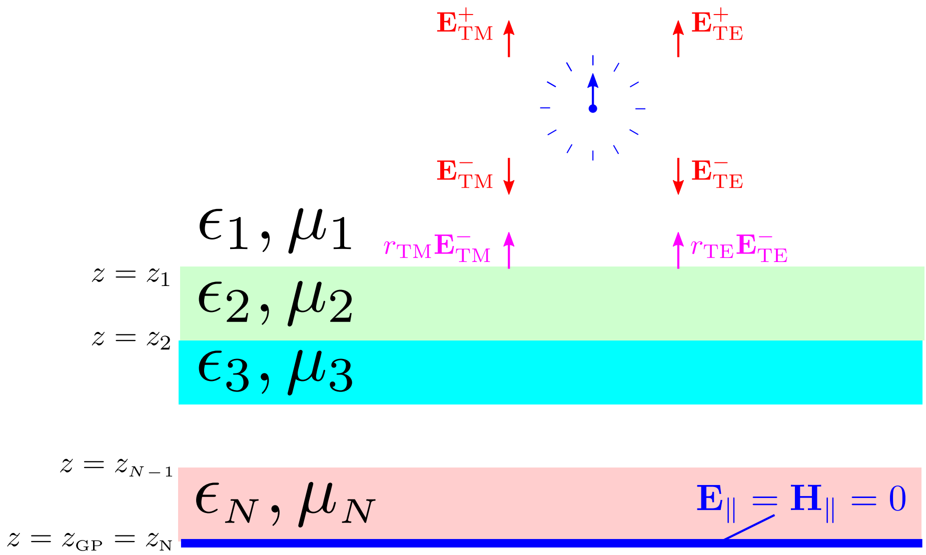

Figure 3: Plane-wave-decomposition strategy for handling multilayer substrate. The fields radiated by a point source (blue) above the substrate are decomposed as a superposition of upward- and downward-traveling plane waves, including both TE- and TM-polarized waves. The downward-traveling waves are reflected at the substrate surface with the usual polarization-dependent Fresnel reflection coefficients $r_{\rm TE,TM}$, and the fields contributed by these reflected waves yield the correction to the free-space Green's function substrate.

2.2 Theory of the substrate DGF, take 2: Plane-wave (Fresnel) scattering picture

An alternative strategy for computing the substrate DGF correction, cartooned in Figure 3, is to think of the fields radiated by a point source above the substrate (blue) as a superposition of plane waves, including both TE- and TM-polarized plane waves (red). The upward-traveling waves radiated by the source ($\mathbf{E}^+_{\rm TE,TM}$) simply radiate away to infinity and do not interact with the substrate, but the downward-traveling waves ($\mathbf{E}^-_{\rm TE,TM}$) reflect from the substrate with polarization-dependent reflection coefficients $r_{\rm TE,TM}$ to yield upward-traveling waves (purple) which constitute the substrate correction to the DGF.

An advantage of this approach is that it subsumes all details of the substrate into the reflection coefficients $r_{\rm TE,TM}$. For simple substrates consisting of one or more homogeneous isotropic material layers these are easily computed in closed form, but the DGF approach here is more general and extends easily to cases involving anisotropic, birefringent, and/or chiral media (in which case the usual TE$\to$TE and TM$\to$TM reflections may be augmented by polarization-mixing terms) and even inhomogeneous substrates of arbitrary complexity for which the reflection coefficients are known empirically.

2.2.1 Plane-wave decomposition of point-source fields

Note: In what follows, $\mathbf{q}=(q_x,q_y)$ is a *two-dimensional* vector and we have[4]

$$q_z \equiv \sqrt{k^2-|\mathbf{q}|^2}, \qquad \mathbf{q}_{\text{3D}} \equiv \left(\begin{array}{c} q_x \\ q_y \\ \pm q_z \end{array}\right), \qquad \pm \equiv \begin{cases} +, & z\ge 0 \\ -, & z<0 \end{cases}.$$

For arbitrary $\mathbf{q}$ I define generalized[5] transverse-electric and transverse-magnetic plane waves propagating in the direction of $\mathbf{q}_{\text{3D}}$:

$$\begin{aligned}
\mathbf{E}^{\pm}_{\text{TE}}(\mathbf{x};k;\mathbf{q}) &\equiv E_0\mathbf{P}(\mathbf{q})e^{i\mathbf{q}\cdot\boldsymbol{\rho}\pm iq_z z}, & \mathbf{H}^{\pm}_{\text{TE}}(\mathbf{x};k;\mathbf{q}) &\equiv H_0\overline{\mathbf{P}}(k,\mathbf{q})e^{i\mathbf{q}\cdot\boldsymbol{\rho}\pm iq_z z}, \\
\mathbf{E}^{\pm}_{\text{TM}}(\mathbf{x};k;\mathbf{q}) &\equiv -E_0\overline{\mathbf{P}}(k,\mathbf{q})e^{i\mathbf{q}\cdot\boldsymbol{\rho}\pm iq_z z}, & \mathbf{H}^{\pm}_{\text{TM}}(\mathbf{x};k;\mathbf{q}) &\equiv H_0\mathbf{P}(\mathbf{q})e^{i\mathbf{q}\cdot\boldsymbol{\rho}\pm iq_z z},
\end{aligned}$$

$$\mathbf{x}=(\boldsymbol{\rho},z), \qquad E_0\equiv 1 \text{ volt}/\mu\text{m}, \qquad H_0\equiv\frac{E_0}{Z_0}.$$

where $\mathbf{P}$ and $\overline{\mathbf{P}}$ are unit-magnitude polarization vectors with the properties that **(1)** both $\mathbf{P}$ and $\overline{\mathbf{P}}$ are orthogonal to $\mathbf{k}_{\text{3D}}$, and **(2)** $\mathbf{P}$ is orthogonal to $\hat{\mathbf{z}}$ (i.e. "transverse").

$$\mathbf{P}(k,\mathbf{q})\equiv\frac{1}{|\mathbf{q}|}\left(\begin{array}{c} -q_y \\ q_x \\ 0 \end{array}\right), \qquad \overline{\mathbf{P}}(k,\mathbf{q})\equiv\frac{1}{k}\Big[\mathbf{q}_{\text{3D}}\times\mathbf{P}(\mathbf{q})\Big]=\frac{1}{k|\mathbf{q}|}\left(\begin{array}{c} \mp q_xq_z \\ \mp q_yq_z \\ q_x^2+q_y^2 \end{array}\right)$$

The trick is now to notice that the columns of the 3×3 matrices in equation (18c,d) may be written as linear combinations of $\mathbf{P}$ and $\overline{\mathbf{P}}$. For example, the leftmost column of $\widetilde{\mathbf{G}}\pm$ is

$$\left(\begin{array}{c} \widetilde{G}_{xx} \\ \widetilde{G}_{yx} \\ \widetilde{G}_{zx} \end{array}\right)=\frac{1}{k^2}\left(\begin{array}{c} k^2-q_x^2 \\ -q_yq_x \\ \mp q_xq_z \end{array}\right)=-\left(\frac{q_y}{|\mathbf{q}|}\right)\mathbf{P}(\mathbf{q})\mp\left(\frac{q_xq_z}{k|\mathbf{q}|}\right)\overline{\mathbf{P}}(\mathbf{q}). \tag{10}$$

The fields of an $\hat{\mathbf{x}}$-directed point electric dipole $\mathbf{p}_0=p_0\hat{\mathbf{x}}$ at $\mathbf{x}_s$, evaluated at point $\mathbf{x}_d$ (for "destination"), then read

$$\mathbf{E}^{\text{ED}}\Big(\mathbf{x}_d;\{p_0\hat{\mathbf{x}},\mathbf{x}_s\}\Big)=ikZ\left(\begin{array}{c} G_{xx} \\ G_{yx} \\ G_{zx} \end{array}\right)(-i\omega p_0)$$

[4] More generally, the symbol $\pm$ here should be understood as $\text{sign}(z_d-z_s)$, i.e. it is positive (negative) when the evaluation point lies above (below) the source point.

[5] These are "generalized" plane waves in the sense that q_z is imaginary for sufficiently large $\mathbf{q}$, in which case the waves are evanescent.

Insert (18b):

$$= (-i\omega p_0)(ikZ) \int \frac{d\mathbf{q}}{(2\pi)^2} \frac{i}{2q_z} \left(\begin{array}{c} \widetilde{G}^{\pm}_{xx} \\ \widetilde{G}^{\pm}_{yx} \\ \widetilde{G}^{\pm}_{zx} \end{array} \right) e^{i\mathbf{q}\cdot(\boldsymbol{\rho}_d-\boldsymbol{\rho}_s)+iq_z|z_d-z_s|}$$

Insert (10):

$$= \frac{k^2 p_0}{\epsilon E_0} \int \frac{d\mathbf{q}}{(2\pi)^2} \Bigg\{ \underbrace{\left(-\frac{iq_y}{2q_z|\mathbf{q}|} \right)}_{C^x_{\text{TE}}} \mathbf{E}^{\pm}_{\text{TE}}(\mathbf{x}_d - \mathbf{x}_s; k; \mathbf{q}) + \underbrace{\left(\mp \frac{iq_x}{2k|\mathbf{q}|} \right)}_{C^{x;\pm}_{\text{TM}}} \mathbf{E}^{\pm}_{\text{TM}}(\mathbf{x}_d - \mathbf{x}_s; k; \mathbf{q}) \Bigg\}$$

Continuing to play this game for point sources of all possible orientations and expressing the results in terms of the generalized plane waves we defined earlier then yields a full plane-wave decomposition of the fields of point electric dipoles oriented in all three Cartesian directions:

$$\mathbf{E}^{\text{ED}}\Big(\mathbf{x}_d; \big\{p_0\hat{\mathbf{x}}, \mathbf{x}_s\big\}\Big) = \left(\frac{k^2 p_0}{\epsilon_0 E_0}\right) \int \frac{d\mathbf{k}}{(2\pi)^2} \Big\{ C^x_{\text{TE}}(\mathbf{k}) \mathbf{E}^{\pm}_{\text{TE}}\Big(\mathbf{x}_d - \mathbf{x}_s; k; \mathbf{q}\Big) + C^{x;\pm}_{\text{TM}}(\mathbf{k}) \mathbf{E}^{\pm}_{\text{TM}}\Big(\mathbf{x}_d - \mathbf{x}_s; k; \mathbf{q}\Big) \Big\} \tag{11a}$$

$$\mathbf{E}^{\text{ED}}\Big(\mathbf{x}_d; \big\{p_0\hat{\mathbf{y}}, \mathbf{x}_s\big\}\Big) = \left(\frac{k^2 p_0}{\epsilon_0 E_0}\right) \int \frac{d\mathbf{k}}{(2\pi)^2} \Big\{ C^y_{\text{TE}}(\mathbf{k}) \mathbf{E}^{\pm}_{\text{TE}}\Big(\mathbf{x}_d - \mathbf{x}_s; k; \mathbf{q}\Big) + C^{y;\pm}_{\text{TM}}(\mathbf{k}) \mathbf{E}^{\pm}_{\text{TM}}\Big(\mathbf{x}_d - \mathbf{x}_s; k; \mathbf{q}\Big) \Big\} \tag{11b}$$

$$\mathbf{E}^{\text{ED}}\Big(\mathbf{x}_d; \big\{p_0\hat{\mathbf{z}}, \mathbf{x}_s\big\}\Big) = \left(\frac{k^2 p_0}{\epsilon_0 E_0}\right) \int \frac{d\mathbf{k}}{(2\pi)^2} \Big\{ C^z_{\text{TE}}(\mathbf{k}) \mathbf{E}^{\pm}_{\text{TE}}\Big(\mathbf{x}_d - \mathbf{x}_s; k; \mathbf{q}\Big) + C^{z}_{\text{TM}}(\mathbf{k}) \mathbf{E}^{\pm}_{\text{TM}}\Big(\mathbf{x}_d - \mathbf{x}_s; k; \mathbf{q}\Big) \Big\} \tag{11c}$$

where the scalar coefficients are

$$\begin{array}{rclcrcl} C^x_{\text{TE}} &=& -\dfrac{iq_y}{2|\mathbf{k}|q_z} & \qquad & C^{x;\pm}_{\text{TM}} &=& \mp\dfrac{iq_x}{2k|\mathbf{k}|} \\ C^y_{\text{TE}} &=& \dfrac{iq_x}{2|\mathbf{k}|q_z} & & C^{y;\pm}_{\text{TM}} &=& \mp\dfrac{iq_y}{2k|\mathbf{k}|} \\ C^z_{\text{TE}} &=& 0 & & C^{z}_{\text{TM}} &=& \dfrac{i|\mathbf{k}|}{2kq_z}. \end{array}$$

In these equations, the $\pm$ sign is $+$ for evaluation points located above the source ($z > z_0$) and $-$ for evaluation points located below the source. In particular, assuming the source lies in the *upper* half-space ($z_0 > 0$), the fields impinging on a dielectric interface at $z = 0$ involve the $-$ sign.

The units of the source-strength prefactor are (C=charge, V=voltage, L=length)

$$\begin{aligned} \left[\left(\frac{k^2 p_0}{\epsilon_0 E_0}\right)\right] &= \Big[k^2 p_0\Big]\Big[\epsilon_0\Big]^{-1}\Big[E_0\Big]^{-1} \\ &= \frac{\text{L}^{-2}\text{C}\cdot\text{L}}{\text{CV}^{-1}\text{L}^{-1}\text{VL}^{-1}} \\ &= \text{length}. \end{aligned}$$

2.2.2 Plane-wave decomposition of DGFs

The point of the above decomposition is that each downward-traveling plane wave radiated by a point source above a substrate is reflected from the substrate with the polarization-dependent reflection coefficients $r_{\text{TE,TM}}(k,\mathbf{q})$ characteristic of the substrate, and thus the scattered fields are

$$\mathbf{E}^{\text{scat,x}}(\boldsymbol{\rho},z)=\left(\frac{k^2p_0}{\epsilon_0}\right)\int\frac{d\mathbf{q}}{(2\pi)^2}\left\{r_{\text{TE}}(\mathbf{q})C^{x}_{\text{TE}}(\mathbf{q})\mathbf{P}(\mathbf{q})+r_{\text{TM}}(\mathbf{q})C^{x;-}_{\text{TM}}(\mathbf{q})\overline{\mathbf{P}}(\mathbf{q})\right\}e^{i\mathbf{q}\cdot\boldsymbol{\rho}+2iq_z z} \tag{12a}$$

$$\mathbf{E}^{\text{scat,y}}(\boldsymbol{\rho},z)=\left(\frac{k^2p_0}{\epsilon_0}\right)\int\frac{d\mathbf{q}}{(2\pi)^2}\left\{r_{\text{TE}}(\mathbf{q})C^{y}_{\text{TE}}(\mathbf{q})\mathbf{P}(\mathbf{q})+r_{\text{TM}}(\mathbf{q})C^{y;-}_{\text{TM}}(\mathbf{q})\overline{\mathbf{P}}(\mathbf{q})\right\}e^{i\mathbf{q}\cdot\boldsymbol{\rho}+2iq_z z} \tag{12b}$$

$$\mathbf{E}^{\text{scat,z}}(\boldsymbol{\rho},z)=\left(\frac{k^2p_0}{\epsilon_0}\right)\int\frac{d\mathbf{q}}{(2\pi)^2}\left\{r_{\text{TE}}(\mathbf{q})C^{z}_{\text{TE}}(\mathbf{q})\mathbf{P}(\mathbf{q})+r_{\text{TM}}(\mathbf{q})C^{z;-}_{\text{TM}}(\mathbf{q})\overline{\mathbf{P}}(\mathbf{q})\right\}e^{i\mathbf{q}\cdot\boldsymbol{\rho}+2iq_z z} \tag{12c}$$

The scattering part of the electric DGF is related to the scattered **E**-field according to $\boldsymbol{\mathcal{G}}^{\text{E}}=\frac{1}{(-i\omega p_0)(i\omega\mu_0)}\mathbf{E}^{\text{scat}}$. or

$$\mathcal{G}^{\text{E}}_{ij}(\boldsymbol{\rho},z)=\int\frac{d\mathbf{k}}{(2\pi)^2}\left\{r_{\text{TE}}(\mathbf{k})C^{j}_{\text{TE}}(\mathbf{k})P_i(\mathbf{k})+r_{\text{TM}}(\mathbf{k})C^{j;-}_{\text{TM}}(\mathbf{k})\overline{P}_i(\mathbf{k})\right\}e^{i\mathbf{k}\cdot\boldsymbol{\rho}+2iq_z z}. \tag{13}$$

A similar derivation yields the scattering part of the magnetic DGF:

$$\mathcal{G}^{\text{M}}_{ij}(\boldsymbol{\rho},z)=\int\frac{d\mathbf{q}}{(2\pi)^2}\left\{r_{\text{TE}}(\mathbf{q})C^{j}_{\text{TE}}(\mathbf{q})\overline{P}_i(\mathbf{q})-r_{\text{TM}}(\mathbf{q})C^{j;-}_{\text{TM}}(\mathbf{q})P_i(\mathbf{q})\right\}e^{i\mathbf{q}\cdot\boldsymbol{\rho}+2iq_z z}. \tag{14}$$

2.3 Reduction of 2D integrals to 1D integrals

It is easy to implement the procedures outlined in the previous two sections to yield numerical values for the 6×6

$$\widetilde{\mathcal{G}}_{ij}(\mathbf{q}) = g_1(|\mathbf{q}|)\delta_{ij} + g_2(|\mathbf{q}|)q_i q_j + g_3(|\mathbf{q}|)\varepsilon_{ijk}q_k \tag{15}$$

$$\begin{aligned}
g_1(\mathbf{q}) &= \frac{1}{2k^2}\big(k^2\delta_{ij} - q_i q_j\big)\widetilde{\mathcal{G}}_{ij} \\
g_2(\mathbf{q}) &= \frac{1}{2k^4}\big(3q_i q_j - k^2\delta_{ij}\big)\widetilde{\mathcal{G}}_{ij} \\
g_3(\mathbf{q}) &= \frac{\varepsilon_{ijk}}{6q_k}\Big(\widetilde{\mathcal{G}}_{ij} - \widetilde{\mathcal{G}}_{ji}\Big)
\end{aligned}$$

2.4 Evaluation of 1D integrals

3 Practice: Running SCUFF-EM calculations with implicit substrates

Mechanically, the process of running full-wave calculations with substrates is the same as for the electrostatic case:

- You write a simple text file, conventionally given file extension `.substrate`, describing the substrate. (The format, which is the same as that used in SCUFF-STATIC, is described in the following section).
- Then you pass the `--SubstrateFile` option to `scuff-em` command-line codes to run calculations in the presence of your multilayered substrate.

3.1 Substrate definition file

The format of the substrate definition file is the same as in the electrostatic case and is repeated here for convenience. Referring to Figure 1, a substrate geometry is specified by

- the z-coordinate of the upper surface of each material layer
- the material properties of each layer
- the z-coordinate of the optional ground plane.

This data is specified to SCUFF-EM in the form of a simple text file (conventionally given file extension `.substrate`) consisting of one line for each layer plus an optional line specifying the ground plane, of the form

```
z1  Material1
z2  Material2
...
zN  MaterialN
zGP GROUNDPLANE
```

where e.g.

- `z1` is the z-coordinate of the upper surface of layer 1
- `Material1` is a SCUFF-EM material designation describing the material of layer 1
- The optional final line, which invokes the fixed keyword `GROUNDPLANE`, specifies that a perfectly-conducting ground plane lives at coordinate $z =$ `zGP`.

If the medium above the uppermost material layer is not vacuum, its material properties may be specified by including a line of the form `MEDIUM UpperMaterial`.

One difference from the electrostatic case is that for full-wave electromagnetism problems with frequency-dependent materials there is no scale invariance, so the length units are no longer arbitrary. In practice, the default length units are determined by the particular SCUFF-EM application code you are running: millimeters for SCUFF-RF and microns for all other codes.

Here are some examples of `.substrate` files:

- An infinite-thickness dielectric slab with $\epsilon_r = 4$ filling the lower half-space:

```
0 CONST_EPS_4
```

- A silicon slab of thickness 1 length unit whose upper surface is the xy plane:

```
 0 SILICON
-1 VACUUM
```

- The same finite-thickness slab as before, but now lying atop a ground plane:

```
 0 SILICON
-1 GROUNDPLANE
```

- A unit-thickness layer of SiO_2 atop an infinite-thickness slab of silicon:

```
 0 SIO2
-1 SILICON
```

- A unit-thickness layer of SiO_2 atop a thickness-2 layer of silicon:

```
 0 SIO2
-1 SILICON
-3 VACUUM
```

- Same as previous item, but now with a ground plane beneath the silicon layer:

```
 0 SIO2
-1 SILICON
-3 GROUNDPLANE
```

A 2D Fourier (plane-wave) representations of homogeneous dyadic Green's functions

Dyadic Green's functions

In an infinite homogeneous medium with relative permittivity and permeability $\{\epsilon_r(\omega), \mu_r(\omega)\}$, a distribution of electric and magnetic currents described by $\boldsymbol{\mathcal{S}}(\mathbf{x}) = \left(\begin{smallmatrix} \mathbf{J}(\mathbf{x}) \\ \mathbf{M}(\mathbf{x})\end{smallmatrix}\right)$ produces electric and magnetic fields $\boldsymbol{\mathcal{F}} = \left(\begin{smallmatrix} \mathbf{E} \\ \mathbf{H}\end{smallmatrix}\right)$ according to

$$\boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{G}} \star \boldsymbol{\mathcal{S}} \tag{16}$$

where $\boldsymbol{\mathcal{G}}$ is the 6x6 dyadic Green's function for the medium and

$$\text{“}\boldsymbol{\mathcal{F}} \equiv \boldsymbol{\mathcal{G}} \star \boldsymbol{\mathcal{S}}'' \qquad \Longrightarrow \qquad \boldsymbol{\mathcal{F}}(\mathbf{x}) = \int \boldsymbol{\mathcal{G}}(\mathbf{x}-\mathbf{x}') \cdot \boldsymbol{\mathcal{S}}(\mathbf{x}') d\mathbf{x}'. \tag{17}$$

I will evaluate convolutions of this form in 2D Fourier space (plane-wave decomposition): representing the fields and sources in Fourier-synthesized form according to

$$\boldsymbol{\mathcal{F}}(\boldsymbol{\rho}, z) = \int \frac{d^2\mathbf{q}}{(2\pi)^2} \widetilde{\boldsymbol{\mathcal{F}}}(\mathbf{q}, z) e^{i\mathbf{q}\cdot\boldsymbol{\rho}}, \qquad \boldsymbol{\mathcal{S}}(\boldsymbol{\rho}, z) \quad = \int \frac{d^2\mathbf{q}}{(2\pi)^2} \widetilde{\boldsymbol{\mathcal{S}}}(\mathbf{q}, z) e^{i\mathbf{q}\cdot\boldsymbol{\rho}},$$

the Fourier components of fields and sources are related by

$$\widetilde{\boldsymbol{\mathcal{F}}}(\mathbf{q}, z) = \int dz' \, \widetilde{\boldsymbol{\mathcal{G}}}(\mathbf{q}, z - z') \widetilde{\boldsymbol{\mathcal{S}}}(\mathbf{q}, z')$$

where

$$\boldsymbol{\mathcal{G}}(\boldsymbol{\rho}, z) = \int \frac{d^2\mathbf{q}}{(2\pi)^2} \widetilde{\boldsymbol{\mathcal{G}}}(\mathbf{q}, z) e^{i\mathbf{q}\cdot\boldsymbol{\rho}} \tag{18a}$$

$$\widetilde{\boldsymbol{\mathcal{G}}}(\mathbf{q}, z) = \frac{i}{2q_z} \begin{pmatrix} ikZ\widetilde{\mathbf{G}}^{\pm} & ik\widetilde{\mathbf{C}}^{\pm} \\ -ik\widetilde{\mathbf{C}}^{\pm} & \frac{ik}{Z}\widetilde{\mathbf{G}}^{\pm} \end{pmatrix} e^{iq_z|z|} \tag{18b}$$

$$\widetilde{\mathbf{G}}^{\pm}(k, \mathbf{q}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \frac{1}{k^2} \begin{pmatrix} q_x^2 & q_x q_y & \pm q_x q_z \\ q_y q_x & q_y^2 & \pm q_y q_z \\ \pm q_z q_x & \pm q_z q_y & q_z^2 \end{pmatrix} \tag{18c}$$

$$\widetilde{\mathbf{C}}^{\pm}(k, \mathbf{q}) = \frac{1}{k} \begin{pmatrix} 0 & \pm q_z & -q_y \\ \mp iq_z & 0 & q_x \\ q_y & -q_x & 0 \end{pmatrix} \tag{18d}$$

$$q_z \equiv \sqrt{k^2 - |\mathbf{q}|^2}, \qquad \pm = \text{sign } z. \tag{18e}$$

Fields of point-source currents

A point electric dipole of strength $\mathbf{p}_0$ at a point $\mathbf{x}_0$ corresponds to a volume electric current distribution of the form

$$\mathbf{J}(\mathbf{x}) = -\frac{\mathbf{p}_0}{i\omega}\delta(\mathbf{x}-\mathbf{x}_0),$$

or, in Fourier space,

$$\mathbf{J}(\mathbf{x}) = \int \frac{d\mathbf{q}}{(2\pi)^2}\widetilde{\mathbf{J}}(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{x}}$$

with

$$\begin{aligned}\widetilde{\mathbf{J}}(\mathbf{q}) &= \int d\mathbf{x}\,\mathbf{J}(\mathbf{x})\,e^{-i\mathbf{q}\cdot\mathbf{x}} \\ &= -\frac{\mathbf{p}_0}{i\omega}e^{-i\mathbf{q}\cdot\mathbf{x}_0}.\end{aligned}$$

Similarly, a point magnetic source of strength $\mathbf{m}_0$ corresponds to a magnetic current distribution with Fourier components

$$\widetilde{\mathbf{M}}(\mathbf{q}) = -\frac{\mathbf{m}_0}{i\omega}e^{-i\mathbf{q}\cdot\mathbf{x}_0}.$$

The Fourier components of the fields $\boldsymbol{\mathcal{F}} = \binom{\mathbf{E}}{\mathbf{H}}$ at height z due to the sources $\boldsymbol{\mathcal{S}} = \binom{\mathbf{K}}{\mathbf{M}}$ at height z_0 read

$$\widetilde{\boldsymbol{\mathcal{F}}}(\mathbf{q};z) = \widetilde{\boldsymbol{\mathcal{G}}}(\mathbf{q},z-z_0)\cdot\widetilde{\boldsymbol{\mathcal{S}}}(\mathbf{q},z_0) \tag{19}$$

or, from (18b)

$$\begin{aligned}\begin{pmatrix}\widetilde{\mathbf{E}}(\mathbf{q},z)\\ \widetilde{\mathbf{H}}(\mathbf{q},z)\end{pmatrix} &= \frac{i}{2q_z}\begin{pmatrix} ikZ\widetilde{\mathbf{G}}^{\pm} & ik\widetilde{\mathbf{C}}^{\pm} \\ -ik\widetilde{\mathbf{C}}^{\pm} & \frac{ik}{Z}\widetilde{\mathbf{G}}^{\pm}\end{pmatrix}\cdot\left(-\frac{1}{i\omega}\right)\begin{pmatrix}\mathbf{p}_0\\ \mathbf{m}_0\end{pmatrix}e^{-i\mathbf{q}\cdot\mathbf{x}_0+iq_z|z-z_0|} \\ &= -\frac{1}{2\omega q_z}\begin{pmatrix} ikZ\widetilde{\mathbf{G}}^{\pm} & ik\widetilde{\mathbf{C}}^{\pm} \\ -ik\widetilde{\mathbf{C}}^{\pm} & \frac{ik}{Z}\widetilde{\mathbf{G}}^{\pm}\end{pmatrix}\begin{pmatrix}\mathbf{p}_0\\ \mathbf{m}_0\end{pmatrix}e^{-i\mathbf{q}\cdot\mathbf{x}_0+iq_z|z-z_0|}.\end{aligned} \tag{20}$$

B Plane-wave reflection coefficients for layered material substrates

B.1 Reflection coefficients for a single material interface

If the substrate consists of just a single semi-infinite material layer with relative material properties $\{\epsilon_r,\mu_r\}$, then the reflection coefficients in (12) are are just the usual Fresnel coefficients:

$$r_{\text{TE}}(k,\mathbf{q}) \equiv \frac{\mu q_z - q_z'}{\mu q_z + q_z'}, \qquad r_{\text{TM}}(k,\mathbf{q}) \equiv \frac{\epsilon q_z - q_z'}{\epsilon q_z + q_z'}.$$

B.2 Reflection coefficients for multilayer substrates