

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

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August 16, 2017

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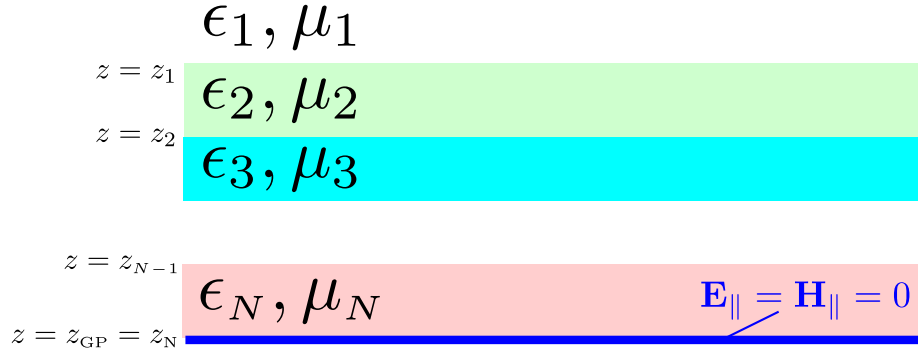


Figure 1: Geometry of the layered substrate. The n th layer has relative permittivity and permeability ϵ_n, μ_n , and its lower surface lies at $z = z_n$. The ground plane, if present, lies at $z = z_{GP}$.

1 Overview

In a previous memo¹ 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 quasi-static 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 n th 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 $z \equiv z_N \equiv z_{GP}$. If the ground plane is absent, layer N is an infinite half-space²

Definition of the substrate DGF

I will use the symbol $\mathbf{\Gamma}(\omega; \mathbf{x}_D, \mathbf{x}_S)$ for the *total* 6×6 dyadic Green's function relating time-harmonic fields at \mathbf{x}_D to sources at \mathbf{x}_S : thus, if $\mathcal{S} \equiv \begin{pmatrix} \mathbf{J} \\ \mathbf{M} \end{pmatrix}$ is the 6-vector distribution of free electric and magnetic currents in the presence of the substrate, then the 6-vector of electric and magnetic fields $\mathcal{F} \equiv \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix}$ is given by

$$\mathcal{F}(\mathbf{x}_D) = \int \mathbf{\Gamma}(\mathbf{x}_D, \mathbf{x}_S) \cdot \mathcal{S}(\mathbf{x}_S) d\mathbf{x}_S.$$

¹“Implicit handling of multilayered dielectric substrates in SCUFF-STATIC”

²As 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 half-space ($z_{N+1} = -\infty$) with the material properties of vacuum ($\epsilon_{N+1} = \mu_{N+1} = 1$).

The 6×6 tensor $\mathbf{\Gamma}$ has a 2×2 block structure:

$$\mathbf{\Gamma} = \begin{pmatrix} \mathbf{\Gamma}^{\text{EE}} & \mathbf{\Gamma}^{\text{EM}} \\ \mathbf{\Gamma}^{\text{ME}} & \mathbf{\Gamma}^{\text{MM}} \end{pmatrix} \quad (1a)$$

with the 3×3 subblocks defined by

$$\Gamma_{ij}^{\text{PQ}}(\omega, \mathbf{x}_D, \mathbf{x}_S) = \begin{pmatrix} i\text{-component of P-type field at } \mathbf{x}_D \text{ due to } j\text{-directed} \\ \text{Q-type point current source at } \mathbf{x}_S, \text{ all fields and} \\ \text{sources having time dependence } \sim e^{-i\omega t} \end{pmatrix} \quad (1b)$$

Homogeneous DGF In an infinite *homogeneous* medium with relative permittivity and permeability $\{\epsilon^r, \mu^r\}$, $\mathbf{\Gamma}$ reduces to its homogeneous form, for which I will use the symbol $\mathbf{\Gamma}^{0r}$ (where the r index labels the medium, which in this case will be one of the layers in Figure 1, i.e. $r \in \{1, 2, \dots, N\}$):

$$\mathbf{x}_D, \mathbf{x}_S \in \text{infinite homogeneous medium } r \implies \mathbf{\Gamma}(\omega; \mathbf{x}_D, \mathbf{x}_S) = \mathbf{\Gamma}^{0r}(\omega; \mathbf{x}_D - \mathbf{x}_S)$$

where

$$\mathbf{\Gamma}^{0r}(\omega, \mathbf{r}) \equiv \begin{pmatrix} ik_r Z_0 Z^r \mathbf{G}(k_r, \mathbf{r}) & ik_r \mathbf{C}(k_r, \mathbf{r}) \\ -ik_r \mathbf{C}(k_r, \mathbf{r}) & \frac{ik_r}{Z_0 Z^r} \mathbf{G}(k_r, \mathbf{r}) \end{pmatrix} \quad (2)$$

$$k_r \equiv \sqrt{\epsilon_0 \epsilon^r \mu_0 \mu^r} \cdot \omega, \quad Z_r \equiv \sqrt{\frac{\mu_0 \mu^r}{\epsilon_0 \epsilon^r}}, \quad G_{ij} = \left(\delta_{ij} - \frac{1}{k^2} \partial_i \partial_j \right) \frac{e^{ik|\mathbf{r}|}}{4\pi|\mathbf{r}|}, \quad C_{ij} = -\frac{1}{ik} \epsilon_{ikl} \partial_k G_{lj}$$

Inhomogeneous DGF On the other hand, in the presence of the multilayered substrate the full DGF $\mathbf{\Gamma}$ receives corrections, which may be thought of as the fields radiated by surface currents induced on the interfacial surfaces of the substrate, and which I will denote by the symbol \mathcal{G} :

$$\mathbf{\Gamma}(\mathbf{x}_D, \mathbf{x}_S) = \mathcal{G}(\mathbf{x}_D, \mathbf{x}_S) + \begin{cases} \mathbf{\Gamma}^{0r}(\mathbf{x}_D - \mathbf{x}_S), & \mathbf{x}_S \in \text{layer } r \\ 0, & \text{otherwise} \end{cases} \quad (3)$$

Like $\mathbf{\Gamma}$, \mathcal{G} is a 6×6 matrix with a 2×2 block structure:

$$\mathcal{G}(\omega; \mathbf{x}_D, \mathbf{x}_S) = \begin{pmatrix} \mathcal{G}^{\text{EE}} & \mathcal{G}^{\text{EM}} \\ \mathcal{G}^{\text{ME}} & \mathcal{G}^{\text{MM}} \end{pmatrix} \quad (4a)$$

with the 3×3 subblocks defined by

$$\mathcal{G}_{ij}^{\text{PQ}} = \begin{pmatrix} \text{P-type field at } \mathbf{x}_D \text{ due to surface currents on} \\ \text{substrate interface layers induced by } j\text{-directed} \\ \text{Q-type source at } \mathbf{x}_S \end{pmatrix} \quad (4b)$$

LIBSUBSTRATE is a code for numerical computation of \mathcal{G} .

Organization of SCUFF-EM implementation and this memo

The full-wave substrate implementation in SCUFF-EM consists of multiple working parts that fit together in a somewhat modular fashion.

Roughly speaking, the computational problem may be divided into two parts:

- (a) For given source and evaluation (or “destination”) points $\{\mathbf{x}_s, \mathbf{x}_d\}$ at a given angular frequency ω in the presence of a multilayer substrate, numerically compute the substrate DGF correction $\mathcal{G}(\omega, \mathbf{x}_d, \mathbf{x}_s)$. This task is independent of SCUFF-EM and is implemented by a standalone library called LIBSUBSTRATE, described in Section 2 of this memo.
- (b) For a SCUFF-EM geometry in the presence of a substrate, compute the substrate corrections to the BEM system matrix \mathbf{M} and RHS vector \mathbf{v} , as well as the substrate corrections to post-processing quantities such as scattered fields. This is done by the file `Substrate.cc` in LIBSCUFF and is described in Section 3 of this memo.

2 LIBSUBSTRATE: Numerical computation of substrate Green's functions

Numerical evaluation of substrate contributions to dyadic Green's functions is handled by a C++ library called LIBSUBSTRATE. Although this library is packaged and distributed with SCUFF-EM and depends on other support libraries in the SCUFF-EM distribution, it is independent of the particular integral-equation formulation implemented by LIBSCUFF, and thus should be of general utility beyond SCUFF-EM.

2.1 Overview of computational strategy

LIBSUBSTRATE decomposes the problem of computing \mathcal{G} into several logical steps, as follows:

1. Solve a linear system to obtain the Fourier-space representation $\tilde{\mathcal{G}}(\mathbf{q})$. Here $\mathbf{q} = (q_x, q_y)$ is a 2D Fourier variable. (Section 2.2.)
2. Reduce the two-dimensional integral over \mathbf{q} to a one-dimensional integral over $|\mathbf{q}| \equiv q$. (Section 2.3.)
3. Evaluate the q integral using established methods for evaluating Sommerfeld integrals. (Section 2.4.)

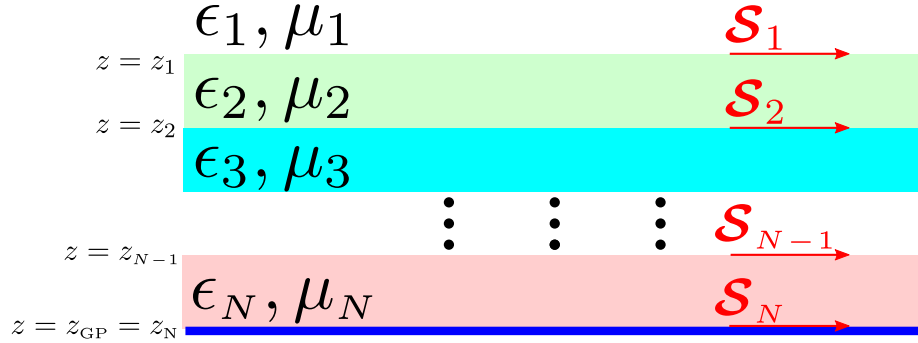


Figure 2: Effective surface-current approach to treatment of multilayer substrate. External field sources induce a distribution of electric and magnetic surface currents $\mathcal{S}_n = \begin{pmatrix} \mathbf{K}_n \\ \mathbf{N}_n \end{pmatrix}$ on the n th material interface, and the fields radiated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

2.2 Computation of Fourier-space DGF $\tilde{\mathcal{G}}(\mathbf{q})$

To compute the substrate correction to the fields of external sources, I 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 $\mathcal{S}_n(\boldsymbol{\rho})$, where $\boldsymbol{\rho} = (x, y)$ and the components of \mathcal{S} are

$$\mathcal{S}_n(\boldsymbol{\rho}) = \begin{pmatrix} K_x(\boldsymbol{\rho}) \\ K_y(\boldsymbol{\rho}) \\ N_x(\boldsymbol{\rho}) \\ N_y(\boldsymbol{\rho}) \end{pmatrix}. \quad (5)$$

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 \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 $\mathcal{F} = \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix}$ reads

$$\mathcal{F}_n(\boldsymbol{\rho}, z) = -\mathbf{\Gamma}^{0n}(z_{n-1}) \star \mathcal{S}_{n-1} + \mathbf{\Gamma}^{0n}(z_n) \star \mathcal{S}_n + \mathcal{F}_n^{\text{ext}}(\boldsymbol{\rho}, z) \quad (6)$$

where $\mathcal{F}_n^{\text{ext}}$ are the externally-sourced (incident) fields due to sources in layer n , $\mathbf{\Gamma}^{0n}$ is the 6×6 homogeneous dyadic Green's function for material layer n ,

and \star is shorthand for the convolution operation

$$“\mathcal{F}(\boldsymbol{\rho}, z) \equiv \Gamma(z') \star \mathcal{S}'' \implies \mathcal{F}(\boldsymbol{\rho}, z) = \int \Gamma(\boldsymbol{\rho} - \boldsymbol{\rho}', z - z') \cdot \mathcal{S}(\boldsymbol{\rho}') d\boldsymbol{\rho}' \quad (7)$$

where the integral extends over the entire interfacial plane. I will evaluate convolutions of this form using the 2D Fourier representation of Γ^{0n} :

$$\Gamma^{0n}(\boldsymbol{\rho}, z) = \int \frac{d^2\mathbf{q}}{(2\pi)^2} \widetilde{\Gamma^{0n}}(\mathbf{q}, z) e^{i\mathbf{q} \cdot \boldsymbol{\rho}} \quad (8a)$$

$$\widetilde{\Gamma^{0n}}(\mathbf{q}, z) = \frac{1}{2} \begin{pmatrix} -\frac{\omega\mu_0\mu_n}{q_{zn}} \tilde{\mathbf{G}}^\pm & +\tilde{\mathbf{C}}^\pm \\ -\tilde{\mathbf{C}}^\pm & -\frac{\omega\epsilon_0\epsilon_n}{q_{zn}} \tilde{\mathbf{G}}^\pm \end{pmatrix} e^{iq_z|z|} \quad (8b)$$

$$\tilde{\mathbf{G}}^\pm(\mathbf{q}, k) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \frac{1}{k^2} \begin{pmatrix} q_x^2 & q_x q_y & \pm q_x q_z \\ q_y q_x & q_y^2 & \pm q_y q_z \\ \pm q_z q_x & \pm q_z q_y & q_z^2 \end{pmatrix} \quad (8c)$$

$$\tilde{\mathbf{C}}^\pm(\mathbf{q}, k) = \begin{pmatrix} 0 & \mp 1 & +q_y/q_z \\ \pm 1 & 0 & -q_x/q_z \\ -q_y/q_z & +q_x/q_z & 0 \end{pmatrix} \quad (8d)$$

$$k_n \equiv \sqrt{\epsilon_0\epsilon_n\mu_0\mu_n} \cdot \omega, \quad q_z \equiv \sqrt{k^2 - |\mathbf{q}|^2}, \quad \pm = \text{sign } z. \quad (8e)$$

With this representation, convolutions like (7) become products in Fourier space:

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

Surface currents from incident fields. To determine the surface currents induced by given incident-field sources, I apply boundary conditions. The boundary condition at $z = z_n$ is that the tangential \mathbf{E}, \mathbf{H} fields be continuous: in Fourier space, we have

$$\tilde{\mathcal{F}}_\parallel(\mathbf{q}, z = z_n^+) = \tilde{\mathcal{F}}_\parallel(\mathbf{q}, z = z_n^-) \quad (9)$$

The fields just **above** the interface ($z \rightarrow z_n^+$) 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:

- 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 (9) reads (temporarily omitting \mathbf{q} arguments)

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

or

$$\mathbf{M}_{n,n-1} \cdot \widetilde{\mathcal{S}}_{n-1} + \mathbf{M}_{n,n} \cdot \widetilde{\mathcal{S}}_n + \mathbf{M}_{n,n+1} \cdot \widetilde{\mathcal{S}}_{n+1} = \widetilde{\mathcal{F}}_{n+1\parallel}^{\text{ext}}(z_n) - \widetilde{\mathcal{F}}_{n\parallel}^{\text{ext}}(z_n) \quad (10)$$

with the 4×4 matrix blocks³

$$\mathbf{M}_{n,n-1} = -\widetilde{\Gamma}^{0n}_{\parallel}(z_n - z_{n-1}) \quad (13a)$$

$$\mathbf{M}_{n,n} = +\widetilde{\Gamma}^{0n}_{\parallel}(0^+) + \widetilde{\Gamma}^{0,n+1}_{\parallel}(0^-) \quad (13b)$$

$$\mathbf{M}_{n,n+1} = -\widetilde{\Gamma}^{0,n+1}_{\parallel}(z_n - z_{n+1}) \quad (13c)$$

Writing down equation (10) equation for all N dielectric interfaces 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:

$$\mathbf{M} \cdot \mathbf{s} = \mathbf{f} \quad (14)$$

³The 4×4 \mathbf{M} blocks here have 2×2 block structure:

$$\mathbf{M}_{n,n} = \sum_{r \in \{n, n+1\}} \frac{1}{2} \begin{pmatrix} -\frac{\omega \epsilon_r}{Z_0 q_{zr}} \mathbf{g}(k_r, \mathbf{q}) & 0 \\ 0 & -\frac{\omega \mu_r Z_0}{q_{zr}} \mathbf{g}(k_r, \mathbf{q}) \end{pmatrix} \quad (11)$$

$$\mathbf{M}_{n,n\pm 1} = \frac{1}{2} \begin{pmatrix} -\frac{\omega \epsilon_r}{Z_0 q_{zr}} \mathbf{g}(k_r, \mathbf{q}) & \mathbf{c}^{\pm} \\ -\mathbf{c}^{\pm} & -\frac{\omega \mu_r Z_0}{q_{zn^*}} \mathbf{g}(k_r, \mathbf{q}) \end{pmatrix} e^{iq_{zr}|z_n - z_{n\pm 1}|} \quad (12)$$

where I put $r \equiv \begin{cases} n, & \text{for } \mathbf{M}_{n,n-1} \\ n+1, & \text{for } \mathbf{M}_{n,n+1} \end{cases}$ and

$$\mathbf{g}(k; \mathbf{q}) = \mathbf{1} - \frac{\mathbf{q}\mathbf{q}^\dagger}{k^2}, \quad \mathbf{c}^{\pm} = \begin{pmatrix} 0 & \mp 1 \\ \pm 1 & 0 \end{pmatrix}$$

where \mathbf{M} is the $4N \times 4N$ block-tridiagonal matrix (13) and where the $4N$ -vectors \mathbf{s} , \mathbf{f} read

$$\mathbf{s} = \begin{pmatrix} \tilde{\mathcal{S}}_1 \\ \tilde{\mathcal{S}}_2 \\ \tilde{\mathcal{S}}_3 \\ \vdots \\ \tilde{\mathcal{S}}_N \end{pmatrix}, \quad \mathbf{f} = \begin{pmatrix} -\tilde{\mathcal{F}}_{1\parallel}(z_1) + \tilde{\mathcal{F}}_{2\parallel}(z_1) \\ -\tilde{\mathcal{F}}_{2\parallel}(z_2) + \tilde{\mathcal{F}}_{3\parallel}(z_2) \\ -\tilde{\mathcal{F}}_{3\parallel}(z_3) + \tilde{\mathcal{F}}_{4\parallel}(z_3) \\ \vdots \\ -\tilde{\mathcal{F}}_{N-1,\parallel}(z_{N-1}) + \tilde{\mathcal{F}}_{N\parallel}(z_{N-1}) \end{pmatrix}.$$

Solving (14) yields the induced surface currents on all layers in terms of the incident fields:

$$\mathbf{s} = \mathbf{W} \cdot \mathbf{f} \quad \text{where} \quad \mathbf{W} \equiv \mathbf{M}^{-1}$$

or, more explicitly,

$$\tilde{\mathcal{S}}_n = \sum_m W_{nm} \mathbf{f}_m \quad (15)$$

Surface currents induced by point sources

For DGF computations the incident fields arise from a single point source—say, a j -directed source in region s . Then the only nonzero length-4 blocks of the RHS vector in (14) are $\mathbf{f}_{s-1}, \mathbf{f}_s$ with components ($\ell = \{1, 2, 4, 5\}$)

$$\left(\mathbf{f}_{s-1}\right)_\ell = -\tilde{\Gamma}_{\ell j}^{0s}(z_{s-1} - z_s), \quad \left(\mathbf{f}_s\right)_\ell = +\tilde{\Gamma}_{\ell j}^{0s}(z_s - z_s) \quad (16)$$

and the surface currents on interface layer n are obtained by solving (15):

$$\begin{aligned} \tilde{\mathcal{S}}_n &= \mathbf{W}_{n,s-1} \mathbf{f}_{s-1} + \mathbf{W}_{n,s} \mathbf{f}_s \\ &= \sum_{p=0}^1 (-1)^{p+1} \mathbf{W}_{n,s-1+p} \cdot \widetilde{\Gamma}_{\parallel,j}^{0s}(z_s - z_{s-1+p}) \end{aligned} \quad (17)$$

Fields due to surface currents

Given the surface currents induced by a j -directed point source at \mathbf{x}_s , I evaluate the fields due to these currents to get the substrate DGF contribution \mathcal{G} . If the evaluation point \mathbf{x}_d lies in region d , then the fields receive contributions from the surface currents at z_{d-1} and z_d , propagated by the homogeneous DGF for region d :

$$\begin{aligned} \tilde{\mathcal{F}}(z_d) &= -\widetilde{\Gamma}^{0d}(z_d - z_{d-1}) \cdot \tilde{\mathcal{S}}_{d-1} + \widetilde{\Gamma}^{0d}(z_d - z_d) \cdot \tilde{\mathcal{S}}_d \\ &= \sum_{q=0}^1 (-1)^{q+1} \widetilde{\Gamma}^{0d}(z_d - z_{d+q-1}) \cdot \tilde{\mathcal{S}}_{d+q-1} \end{aligned}$$

(The minus sign in the first term arises because, in my convention, surface currents on the upper surface of a region contribute to the fields in that region with a minus sign). Inserting (17), the i component here—which is the ij component of the substrate DGF—is

$$\tilde{\mathcal{G}}_{ij}(z_D, z_S) = \sum_{p,q=0}^1 (-1)^{p+q} \widetilde{\mathbf{\Gamma}^{0d}_{i,\parallel}}(z_D - z_{d-1+q}) \mathbf{W}_{d-1+q,s-1+p} \widetilde{\mathbf{\Gamma}^{0s}_{\parallel,j}}(z_{s-1+p} - z_S). \quad (18)$$

The calculation of equation (18) is carried out by the routine `GetGTwiddle` in `LIBSUBSTRATE`.

2.3 Reduction of 2D integrals over \mathbf{q} to 1D (Sommerfeld) integrals over q

The real-space DGF correction is the inverse Fourier transform of (18):

$$\mathcal{G}(\boldsymbol{\rho}, z_D, z_S) = \int \frac{d^2 \mathbf{q}}{(2\pi)^2} \tilde{\mathcal{G}}(\mathbf{q}; z_D, z_S) e^{i\mathbf{q} \cdot \boldsymbol{\rho}}$$

or, in polar coordinates $(q_x, q_y) = (q \cos \theta_{\mathbf{q}}, q \sin \theta_{\mathbf{q}})$,

$$= \int_0^\infty \frac{q dq}{2\pi} \int_0^{2\pi} \frac{d\theta_q}{2\pi} \tilde{\mathcal{G}}(\mathbf{q}; z_D, z_S) e^{iq\rho \cos(\theta_q - \theta_\rho)}.$$

The goal of this section is to integrate out the angular variable θ_q to reduce the 2D integral over \mathbf{q} to a 1D integral over $q = |\mathbf{q}|$.

Scalar \times matrix structure of $\tilde{\mathcal{G}}$ I begin by noting that $\tilde{\mathcal{G}}(\mathbf{q})$ may be decomposed as a sum of scalar functions of $q = |\mathbf{q}|$ times q -independent matrix-valued functions of $\theta_{\mathbf{q}}$:

$$\tilde{\mathcal{G}}(\mathbf{q}) = \sum_{n=1}^{18} \tilde{g}^{(n)}(q) \boldsymbol{\Lambda}^{(n)}(\theta_{\mathbf{q}}) \quad (19)$$

For example, the upper two quadrants read

$$\begin{aligned}
\widetilde{\mathcal{G}}^{\text{EE}}(\mathbf{q}) &= \underbrace{\widetilde{g}^{\text{EE}0\parallel}(q) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}}_{\Lambda^{0\parallel}} + \underbrace{\widetilde{g}^{\text{EE}0z}(q) \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}}_{\Lambda^{0z}} \\
&+ \underbrace{\widetilde{g}^{\text{EE}1\text{A}}(q) \begin{pmatrix} 0 & 0 & \cos \theta_{\mathbf{q}} \\ 0 & 0 & \sin \theta_{\mathbf{q}} \\ 0 & 0 & 0 \end{pmatrix}}_{\Lambda^1(\theta_{\mathbf{q}})} + \underbrace{\widetilde{g}^{\text{EE}1\text{B}}(q) \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \cos \theta_{\mathbf{q}} & \sin \theta_{\mathbf{q}} & 0 \end{pmatrix}}_{\Lambda^{1\dagger}(\theta_{\mathbf{q}})} \\
&+ \underbrace{\widetilde{g}^{\text{EE}2}(q) \begin{pmatrix} \cos^2 \theta_{\mathbf{q}} & \cos \theta_{\mathbf{q}} \sin \theta_{\mathbf{q}} & 0 \\ \cos \theta_{\mathbf{q}} \sin \theta_{\mathbf{q}} & \sin^2 \theta_{\mathbf{q}} & 0 \\ 0 & 0 & 0 \end{pmatrix}}_{\Lambda^{2A}(\theta_{\mathbf{q}})} \\
\widetilde{\mathcal{G}}^{\text{EM}}(\mathbf{q}) &= \underbrace{g^{\text{EM}0\parallel}(q) \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}}_{\Lambda^{0\times}} + \underbrace{g^{\text{EM}2}(q) \begin{pmatrix} \cos \theta_{\mathbf{q}} \sin \theta_{\mathbf{q}} & \sin^2 \theta_{\mathbf{q}} & 0 \\ -\cos^2 \theta_{\mathbf{q}} & -\cos \theta_{\mathbf{q}} \sin \theta_{\mathbf{q}} & 0 \\ 0 & 0 & 0 \end{pmatrix}}_{\Lambda^{2\times}} \\
&+ \underbrace{g^{\text{EM}1\text{A}}(q) \begin{pmatrix} 0 & 0 & -\sin \theta_{\mathbf{q}} \\ 0 & 0 & +\cos \theta_{\mathbf{q}} \\ 0 & 0 & 1 \end{pmatrix}}_{\Lambda^{1\times}} + \underbrace{g^{\text{EM}1\text{B}}(q) \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -\sin \theta_{\mathbf{q}} & \cos \theta_{\mathbf{q}} & 1 \end{pmatrix}}_{\Lambda^{1\times\dagger}}
\end{aligned}$$

and the expressions for $\widetilde{\mathcal{G}}^{\text{ME}}$ and $\widetilde{\mathcal{G}}^{\text{MM}}$ are similar, involving the same Λ matrices with different \widetilde{g} prefactors.

The real-space substrate DGF reads

$$\mathcal{G}(\boldsymbol{\rho}, z_{\text{D}}, z_{\text{S}}) = \int_0^\infty \frac{q dq}{2\pi} \int_0^{2\pi} \frac{d\theta_q}{2\pi} \widetilde{\mathcal{G}}(\mathbf{q}; z_{\text{D}}; z_{\text{S}}) e^{iq\rho \cos(\theta_q - \theta_\rho)}.$$

Insert (19):

$$= \sum_n \int_0^\infty \frac{q dq}{2\pi} \widetilde{g}^{(n)}(q) \int_0^{2\pi} \frac{d\theta_q}{2\pi} \Lambda^{(n)}(\theta_q) e^{iq\rho(\theta_q - \theta_\rho)}$$

Evaluate θ_q integrals using Table 3:

$$= \sum_m \Lambda^{(m)}(\theta_\rho) \int_0^\infty \widetilde{g}^{(m)}(q) dq$$

$$\frac{1}{2\pi} \int_0^{2\pi} e^{iq\rho \cos(\theta_q - \theta_\rho)} \left\{ \begin{array}{c} 1 \\ \cos \theta_q \\ \sin \theta_q \\ \cos^2 \theta_q \\ \cos \theta_q \sin \theta_q \\ \sin^2 \theta_q \end{array} \right\} d\theta_q = \left\{ \begin{array}{c} J_0(q\rho) \\ iJ_1(q\rho) \cos \theta_\rho \\ iJ_1(q\rho) \sin \theta_\rho \\ -J_2(q\rho) \cos^2 \theta_\rho + \frac{J_1(q\rho)}{q\rho} \\ -J_2(q\rho) \cos \theta_\rho \sin \theta_\rho \\ -J_2(q\rho) \sin^2 \theta_\rho + \frac{J_1(q\rho)}{q\rho} \end{array} \right\},$$

Figure 3: Table of integrals used to reduce 2D integrals over \mathbf{q} to 1D integrals over $|q|$.

$$\tilde{\mathbf{g}}^{\text{EE0}\parallel}(q) = \frac{q}{2\pi} \left[\tilde{g}^{\text{EE0}\parallel}(q) J_0(q\rho) + \tilde{g}^{\text{EE2}}(q) \frac{J_1(q\rho)}{q\rho} \right]$$

2.4 Evaluation of Sommerfeld integrals

3 SCUFF-EM integration: Substrate contributions to BEM matrix and RHS vector

$$\begin{aligned}\mathcal{G}^{\text{PQ}}(\rho, \theta, z_{\text{D}}, z_{\text{S}}) &= \sum_{\nu p} g^{\text{PQ}\nu p}(\rho, z_{\text{D}}, z_{\text{S}}) \mathbf{\Lambda}^{\text{PQ}\nu p}(\theta) \\ g^{\text{PQ}\nu p}(\rho) &= \int \frac{q dq}{(2\pi)} \tilde{g}^{\text{PQ}\nu p}(q) J_{\nu}(q\rho) e^{i\alpha(q, z_{\text{D}}, z_{\text{S}})} \mathbf{\Lambda}^{\text{PQ}\nu p}(\theta)\end{aligned}$$

$$M_{\alpha\beta}^{\text{PQ}} \left\langle \mathbf{b}_{\alpha} \left| \mathcal{G}^{\text{PQ}} \right| \mathbf{b}_{\beta} \right\rangle$$

4 Unit-test framework

The LIBSUBSTRATE standalone library comes with a unit-test suite to test core functionality related to calculation of substrate DGFs. Separately, the unit-test suite for LIBSCUFF includes tests to check the integration of LIBSUBSTRATE into LIBSCUFF.

4.1 LIBSUBSTRATE unit tests

4.1.1 tGTwiddle

The unit-test code `tGTwiddle.cc` tests that the full Fourier-space DGF $\tilde{\Gamma}(\mathbf{q}, z_D, z_S)$ satisfies the appropriate boundary conditions at each layer of the layered substrate, namely

$$C^+(P, i, \ell) \tilde{\Gamma}_{ij}^{\text{PQ}}(\mathbf{q}, z_\ell + \eta, z_S) C^-(P, i, \ell) \tilde{\Gamma}_{ij}^{\text{PQ}}(\mathbf{q}, z_\ell - \eta, z_S) \quad (20)$$

where

$$C^\pm(P, i, \ell) = \begin{cases} 1, & i \in \{x, y\} \\ \epsilon_\ell^\pm, & i = z, P = E \\ \mu_\ell^\pm, & i = z, P = H \end{cases}$$

where $\{\epsilon, \mu\}_\ell^\pm$ are the material properties for the layer above/below z_ℓ , i.e. (Figure ??)

$$\{\epsilon_\ell, \mu_\ell\}^+ = \{\epsilon_\ell, \mu_\ell\}, \quad \{\epsilon_\ell, \mu_\ell\}^- = \{\epsilon_{\ell+1}, \mu_{\ell+1}\}.$$

If a ground plane is present, we have the additional condition

$$\tilde{\Gamma}_{ij}^{\text{PQ}}(q, z_{\text{GP}}, z_S) = 0 \quad \text{for } i \in \{x, y\}. \quad (21)$$

Conditions (??) and (??) must hold *independently* of the indices $\mathbf{Q} \in \{E, H\}$ and $j \in \{1, 2, 3\}$ and of the values of \mathbf{q} and z_S .