Computation of Green's Functions and LDOS in SCUFF-EM

Homer Reid

September 27, 2014

Contents

1 Green's functions and LDOS in the non-periodic case

The scattering parts of the electric and magnetic dyadic Green's functions (DGFs) of a geometry are defined by

$$\mathcal{G}^{\mathrm{E}}_{ij}(\omega;\mathbf{x},\mathbf{x}') \equiv \frac{1}{ikZ_0Z^r}\left(\begin{array}{l}i\text{-component of scattered }\mathbf{E}\text{-field at }\mathbf{x}\text{ due to a unit-}\\ \text{strength }j\text{-directed point }\textbf{electric}\text{ dipole radiator at}\\ \mathbf{x}'\text{, all quantities having time dependence }\sim e^{-i\omega t}\end{array}\right)$$

$$\mathcal{G}^{\mathrm{M}}_{ij}(\omega;\mathbf{x},\mathbf{x}') \equiv \frac{1}{ik}\left(\begin{array}{l}i\text{-component of scattered }\mathbf{H}\text{-field at }\mathbf{x}\text{ due to a unit-}\\ \text{strength }j\text{-directed point }\textbf{magnetic}\text{ dipole radiator}\\ \text{at }\mathbf{x}'\text{, all quantities having time dependence }\sim e^{-i\omega t}\end{array}\right)$$

Here $k=\sqrt{\epsilon^r\mu^r}\cdot\omega$ and $Z^r=\sqrt{\mu^r/\epsilon^r}$ are the wavenumber and relative wave impedance of the material medium in which point $\mathbf{x}$ resides (ϵ^r,μ^r are its relative permittivity and permeability) and $Z_0\approx 377\,\Omega$ is the impedance of vacuum. The prefactors $\frac{1}{ikZ_0Z^r}$ and $\frac{1}{ik}$ are inserted to ensure that $\boldsymbol{\mathcal{G}}^{\mathrm{E,M}}$ have dimensions of inverse length.

The enhancement of the local density of states (LDOS) at frequency ω and at a point $\mathbf{x}$ in a scattering geometry is related to the scattering DGFs according to[1]

$$\mathtt{LDOS}(\omega;\mathbf{x}) \equiv \frac{\rho(\omega;\mathbf{x})}{\rho_0(\omega)} \equiv \frac{\pi}{k_0^2}\mathrm{Tr}\ \mathrm{Im}\left[\boldsymbol{\mathcal{G}}^{\mathrm{E}}(\omega;\mathbf{x},\mathbf{x})+\boldsymbol{\mathcal{G}}^{\mathrm{M}}(\omega;\mathbf{x},\mathbf{x})\right]$$

where $\rho_0(\omega)\equiv k_0^3/(\pi c)$ is the free-space LDOS and $k_0=\omega/c$ is the free-space wavenumber at the frequency in question.

In SCUFF-EM the dyadic GFs may be computed easily by solving a scattering problem in which the incident fields arise from a point dipole radiator at a source point $\mathbf{x}_{\mathrm{S}}$. For example, to compute $\mathcal{G}^{\mathrm{E}}$ we take the incident fields to be the fields of a unit-strength j-directed point electric dipole source at $\mathbf{s}^{\mathrm{S}}$:

$$\mathbf{E}^{\mathrm{inc}}(\mathbf{x})=\mathbf{E}^{\mathrm{ED}}\Big(\mathbf{x};\{\mathbf{x}_{\mathrm{S}},\hat{\mathbf{x}}_j\}\Big),\qquad \mathbf{H}^{\mathrm{inc}}(\mathbf{x})=\mathbf{H}^{\mathrm{ED}}\Big(\mathbf{x};\{\mathbf{x}_{\mathrm{S}},\hat{\mathbf{x}}_j\}\Big) \tag{1}$$

where $\{\mathbf{E},\mathbf{H}\}^{\mathrm{ED}}\Big(\mathbf{x};\{\mathbf{x}_0,\mathbf{p}_0\}\Big)$ are the fields of a point electric dipole radiator at $\mathbf{x}_0$ with dipole moment $\mathbf{p}_0$. (Expressions for these fields are given in Appendix A). Then we simply solve an ordinary SCUFF-EM scattering problem with the incident fields given by equation (1) and compute the scattered—not total!—fields at the evaluation point $\mathbf{x}_{\mathrm{D}}$. The three components of the $\mathbf{E}$-field at $\mathbf{x}_{\mathrm{D}}$, divided by ikZ_0Z_r, yield the three vertical entries of the jth column of the 3×3 matrix $\boldsymbol{\mathcal{G}}^{\mathrm{E}}(\omega;\mathbf{x}_{\mathrm{D}},\mathbf{x}_{\mathrm{S}}.)$ Calculating $\boldsymbol{\mathcal{G}}^{\mathrm{M}}$ is similar except that we use a point magnetic source to supply the incident field and compute the scattered $\mathbf{H}$ field instead of the scattered $\mathbf{E}$ field.

[1] K Joulain et al.,"Definition and measurement of the local density of electromagnetic states close to an interface," Physical Review B **68** 245405 (2003)

2 Extension to the periodic case

In the Bloch-periodic module of SCUFF-EM, *all* fields and currents are assumed to be Bloch-periodic, i.e. if $Q(\mathbf{x})$ denotes any field or current component at $\mathbf{x}$, then we have the built-in assumption

$$Q(\mathbf{x}+\mathbf{L}) = e^{i\mathbf{k}_{\mathrm{B}}\cdot\mathbf{L}}Q(\mathbf{x}) \tag{2}$$

where $\mathbf{L}$ is any lattice vector and $\mathbf{k}_{\mathrm{B}}$ is the Bloch wavevector.

The fields of a point dipole, equation (1), do *not* satisfy (2), and hence may not be used in Bloch-periodic SCUFF-EM calculations. Instead, what we can simulate in the periodic case are the fields of an infinite phased *array* of point electric dipoles,

$$\mathbf{E}^{\mathrm{EDA}}\Big(\mathbf{x};\{\mathbf{x}_0,\mathbf{p}_0,\mathbf{k}_{\mathrm{B}}\}\Big) = \sum_{\mathbf{L}} e^{i\mathbf{k}_{\mathrm{B}}\cdot\mathbf{L}}\,\mathbf{E}^{\mathrm{ED}}\Big(\mathbf{x};\{\mathbf{x}_0+\mathbf{L},\mathbf{p}_0\}\Big), \tag{3a}$$

$$\mathbf{H}^{\mathrm{EDA}}\Big(\mathbf{x};\{\mathbf{x}_0,\mathbf{p}_0,\mathbf{k}_{\mathrm{B}}\}\Big) = \sum_{\mathbf{L}} e^{i\mathbf{k}_{\mathrm{B}}\cdot\mathbf{L}}\,\mathbf{H}^{\mathrm{ED}}\Big(\mathbf{x};\{\mathbf{x}_0+\mathbf{L},\mathbf{p}_0\}\Big), \tag{3b}$$

(where "EDA" stands for "electric dipole array"). The quantities we can compute in a single SCUFF-EM scattering calculation are now the periodically phased versions of the DGFs, i.e. (suppressing ω arguments),

$$\overline{\mathcal{G}^{\mathrm{E}}_{ij}}(\mathbf{x},\mathbf{x}',\mathbf{k}_{\mathrm{B}}) \equiv \sum_{\mathbf{L}} e^{i\mathbf{k}_{\mathrm{B}}\cdot\mathbf{L}}\mathcal{G}^{\mathrm{E}}_{ij}(\mathbf{x},\mathbf{x}'-\mathbf{L}), \tag{4}$$

with $\overline{\mathcal{G}^{\mathrm{M}}_{ij}}$ defined similarly. (Here and elsewhere, barred symbols denote Bloch-periodic quantities.) To recover the non-periodic Green's function—that is, the response of our periodic geometry to a *non-periodic* point source—we must perform a Brillouin-zone integration:[2]

$$\mathcal{G}^{\mathrm{E}}_{ij}(\mathbf{x},\mathbf{x}') = \frac{1}{\mathcal{V}_{\mathrm{BZ}}}\int_{\mathrm{BZ}} \overline{\mathcal{G}^{\mathrm{E}}_{ij}}(\mathbf{x},\mathbf{x}',\mathbf{k}_{\mathrm{B}})\,d\mathbf{k}_{\mathrm{B}}. \tag{5}$$

and similarly for $\mathcal{G}^{\mathrm{M}}$.

Evaluation of BZ integrals

The SCUFF-EM API offers a routine for computing the integrand of (5) for given evaluation and source points $\mathbf{x},\mathbf{x}'$ and Bloch vector $\mathbf{k}_{\mathrm{B}}$. To get the full Green's function on the LHS requires a numerical cubature over the Brillouin zone.

[2] To derive these equations, multiply both sides of (4) by $e^{-i\mathbf{k}_{\mathrm{B}}\cdot\mathbf{L}'}$, integrate both sides over the Brillouin zone, and use the condition

$$\int_{\mathrm{BZ}} e^{i\mathbf{k}_{\mathrm{B}}\cdot(\mathbf{L}-\mathbf{L}')}\,d\mathbf{k} = \mathcal{V}_{\mathrm{BZ}}\,\delta(\mathbf{L},\mathbf{L}')$$

where $\mathcal{V}_{\mathrm{BZ}}$ is the Brillouin-zone volume [for example, a square lattice with basis vectors $\{\mathbf{L}_1,\mathbf{L}_2\} = \{L_x\hat{\mathbf{x}}, L_y\hat{\mathbf{y}}\}$ has $\mathcal{V}_{\mathrm{BZ}} = 4\pi^2/(L_xL_y)$]. Setting $\mathbf{L}'=0$ recovers (5).

For a 2D square lattice with lattice vectors $\mathbf{L}_1 = L_x\hat{\mathbf{x}}, \mathbf{L}_2 = L_y\hat{\mathbf{x}}$, a set of reciprocal-lattice basis vectors is $\mathbf{\Gamma}_1 = \left(\frac{2\pi}{L_x}\right)\hat{\mathbf{x}}, \mathbf{\Gamma}_2 = \left(\frac{2\pi}{L_y}\right)\hat{\mathbf{y}}$, and Brillouin-zone integrals take the form

$$\frac{1}{\mathcal{V}_{\text{BZ}}}\int_{\text{BZ}} f(\mathbf{k}_{\text{B}})\,d\mathbf{k}_{\text{B}} = 4\int_0^{1/2} du_1 \int_0^{1/2} du_2\, f\Big(u_1\mathbf{\Gamma}_1 + u_y\mathbf{\Gamma}_2\Big)$$

3 API Routines for computing dyadic Green's functions

The SCUFF-EM API routine that computes the quantity $\overline{\mathcal{G}^{\mathrm{E}}_{ij}}(\mathbf{x}, \mathbf{x}', k^{\mathrm{B}})$ in equation (5) is

```
void RWGGeometry::GetDyadicGFs(double XEval[3], double XSource[3],
                               cdouble Omega, double kBloch[2],
                               HMatrix *M, HVector *KN,
                               cdouble GEScat[3][3],
                               cdouble GMScat[3][3],
                               cdouble GETot[3][3],
                               cdouble GMTot[3][3]);
```

For cases in which $\mathbf{x} = \mathbf{x}'$ and we need only the scattering parts of the DGFs, there is a simpler interface:

```
void RWGGeometry::GetDyadicGFs(double X[3], cdouble Omega,
                               double *kBloch,
                               HMatrix *M, HVector *KN,
                               cdouble GEScat[3][3],
                               cdouble GMScat[3][3]);
```

In this routine, the input parameters are as follows:

- `X[0..2]` are the Cartesian coordinates of the evaluation point
- `Omega` is the angular frequency in units of 3×10^{14} rad/sec
- `kBloch[0,1]` are the x and y components of the Bloch vector
- `M` is the LU-factorized BEM matrix—that is, the result of calling `AssembleBEMMatrix()` followed by `LUFactorize()`)
- `KN` is a user-allocated RHS vector (allocated, for example, by saying `KN=G->AllocateRHSVector`) which is used internally as a workspace and needs only to be allocated, not initialized in any way

The output parameters are:

- `GEScat[i][j], GMScat[i][j]]` are the Cartesian components of the electric and magnetic scattering DGFs.

A Fields of a phased array of point dipole radiators

To compute dyadic Green's functions in periodic geometries, SCUFF-LDOS solves a scattering problem in which the incident fields originate from a an infinite phased array of point sources. Here I describe the calculation of these infinite fields. This calculation is implemented by the `PointSource` class in the LIBINCFIELD module in SCUFF-EM.

Fields of a single point dipole

First consider a single point electric dipole radiator (not an array) with dipole moment $\mathbf{p}_0$ at a point $\mathbf{x}_0$ in a medium with relative permittivity and permeability ϵ^r, μ^r (as usual suppressing time-dependence factors of $e^{-i\omega t}$). The fields at $\mathbf{x}$ due to this source are

$$\begin{aligned}
\mathbf{E}^{\text{ED}}(\mathbf{x};\mathbf{x}_0,\mathbf{p}_0) &= \frac{|\mathbf{p}_0|}{\epsilon_0\epsilon^r}\cdot\frac{e^{ikr}}{4\pi r^3}\cdot\Big[f_1(ikr)\hat{\mathbf{p}}_\mathbf{0}+f_2(ikr)(\hat{\mathbf{r}}\cdot\hat{\mathbf{p}}_\mathbf{0})\hat{\mathbf{r}}\Big]\\
\mathbf{H}^{\text{ED}}(\mathbf{x};\mathbf{x}_0,\mathbf{p}_0) &= \frac{1}{Z_0Z^r}\cdot\frac{|\mathbf{p}_0|}{\epsilon_0\epsilon^r}\cdot\frac{e^{ikr}}{4\pi r^3}\cdot\Big[f_3(ikr)(\hat{\mathbf{r}}\times\hat{\mathbf{p}}_\mathbf{0})\Big]
\end{aligned}$$

$$\mathbf{r}=|\mathbf{x}-\mathbf{x}_0|,\qquad r=|\mathbf{r}|,\qquad \hat{\mathbf{r}}=\frac{\mathbf{r}}{r},$$

$$f_1(x)=-1+x-x^2,\qquad f_2(x)=3-3x+x^2,\qquad f_3(x)=x-x^2.$$

An alternative way to understand these fields is to think of the point dipole $\mathbf{p}_0$ at $\mathbf{x}_0$ as a localized volume current distribution,

$$\mathbf{J}(\mathbf{x})=-i\omega\mathbf{p}_0\delta(\mathbf{x}-\mathbf{x}_0) \tag{6}$$

in which case it is easy to compute the fields at $\mathbf{x}$ by convolving with the usual (free-space) dyadic Green's functions relating currents to fields:

$$\begin{aligned}
E_i(\mathbf{x}) &= \int\Gamma^{\text{EE}}_{ij}(\mathbf{x},\mathbf{x}')J_j(\mathbf{x}')d\mathbf{x}'\\
&= -i\omega\Gamma^{\text{EE}}_{ij}(\mathbf{x},\mathbf{x}_0)p_{0j}\\
&= (-i\omega)(ikZ_0Z^r)G_{ij}(\mathbf{x},\mathbf{x}_0)p_{0j}\\
&= +k^2\cdot\frac{|\mathbf{p}_0|}{\epsilon_0\epsilon^r}\cdot G_{ij}(\mathbf{x},\mathbf{x}_0)\hat{p}_{0j}
\end{aligned} \tag{7a}$$

$$\begin{aligned}
H_i(\mathbf{x}) &= \int\Gamma^{\text{ME}}_{ij}(\mathbf{x},\mathbf{x}')J_j(\mathbf{x}')d\mathbf{x}'\\
&= -i\omega\Gamma^{\text{ME}}_{ij}(\mathbf{x},\mathbf{x}_0)p_{0j}\\
&= (-i\omega)(-ik)C_{ij}(\mathbf{x},\mathbf{x}_0)p_{0j}\\
&= -\frac{k^2}{Z_0Z^r}\cdot\frac{|\mathbf{p}|}{\epsilon_0\epsilon^r}\cdot C_{ij}(\mathbf{x},\mathbf{x}_0)\hat{p}_{0j}
\end{aligned} \tag{7b}$$

where the $\mathbf{G}$ and $\mathbf{C}$ dyadics are related to the scalar Helmholtz Green's function according to

$$G_{ij}(\mathbf{r}) = \Big[\delta_{ij} + \frac{1}{k^2}\partial_i\partial_j\Big]G_0(\mathbf{r}), \qquad C_{ij}(\mathbf{r}) = \frac{1}{ik}\varepsilon_{ijk}\partial_k G_0(\mathbf{r}). \tag{8}$$

Note that the $\mathbf{E}$ and $\mathbf{H}$ fields due to an electric current distribution $\mathbf{J}$ are

$$\mathbf{E}(\mathbf{x}) = ikZ_0\int \mathbf{G}(\mathbf{x}-\mathbf{x}')\cdot\mathbf{J}(\mathbf{x}'), \qquad \mathbf{H}(\mathbf{x}) = -ik\int \mathbf{C}(\mathbf{x}-\mathbf{x}')\cdot\mathbf{J}(\mathbf{x}'). \tag{9}$$

Fields of a phased array of point dipoles, take 1

Now consider the fields of a phased array of electric dipoles of dipole moment $\mathbf{p}_0$ located at $\mathbf{x}_0$ in the lattice unit cell. A first way to get the fields of this array is to start with equations (7) and (8), but replace the non-periodic scalar Green's function G_0 with its Bloch-periodic version,

$$G_0(\mathbf{x}-\mathbf{x}') \qquad \longrightarrow \qquad \overline{G_0}(\mathbf{x},\mathbf{x}';\mathbf{k}_{\text{B}}) \equiv \sum_{\mathbf{L}} e^{i\mathbf{k}_{\text{B}}\cdot\mathbf{L}}\, G_0(\mathbf{x}-\mathbf{x}'-\mathbf{L}).$$

Then the components of the fields of an electric dipole array, equation (3), read

$$\begin{aligned} E_i^{\text{EDA}}(\mathbf{x}) &= k^2\cdot\frac{|\mathbf{p}_0|}{\epsilon_0\epsilon^r}\left[\delta_{ij} + \frac{1}{k^2}\partial_i\partial_j\right]\overline{G}_0(\mathbf{x}-\mathbf{x}')\hat{p}_{0j} \\ H_i^{\text{EDA}}(\mathbf{x}) &= \frac{ik}{Z_0 Z^r}\cdot\frac{|\mathbf{p}_0|}{\epsilon_0\epsilon^r}\cdot\epsilon_{ijk}\partial_k\overline{G}_0(\mathbf{x}-\mathbf{x}')\hat{p}_{0j}. \end{aligned}$$

Fields of a phased array of point dipoles, take 2

An alternative way to get the fields of a point array of dipoles, which is useful for the half-space calculation of the following section, is to start with the two-dimensional Fourier representation of the (non-periodic) homogeneous dyadic Green's functions. These follow from the two-dimensional Fourier representation of of the non-periodic scalar Green's function:

$$G_0(\mathbf{r}) = \frac{e^{ik_0|\mathbf{r}|}}{4\pi|\mathbf{r}|} = \frac{i\pi}{2}\int_{\mathbb{R}^2}\frac{d^2\mathbf{k}}{(2\pi)^2}\frac{e^{i(k_x x + k_y y + ik_z|z|)}}{k_z}, \qquad k_z \equiv \sqrt{k_0^2 - k_x^2 - k_y^2}$$

Applying (8), we obtain the 2D Fourier expansion of the dyadic Green's functions:

$$\mathbf{G}(\boldsymbol{\rho},z) = \int_{\mathbb{R}^2}\frac{d\mathbf{k}}{(2\pi)^2}\mathbf{g}(\boldsymbol{\rho},z;\mathbf{k}), \qquad \mathbf{C}(\boldsymbol{\rho},z) = \int_{\mathbb{R}^2}\frac{d\mathbf{k}}{(2\pi)^2}\mathbf{c}(\boldsymbol{\rho},z;\mathbf{k}), \tag{10}$$

$$\mathbf{g}(\boldsymbol{\rho},z;\mathbf{k}) = \left(\frac{i\pi}{2k_0^2 k_z}\right)\begin{pmatrix} k_0^2 - k_x^2 & -k_x k_y & \mp k_z k_x \\ -k_y k_x & k_0^2 - k_y^2 & \mp k_z k_y \\ \mp k_x k_z & \mp k_y k_z & k_0^2 - k_z^2 \end{pmatrix} e^{i\mathbf{k}\cdot\boldsymbol{\rho}}e^{ik_z|z|} \tag{11a}$$

$$\mathbf{c}(\boldsymbol{\rho},z;\mathbf{k}) = \left(\frac{i\pi}{2k_0 k_z}\right)\begin{pmatrix} 0 & \pm k_z & -k_y \\ \mp k_z & 0 & k_x \\ k_y & -k_x & 0 \end{pmatrix} e^{i\mathbf{k}\cdot\boldsymbol{\rho}}e^{ik_z|z|} \tag{11b}$$

where the $\pm$ sign is $\text{sign}(z)$. Now reinterpret the infinite integrals over the entire k_x, k_y plane in (10) as finite integrals over just the Brillouin zone;

$$\mathbf{G}(\boldsymbol{\rho}, z) = \int_0^{\Gamma_x} dk_x \int_0^{\Gamma_y} dk_y \, \frac{d\mathbf{k}}{(2\pi)^2} \overline{\mathbf{g}}(\boldsymbol{\rho}, z; \mathbf{k}), \qquad \mathbf{C}(\boldsymbol{\rho}, z) = \int_0^{\Gamma_x} dk_x \int_0^{\Gamma_y} dk_y \, \frac{d\mathbf{k}}{(2\pi)^2} \overline{\mathbf{c}}(\boldsymbol{\rho}, z; \mathbf{k}), \tag{12}$$

$$\begin{aligned} \overline{\mathbf{g}}(\boldsymbol{\rho}, z; k_x, k_y) &= \sum_{n_x, n_y = -\infty}^{\infty} \mathbf{g}\Big(\boldsymbol{\rho}, z; k_x + n_x \boldsymbol{\Gamma}_x, k_y + n_y \boldsymbol{\Gamma}_y\Big), \\ \overline{\mathbf{c}}(\boldsymbol{\rho}, z; k_x, k_y) &= \sum_{n_x, n_y = -\infty}^{\infty} \mathbf{c}\Big(\boldsymbol{\rho}, z; k_x + n_x \boldsymbol{\Gamma}_x, k_y + n_y \boldsymbol{\Gamma}_y\Big). \end{aligned}$$

If I think of (12) as equations of the form (5), i.e. equations relating non-barred quantities to Brillouin-zone integrals over barred quantities, I can identify the Bloch-periodic versions of the dyadic Green's functions as

$$\overline{\mathbf{G}}\Big(\boldsymbol{\rho}, z; \mathbf{k}^{\text{B}}\Big) = \frac{\mathcal{V}^{\text{BZ}}}{(2\pi)^2} \overline{\mathbf{g}}\big(\boldsymbol{\rho}, z; \mathbf{k}^{\text{B}}\big), \qquad \overline{\mathbf{C}}\Big(\boldsymbol{\rho}, z; \mathbf{k}^{\text{B}}\Big) = \frac{\mathcal{V}^{\text{BZ}}}{(2\pi)^2} \overline{\mathbf{c}}\big(\boldsymbol{\rho}, z; \mathbf{k}^{\text{B}}\big).$$

B Analytical expressions for the dyadic Green's functions of a dielectric half-space

For testing purposes it is useful to have analytical expressions for the dyadic Green's functions above an infinite half space. These are obtained via a two-step process:

1. First we express the fields of a point source above a dielectric half-space as a superposition of plane waves; in particular, the fields impinging upon the half-space are a linear combination of downward-traveling plane waves.
2. Then we reason that each individual plane wave is reflected from the interface with the usual Fresnel reflection coefficient, and thus the scattered field is just the same superposition of plane waves with which we began, except that **(1)** now the plane waves are traveling *upward*, and **(2)** each plane wave comes multiplied by the Fresnel reflection coefficients for the dielectric interface.

This procedure is worked out in more detail in the following sections.

B.1 Plane-wave decomposition of non-periodic point-source fields

Note: In what follows, $\mathbf{k}=(k_x,k_y)$ is a *two-dimensional* vector and we have

$$k_z \equiv \sqrt{k_0^2-|\mathbf{k}|^2}, \qquad \mathbf{k}_{\text{3D}} \equiv \left(\begin{array}{c} k_x \\ k_y \\ \pm k_z \end{array}\right), \qquad \pm \equiv \begin{cases} +, & z\ge 0 \\ -, & z<0 \end{cases}.$$

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

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

$$E_0 \equiv 1\text{ volt}/\mu\text{m}, \qquad H_0 \equiv \frac{E_0}{Z_0}.$$

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").

$$\mathbf{P}(\mathbf{k}) \equiv \frac{1}{|\mathbf{k}|}\left(\begin{array}{c} -k_y \\ k_x \\ 0 \end{array}\right), \qquad \overline{\mathbf{P}}(\mathbf{k}) \equiv \frac{1}{k_0}\Big[\mathbf{k}_{\text{3D}}\times\mathbf{P}(\mathbf{k})\Big] = \frac{1}{k_0|\mathbf{k}|}\left(\begin{array}{c} \mp k_x k_z \\ \mp k_y k_z \\ k_x^2+k_y^2 \end{array}\right)$$

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

The trick is now to notice that the columns of the 3×3 matrices in equation (11) may be written as linear combinations of $\mathbf{P}$ and $\overline{\mathbf{P}}$. For example, the leftmost column of the matrix that enters the definition of $\mathbf{g}$ is

$$\left(\begin{array}{c} k_0^2-k_x^2 \\ -k_yk_x \\ \mp k_xk_z\end{array}\right) = -\left(\frac{k_0^2k_y}{|\mathbf{k}|}\right)\mathbf{P}(\mathbf{k}) \mp \left(\frac{k_0k_xk_z}{|\mathbf{k}|}\right)\overline{\mathbf{P}}(\mathbf{k}). \tag{13}$$

The fields of an $\hat{\mathbf{x}}$-directed point dipole source $\mathbf{p}_0 = p_0\hat{\mathbf{x}}$ (a single point source, not an array) located a height z_0 above the xy plane then read, from (9) and (6),

$$\mathbf{E}^{\text{ED}}\Big(\mathbf{x};\{z_0\hat{\mathbf{z}};\hat{\mathbf{x}}\}\Big) = ik_0Z_0\left(\begin{array}{c} G_{xx} \\ G_{yx} \\ G_{zx}\end{array}\right)(-i\omega p_0) = \frac{p_0}{\epsilon_0}k_0^2\left(\begin{array}{c} G_{xx} \\ G_{yx} \\ G_{zx}\end{array}\right)$$

Insert (10):

$$\mathbf{E}^{\text{ED}}\Big(\mathbf{x};\{z_0\hat{\mathbf{z}};\hat{\mathbf{x}}\}\Big) = \frac{p_0}{\epsilon_0}k_0^2\int_{\mathbb{R}^2}\frac{d\mathbf{k}}{(2\pi)^2}\left(\begin{array}{c} g_{xx} \\ g_{yx} \\ g_{zx}\end{array}\right)$$

Insert (11) and (13:

$$= \frac{p_0}{\epsilon_0}k_0^2\int_{\mathbb{R}^2}\frac{d\mathbf{k}}{(2\pi)^2}\left(\frac{i\pi}{2k_0^2k_z}\right)\left[-\left(\frac{k_0^2k_y}{|\mathbf{k}|}\right)\mathbf{P}(\mathbf{k}) \mp \left(\frac{k_0k_xk_z}{|\mathbf{k}|}\right)\overline{\mathbf{P}}(\mathbf{k})\right]e^{i\mathbf{k}\cdot\boldsymbol{\rho}}e^{ik_z|z-z_0|}.$$

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 a point source:

$$\mathbf{E}^{\text{ED}}\Big(\mathbf{x};\big\{z_0\hat{\mathbf{z}},\hat{\mathbf{x}}\big\}\Big) = \left(\frac{p_0}{\epsilon_0E_0}\right)\int\frac{d\mathbf{k}}{(2\pi)^2}\Big\{C^{x}_{\text{TE}}(\mathbf{k})\mathbf{E}^{\pm}_{\text{TE}}\Big(\mathbf{x}-z_0\hat{\mathbf{z}};\mathbf{k}\Big) + C^{x;\pm}_{\text{TM}}(\mathbf{k})\mathbf{E}^{\pm}_{\text{TM}}\Big(\mathbf{x}-z_0\hat{\mathbf{z}};\mathbf{k}\Big)\Big\} \tag{14a}$$

$$\mathbf{E}^{\text{ED}}\Big(\mathbf{x};\big\{z_0\hat{\mathbf{z}},\hat{\mathbf{y}}\big\}\Big) = \left(\frac{p_0}{\epsilon_0E_0}\right)\int\frac{d\mathbf{k}}{(2\pi)^2}\Big\{C^{y}_{\text{TE}}(\mathbf{k})\mathbf{E}^{\pm}_{\text{TE}}\Big(\mathbf{x}-z_0\hat{\mathbf{z}};\mathbf{k}\Big) + C^{y;\pm}_{\text{TM}}(\mathbf{k})\mathbf{E}^{\pm}_{\text{TM}}\Big(\mathbf{x}-z_0\hat{\mathbf{z}};\mathbf{k}\Big)\Big\} \tag{14b}$$

$$\mathbf{E}^{\text{ED}}\Big(\mathbf{x};\big\{z_0\hat{\mathbf{z}},\hat{\mathbf{z}}\big\}\Big) = \left(\frac{p_0}{\epsilon_0E_0}\right)\int\frac{d\mathbf{k}}{(2\pi)^2}\Big\{C^{z}_{\text{TE}}(\mathbf{k})\mathbf{E}^{\pm}_{\text{TE}}\Big(\mathbf{x}-z_0\hat{\mathbf{z}};\mathbf{k}\Big) + C^{z}_{\text{TM}}(\mathbf{k})\mathbf{E}^{\pm}_{\text{TM}}\Big(\mathbf{x}-z_0\hat{\mathbf{z}};\mathbf{k}\Big)\Big\} \tag{14c}$$

where the scalar coefficients are

$$\begin{array}{rclcrcl} C^{x}_{\text{TE}} &=& -\dfrac{i\pi k_0^2k_y}{2|\mathbf{k}|k_z} && C^{x;\pm}_{\text{TM}} &=& \pm\dfrac{i\pi k_0k_x}{2|\mathbf{k}|} \\ C^{y}_{\text{TE}} &=& \dfrac{i\pi k_0^2k_x}{2|\mathbf{k}|k_z} && C^{y;\pm}_{\text{TM}} &=& \pm\dfrac{i\pi k_0k_y}{2|\mathbf{k}|} \\ C^{z}_{\text{TE}} &=& 0 && C^{z}_{\text{TM}} &=& \dfrac{i\pi k_0|\mathbf{k}|}{2k_z}. \end{array}$$

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)

$$\begin{aligned}\left[\left(\frac{p_0}{\epsilon_0 E_0}\right)\right] &= \Big[p_0\Big]\Big[\epsilon_0\Big]^{-1}\Big[E_0\Big]^{-1} \\ &= \frac{\mathrm{C}\cdot\mathrm{L}}{\mathrm{CV}^{-1}\mathrm{L}^{-1}\mathrm{VL}^{-1}} \\ &= (\text{length})^3.\end{aligned}$$

B.2 Plane-wave decomposition of non-periodic DGFs

The point of the above decomposition is that each plane wave is reflected from a dielectric interface at $z = 0$ with the usual Fresnel reflection coefficients $r^{\text{TE,TM}}(\mathbf{k})$, and thus the scattered fields (evaluated at the location of the source point) due to an $x-, y-$, or z-directed dipole at height z_0 are

$$\mathbf{E}^{\text{scat,x}} = \left(\frac{p_0}{\epsilon_0 E_0}\right)\int \frac{d\mathbf{k}}{(2\pi)^2}\left\{r_{\text{TE}}(\mathbf{k})C^{x}_{\text{TE}}(\mathbf{k})\mathbf{E}^{+}_{\text{TE}}\Big(2z_0\hat{\mathbf{z}};\mathbf{k}\Big) + r_{\text{TM}}(\mathbf{k})C^{x;-}_{\text{TM}}(\mathbf{k})\mathbf{E}^{+}_{\text{TM}}\Big(2z_0\hat{\mathbf{z}};\mathbf{k}\Big)\right\} \tag{15a}$$

$$\mathbf{E}^{\text{scat,y}} = \left(\frac{p_0}{\epsilon_0 E_0}\right)\int \frac{d\mathbf{k}}{(2\pi)^2}\left\{r_{\text{TE}}(\mathbf{k})C^{y}_{\text{TE}}(\mathbf{k})\mathbf{E}^{+}_{\text{TE}}\Big(2z_0\hat{\mathbf{z}};\mathbf{k}\Big) + r_{\text{TM}}(\mathbf{k})C^{y;-}_{\text{TM}}(\mathbf{k})\mathbf{E}^{+}_{\text{TM}}\Big(2z_0\hat{\mathbf{z}};\mathbf{k}\Big)\right\} \tag{15b}$$

$$\mathbf{E}^{\text{scat,z}} = \left(\frac{p_0}{\epsilon_0 E_0}\right)\int \frac{d\mathbf{k}}{(2\pi)^2}\left\{r_{\text{TE}}(\mathbf{k})C^{z}_{\text{TE}}(\mathbf{k})\mathbf{E}^{+}_{\text{TE}}\Big(2z_0\hat{\mathbf{z}};\mathbf{k}\Big) + r_{\text{TM}}(\mathbf{k})C^{z}_{\text{TM}}(\mathbf{k})\mathbf{E}^{+}_{\text{TM}}\Big(2z_0\hat{\mathbf{z}};\mathbf{k}\Big)\right\} \tag{15c}$$

where the Fresnel coefficients are

$$r_{\text{TE}}(\mathbf{k}) = \frac{\sqrt{k_0^2-\mathbf{k}^2} - \sqrt{\epsilon k_0^2 - \mathbf{k}^2}}{\sqrt{k_0^2-\mathbf{k}^2} + \sqrt{\epsilon k_0^2 - \mathbf{k}^2}}, \qquad r_{\text{TM}}(\mathbf{k}) = \frac{\epsilon\sqrt{k_0^2-\mathbf{k}^2} - \sqrt{\epsilon k_0^2 - \mathbf{k}^2}}{\epsilon\sqrt{k_0^2-\mathbf{k}^2} + \sqrt{\epsilon k_0^2 - \mathbf{k}^2}}.$$

Note that the $\mathbf{E}_{\text{TE,TM}}$ here involve the $+$ sign, since the reflected waves are upward-traveling; but the C coefficients involve the $-$ sign, because these were the coefficients of the original downward-traveling plane waves that impinged on the interface.

B.3 Plane-wave decomposition of periodic DGFs

To obtain expressions for the incident and scattered fields of a Bloch-phased *array* of point sources, we first rewrite expressions (14) and (15) for the non-periodic incident and scattered fields as integrals over the Brillouin zone. For example, the fields of a (non-periodic) $\mathbf{x}$-directed source at $\mathbf{x}_0 = z_0\hat{\mathbf{z}}$ are

$$\begin{aligned}
&\mathbf{E}^{\text{ED}}\Big(\mathbf{x};\big\{z_0\hat{\mathbf{z}},\hat{\mathbf{x}}\big\}\Big) \\
&\qquad = \left(\frac{p_0}{\epsilon_0 E_0}\right)\int_{\text{BZ}}\frac{d\mathbf{k}_{\text{B}}}{(2\pi)^2}\sum_{\mathbf{\Gamma}}\Big\{C^{x}_{\text{TE}}(\mathbf{k}_{\text{B}}+\mathbf{\Gamma})\mathbf{E}^{\pm}_{\text{TE}}\Big(\mathbf{x}-z_0\hat{\mathbf{z}};\mathbf{k}_{\text{B}}+\mathbf{\Gamma}\Big) \\
&\qquad\qquad + C^{x;\pm}_{\text{TM}}(\mathbf{k}+\mathbf{\Gamma})\mathbf{E}^{\pm}_{\text{TM}}\Big(\mathbf{x}-z_0\hat{\mathbf{z}};\mathbf{k}_{\text{B}}+\mathbf{\Gamma}\Big)\Big\}
\end{aligned}$$

and the corresponding scattered fields evaluated at the location of the dipole are

$$\begin{aligned}
&\mathbf{E}^{\text{scat}} \\
&\quad = \left(\frac{p_0}{\epsilon_0 E_0}\right)\int_{\text{BZ}}\frac{d\mathbf{k}_{\text{B}}}{(2\pi)^2}\sum_{\mathbf{\Gamma}}\Big\{r_{\text{TE}}(\mathbf{k}_{\text{B}}+\mathbf{\Gamma})C^{x}_{\text{TE}}(\mathbf{k}_{\text{B}}+\mathbf{\Gamma})\mathbf{E}^{+}_{\text{TE}}\Big(2z_0\hat{\mathbf{z}};\mathbf{k}_{\text{B}}+\mathbf{\Gamma}\Big) \\
&\qquad\qquad + r_{\text{TM}}(\mathbf{k}_{\text{B}}+\mathbf{\Gamma})C^{x;-}_{\text{TM}}(\mathbf{k}+\mathbf{\Gamma})\mathbf{E}^{+}_{\text{TM}}\Big(2z_0\hat{\mathbf{z}};\mathbf{k}_{\text{B}}+\mathbf{\Gamma}\Big).\Big\}
\end{aligned}$$

Here k_{B} lives in the Brillouin zone—it is a Bloch vector—and the sum is over all reciprocal lattice vectors $\mathbf{\Gamma}$.

C Rewriting infinite 2D k-integrals as Brillouin-zone integrals

One frequently encounters quantities expressed as infinite $\mathbf{k}-$space integrals, i.e. integrals over a two-dimensional wavevector $\mathbf{k}$ that ranges over all of $\mathbb{R}_2$:

$$I = \int_{\mathbb{R}^2} \frac{d^2\mathbf{k}}{(2\pi)^2} Q(\mathbf{k}).$$

Examples include equations (10) and To rewrite such integrals in a form that facilitates comparison with SCUFF-LDOS calculations, it is convenient to recast such integrals as Brillouin-zone integrations:

$$I = \int_{\text{BZ}} \frac{d^2\mathbf{k}}{(2\pi)^2} \overline{Q}(\mathbf{k}),$$

where $\overline{Q}(\mathbf{k})$ is the sum of the integrand function $Q(\mathbf{k})$ evaluated at $\mathbf{k}$ and all images of $\mathbf{k}$ under translation by reciprocal-lattice vectors

$$\overline{Q}(\mathbf{x}) = \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} Q\big(\mathbf{k} + n_1\boldsymbol{\Gamma}_1 + n_2\boldsymbol{\Gamma}_2\big)$$

where $\boldsymbol{\Gamma}_1, \boldsymbol{\Gamma}_2$ are a basis for the reciprocal lattice. (We have here considered the 2D-periodic case, but the 1D-periodic case is similar).