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

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Contents

1 Notation and conventions

Before doing anything we recall our notation and conventions for dyadic Green's functions (DGFs) and local densities of states (LDOS).

Dyadic Green's functions

I use the symbol $\mathbf{\Gamma} = \begin{pmatrix} \mathbf{\Gamma}^{\mathrm{EE}} & \mathbf{\Gamma}^{\mathrm{EM}} \\ \mathbf{\Gamma}^{\mathrm{ME}} & \mathbf{\Gamma}^{\mathrm{MM}} \end{pmatrix}$ for the 6x6 dyadic Green's function giving the electric and magnetic fields produced by time-harmonic electric and magnetic volume currents $\mathbf{J}, \mathbf{M}$:

$$\left\{ \begin{array}{c} E_i(\mathbf{x}) \\ H_i(\mathbf{x}) \end{array} \right\} = \int \left(\begin{array}{cc} \Gamma^{\mathrm{EE}}_{ij}(\omega;\mathbf{x};\mathbf{x}') & \Gamma^{\mathrm{EM}}_{ij}(\omega;\mathbf{x};\mathbf{x}') \\ \Gamma^{\mathrm{ME}}_{ij}(\omega;\mathbf{x};\mathbf{x}') & \Gamma^{\mathrm{MM}}_{ij}(\omega;\mathbf{x};\mathbf{x}') \end{array} \right) \left(\begin{array}{c} J_j(\mathbf{x}') \\ M_j(\mathbf{x}') \end{array} \right) dV,$$

where all fields and currents are understood to have time dependence $\sim e^{-i\omega t}$. In general $\mathbf{\Gamma}$ can be decomposed as the sum of a homogeneous part (direct contribution of sources to fields in an infinite homogeneous medium) plus a scattering part:

$$\mathbf{\Gamma} = \mathbf{\Gamma}^0 + \mathbf{\Gamma}^{\mathrm{scat}} \tag{1}$$

The homogeneous part may be written down in closed analytical form (see below), while the scattering part typically requires a numerical solver like SCUFF-EM.

Homogenenous DGFs

In a homogeneous material region with relative permittivity and permeability $\{\epsilon^r, \mu^r\}$, the four quadrants of the 6×6 tensor $\mathbf{\Gamma}^0$ may be expressed in terms of two 3×3 tensors $\mathbb{G}, \mathbb{C}$:

$$\mathbf{\Gamma}^{0,\mathrm{EE}} = ikZ_0Z^r\mathbb{G} \tag{2a}$$

$$\mathbf{\Gamma}^{0,\mathrm{EM}} = ik\mathbb{C} \tag{2b}$$

$$\mathbf{\Gamma}^{0,\mathrm{ME}} = -ik\mathbb{C} \tag{2c}$$

$$\mathbf{\Gamma}^{0,\mathrm{MM}} = \frac{ik}{Z_0Z^r}\mathbb{G} \tag{2d}$$

where $k = \sqrt{\epsilon^r\mu^r} \cdot \omega/c$ is the photon wavenumber in the medium (c is the vacuum speed of light), $Z^r = \sqrt{\frac{\mu^r}{\epsilon^r}}$ is the dimensionless relative wave impedance, $Z_0 \approx 377\,\Omega$ is the impedance of free space, and the $\mathbb{G}$ and $\mathbb{C}$ tensors are

$$\mathbb{G}_{ij}(k,\mathbf{r}) = \frac{e^{ikr}}{4\pi(ik)^2r^3}\left[\Big(1 - ikr + (ikr)^2\Big)\delta_{ij} + \Big(-3 + 3ikr - (ikr)^2\Big)\frac{r_ir_j}{r^2}\right] \tag{3a}$$

$$\mathbb{C}_{ij}(k,\mathbf{r}) = \frac{e^{ikr}}{4\pi(ik)r^3}\varepsilon_{ijk}r_k. \tag{3b}$$

Note that $\mathbb{G}$ and $\mathbb{C}$ have units of inverse length.

The prefactors in (2a,d) may be written in the alternative forms

$$ikZ_0Z_r = i\omega\mu_0\mu^r, \qquad \frac{ik}{Z_0Z_r} = i\omega\epsilon_0\epsilon^r$$

where $\{\epsilon_0, \mu_0\}$ are permittivity and permeability of free space. I prefer the forms in (2) because then I don't have to remember the annoying values or units of $\{\epsilon_0, \mu_0\}$

In the limit $\mathbf{r} \to 0$, the real part of $\mathbb{G}$ blows up, but the imaginary part remains finite and equal to

$$\text{Im } \mathbb{G}_{ij}(k, 0) = \frac{\text{Re } k}{6\pi}\delta_{ij}. \tag{4}$$

LDOS from DGFs

The electric and magnetic local densities of states at a point $\mathbf{r}$ are related to the DGFs according to

$$\rho^{\text{E}}(\omega; \mathbf{r}) = \left(\frac{k}{\pi c}\right) \cdot \left[\frac{1}{ikZ_0Z^r}\text{Tr Im } \mathbf{\Gamma}^{\text{EE}}(\omega; \mathbf{r}, \mathbf{r})\right] \tag{5a}$$

$$\rho^{\text{M}}(\omega; \mathbf{r}) = \left(\frac{k}{\pi c}\right) \cdot \left[\frac{Z_0Z^r}{ik}\text{Tr Im } \mathbf{\Gamma}^{\text{MM}}(\mathbf{r}, \mathbf{r})\right] \tag{5b}$$

where k, Z^r are the wavelength and relative wave impedance of the medium at $\mathbf{r}$.

My rationale for writing the prefactors in (5) the way I do is that the quantities in square brackets have dimensions of inverse length (indeed, in the homogeneous case the quantities in square brackets are both equal to Tr Im $\mathbb{G}$), making it easy to check the units of ρ:

$$\left[\rho^{\text{E,M}}\right] = \left[\frac{k}{\pi c}\right]\left[\frac{1}{\text{length}}\right] = \left[\frac{1}{\text{length}^3 \cdot \text{frequency}}\right]$$

Vacuum LDOS

To get the vacuum LDOS, I insert (2) into (5) and use (4) to get

$$\rho_0^{\text{E}}(\omega) = \rho_0^{\text{M}}(\omega) = \frac{k^2}{2\pi^2 c} = \frac{\omega^3}{2\pi^3 c^3}.$$

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

In the presence of scatterers, the homogeneous DGFs are augmented by contributions from currents induced on the surfaces of material interfaces, cf. (1). In analogy to equations (2a,d), I define electric and magnetic scattering versions of the $\mathbb{G}$ tensor:

$$\begin{aligned}
\mathcal{G}^{\text{E}}_{ij}(\omega;\mathbf{x},\mathbf{x}') &\equiv \frac{1}{ikZ_0Z^r}\mathbf{\Gamma}^{\text{EE,scat}}_{ij}(\omega;\mathbf{x},\mathbf{x}') \\
&= \frac{1}{ikZ_0Z^r}\left(\begin{array}{l} i\text{-component of scattered } \mathbf{E}\text{-field at } \mathbf{x} \text{ due to a unit-} \\ \text{strength } j\text{-directed point } \textbf{electric} \text{ dipole radiator at} \\ \mathbf{x}'\text{, all quantities having time dependence} \sim e^{-i\omega t} \end{array}\right) \\
\mathcal{G}^{\text{M}}_{ij}(\omega;\mathbf{x},\mathbf{x}') &\equiv \frac{Z_0Z^r}{ik}\mathbf{\Gamma}^{\text{MM,scat}}_{ij}(\omega;\mathbf{x},\mathbf{x}') \\
&= \frac{Z_0Z^r}{ik}\left(\begin{array}{l} i\text{-component of scattered } \mathbf{H}\text{-field at } \mathbf{x} \text{ due to a unit-} \\ \text{strength } j\text{-directed point } \textbf{magnetic} \text{ dipole radiator} \\ \text{at } \mathbf{x}'\text{, all quantities having time dependence} \sim e^{-i\omega t} \end{array}\right)
\end{aligned}$$

Like $\mathbb{G}$, the tensors $\boldsymbol{\mathcal{G}}^{\text{E,M}}$ have dimensions of inverse length.

The enhancements of the electric and magnetic LDOS at frequency ω at a point $\mathbf{x}$ in a scattering geometry are related to these scattering DGFs according to

$$\rho^{\text{E}}_{\text{scat}}(\omega;\mathbf{x}) \equiv \frac{k}{\pi c}\text{Tr Im } \boldsymbol{\mathcal{G}}^{\text{E}}(\omega;\mathbf{x},\mathbf{x}), \qquad \rho^{\text{M}}_{\text{scat}}(\omega;\mathbf{x}) \equiv \frac{k}{\pi c}\text{Tr Im } \boldsymbol{\mathcal{G}}^{\text{M}}(\omega;\mathbf{x},\mathbf{x}).$$

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 $\mathbf{x}_{\text{S}}$. For example, to compute $\mathcal{G}^{\text{E}}$ we take the incident fields to be the fields of a unit-strength j-directed point electric dipole source at $\mathbf{x}_{\text{S}}$:

$$\mathbf{E}^{\text{inc}}(\mathbf{x}) = \mathbf{E}^{\text{ED}}\Big(\mathbf{x};\{\mathbf{x}_{\text{S}},\hat{\mathbf{x}}_j\}\Big), \qquad \mathbf{H}^{\text{inc}}(\mathbf{x}) = \mathbf{H}^{\text{ED}}\Big(\mathbf{x};\{\mathbf{x}_{\text{S}},\hat{\mathbf{x}}_j\}\Big) \tag{6}$$

where $\{\mathbf{E},\mathbf{H}\}^{\text{ED}}\Big(\mathbf{x};\{\mathbf{x}_0,\mathbf{p}_0\}\Big)$ are the fields at $\mathbf{x}$ due to 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 (6) and compute the scattered—not total!—fields at the evaluation point $\mathbf{x}_{\text{D}}$. The three components of the $\mathbf{E}$-field at $\mathbf{x}_{\text{D}}$, divided by ikZ_0Z_r, yield the three vertical entries of the jth column of the 3×3 matrix $\boldsymbol{\mathcal{G}}^{\text{E}}(\omega;\mathbf{x}_{\text{D}},\mathbf{x}_{\text{S}}.)$ Calculating $\boldsymbol{\mathcal{G}}^{\text{M}}$ 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.

3 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

$$Q(\mathbf{x}+\mathbf{L}) = e^{i\mathbf{k}_{\text{B}}\cdot\mathbf{L}}Q(\mathbf{x}) \tag{7}$$

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

The fields of a point dipole, equation (6), do *not* satisfy (7), 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,

$$\mathbf{E}^{\text{EDA}}\Big(\mathbf{x};\{\mathbf{x}_0,\mathbf{p}_0,\mathbf{k}_{\text{B}}\}\Big) = \sum_{\mathbf{L}} e^{i\mathbf{k}_{\text{B}}\cdot\mathbf{L}}\,\mathbf{E}^{\text{ED}}\Big(\mathbf{x};\{\mathbf{x}_0+\mathbf{L},\mathbf{p}_0\}\Big), \tag{8a}$$

$$\mathbf{H}^{\text{EDA}}\Big(\mathbf{x};\{\mathbf{x}_0,\mathbf{p}_0,\mathbf{k}_{\text{B}}\}\Big) = \sum_{\mathbf{L}} e^{i\mathbf{k}_{\text{B}}\cdot\mathbf{L}}\,\mathbf{H}^{\text{ED}}\Big(\mathbf{x};\{\mathbf{x}_0+\mathbf{L},\mathbf{p}_0\}\Big), \tag{8b}$$

(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),

$$\overline{\mathcal{G}^{\text{E}}_{ij}}(\mathbf{x},\mathbf{x}',\mathbf{k}_{\text{B}}) \equiv \sum_{\mathbf{L}} e^{i\mathbf{k}_{\text{B}}\cdot\mathbf{L}}\mathcal{G}^{\text{E}}_{ij}(\mathbf{x},\mathbf{x}'+\mathbf{L}), \tag{9}$$

with $\overline{\mathcal{G}^{\text{M}}_{ij}}$ 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:[1]

$$\mathcal{G}^{\text{E}}_{ij}(\mathbf{x},\mathbf{x}') = \frac{1}{\mathcal{V}_{\text{BZ}}}\int_{\text{BZ}} \overline{\mathcal{G}^{\text{E}}_{ij}}(\mathbf{x},\mathbf{x}',\mathbf{k}_{\text{B}})\,d\mathbf{k}_{\text{B}} \tag{10}$$

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

Reciprocity of homogeneous Green's functions

The non-periodic Green's functions $\mathbb{G},\mathbb{C}$ satisfy the reciprocity relations

$$\mathbb{K}_{ji}(\mathbf{r}) = \mathbb{K}_{ij}(-\mathbf{r}).$$

[1] To derive these equations, multiply both sides of (9) by $e^{-i\mathbf{k}_{\text{B}}\cdot\mathbf{L}'}$, integrate both sides over the Brillouin zone, and use the condition

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

where $\mathcal{V}_{\text{BZ}}$ 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 $\mathcal{V}_{\text{BZ}} = 4\pi^2/(L_xL_y)$]. Setting $\mathbf{L}'=0$ recovers (10).

$(\mathbb{K} = \mathbb{G}, \mathbb{C})$. Their periodic counterparts satisfy

$$\begin{aligned}
\overline{\mathbb{K}}_{ji}(\mathbf{r}; \mathbf{k}_{\rm B}) &= \sum_{\mathbf{L}} e^{i\mathbf{k}_{\rm B}\cdot\mathbf{L}} \mathbb{K}_{ji}(\mathbf{r} - \mathbf{L}) \\
&= \sum_{\mathbf{L}} e^{i\mathbf{k}_{\rm B}\cdot\mathbf{L}} \mathbb{K}_{ij}(-\mathbf{r} + \mathbf{L}) \\
&= \sum_{\mathbf{L}} e^{-i\mathbf{k}_{\rm B}\cdot\mathbf{L}} \mathbb{K}_{ij}(-\mathbf{r} - \mathbf{L}) \\
&= \overline{\mathbb{K}}_{ij}(-\mathbf{r}; -\mathbf{k}_{\rm B}).
\end{aligned}$$

Evaluation of BZ integrals

The SCUFF-EM API offers a routine for computing the integrand of (10) for given evaluation and source points $\mathbf{x}, \mathbf{x}'$ and Bloch vector $\mathbf{k}_{\rm B}$. To get the full Green's function on the LHS requires a numerical cubature over the Brillouin zone.

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

$$\frac{1}{\mathcal{V}_{\rm BZ}} \int_{\rm BZ} f(\mathbf{k}_{\rm B})\, d\mathbf{k}_{\rm B} = 4\int_0^{1/2} du_1 \int_0^{1/2} du_2\, f\Big(u_1\mathbf{\Gamma}_1 + u_2\mathbf{\Gamma}_2\Big)$$

4 Vector-matrix-vector product formula for dyadic Green's functions

In the discretized BEM framework we can write convenient vector-matrix-vector product formulas for the scattering parts of the electric and magnetic DGFs. I first derive these for the non-periodic case, then discuss the modifications required to extend to periodic geometries.

4.1 The non-periodic case

VMVP formula for $\boldsymbol{\mathcal{G}}^{\mathrm{E}}$

Consider first the electric DGF $\boldsymbol{\mathcal{G}}^{\mathrm{E}}_{ij}(\mathbf{x}_{\mathrm{D}},\mathbf{x}_{\mathrm{S}})$, where the subscripts stand for "destination" and "source." To get at this, we must solve a scattering problem in which the incident fields are the fields radiated by a j-directed point dipole source $\mathbf{p}=p_0\hat{\mathbf{n}}_j$ at $\mathbf{x}_{\mathrm{S}}$:

$$\left\{\begin{array}{c} E^{\mathrm{inc}}_\ell(\mathbf{x}) \\ \\ H^{\mathrm{inc}}_\ell(\mathbf{x})\end{array}\right\} = -i\omega p_0 \left\{\begin{array}{c} \Gamma^{\mathrm{EE}}_{\ell j}(\mathbf{x},\mathbf{x}_{\mathrm{S}}) \\ \\ \Gamma^{\mathrm{ME}}_{\ell j}(\mathbf{x},\mathbf{x}_{\mathrm{S}})\end{array}\right\} = (-i\omega p_0)\left\{\begin{array}{r} ikZ_0Z^r\mathbb{G}_{\ell j}(\mathbf{x},\mathbf{x}_{\mathrm{S}}) \\ \\ -ik\mathbb{C}_{\ell j}(\mathbf{x},\mathbf{x}_{\mathrm{S}})\end{array}\right\} \tag{11}$$

The scattered electric field at $\mathbf{x}_{\mathrm{D}}$ is obtained from the surface currents $\mathbf{K},\mathbf{N}$ according to

$$E^{\mathrm{scat}}_i(\mathbf{x}_{\mathrm{D}}) = \int \left\{\begin{array}{c} \Gamma^{\mathrm{EE}}_{i\ell}(\mathbf{x}_{\mathrm{D}},\mathbf{x}) \\ \\ \Gamma^{\mathrm{EM}}_{i\ell}(\mathbf{x}_{\mathrm{D}},\mathbf{x})\end{array}\right\}^T \left\{\begin{array}{c} K_\ell(\mathbf{x}) \\ \\ N_\ell(\mathbf{x})\end{array}\right\} d\mathbf{x} \tag{12}$$

$$= \int \left\{\begin{array}{r} ikZ_0Z^r\mathbb{G}_{i\ell}(\mathbf{x}_{\mathrm{D}},\mathbf{x}) \\ \\ +ik\mathbb{C}_{i\ell}(\mathbf{x}_{\mathrm{D}},\mathbf{x})\end{array}\right\}^T \left\{\begin{array}{c} K_\ell(\mathbf{x}) \\ \\ N_\ell(\mathbf{x})\end{array}\right\} d\mathbf{x} \tag{13}$$

Insert the expansions $\mathbf{K}(\mathbf{x})=\sum k_a\mathbf{b}_a(\mathbf{x})$, $\mathbf{N}(\mathbf{x})=-Z_0\sum n_a\mathbf{b}_a(\mathbf{x})$:

$$= \sum_a \left\{\begin{array}{c} ikZ_0Z^r g_a(\mathbf{x}_{\mathrm{D}},\hat{\mathbf{n}}_i) \\ \\ -ikZ_0 c_a(\mathbf{x}_{\mathrm{D}},\hat{\mathbf{n}}_i)\end{array}\right\}^T \left\{\begin{array}{c} k_a \\ \\ n_a\end{array}\right\} \tag{14}$$

where I defined

$$g_a(\mathbf{x}_{\mathrm{D}},\hat{\mathbf{n}}_i) \equiv \int \mathbb{G}_{i\ell}(\mathbf{x}_{\mathrm{D}},\mathbf{x})b_{a\ell}(\mathbf{x})\,d\mathbf{x}, \qquad c_a(\mathbf{x}_{\mathrm{D}},\hat{\mathbf{n}}_i) \equiv \int \mathbb{C}_{i\ell}(\mathbf{x}_{\mathrm{D}},\mathbf{x})b_{a\ell}(\mathbf{x})\,d\mathbf{x}.$$

The surface-current expansion coefficients are obtained by solving the BEM system:

$$\left(\begin{array}{c} k_a \\ n_a\end{array}\right) = -W_{ab}\left(\begin{array}{c} e_b \\ h_b\end{array}\right). \tag{15}$$

Here $\mathbf{W}$ is the inverse BEM matrix and e_b, h_b are the projections of the incident field onto the basis functions:

$$\begin{aligned}
e_b \equiv \frac{1}{Z_0}\Big\langle \mathbf{b}_m \Big| \mathbf{E}^{\text{inc}} \Big\rangle &= (-i\omega p_0)(ikZ^r) \underbrace{\int b_{b\ell}(\mathbf{x}) \mathbb{G}_{\ell j}(\mathbf{x}, \mathbf{x}_{\text{S}})\, dx}_{g_b(\mathbf{x}_{\text{S}}, \hat{\mathbf{n}}_j)} \\
&= (-i\omega p_0)(ikZ^r) g_b(\mathbf{x}_{\text{S}}, \hat{\mathbf{n}}_j) \qquad \text{(16a)} \\
h_b \equiv \quad \Big\langle \mathbf{b}_m \Big| \mathbf{H}^{\text{inc}} \Big\rangle &= (-i\omega p_0)(ik) \underbrace{\left[-\int b_{b\ell}(\mathbf{x}) \mathbb{C}_{\ell j}(\mathbf{x}, \mathbf{x}_{\text{S}})\, dx \right]}_{-c_b(\mathbf{x}_{\text{S}}, \hat{\mathbf{n}}_j)} \\
&= -(-i\omega p_0)(ik) c_b(\mathbf{x}_{\text{S}}, \hat{\mathbf{n}}_j). \qquad \text{(16b)}
\end{aligned}$$

Note that the g_b, c_b quantities are the same as the g_a, c_a computed above; this follows from reciprocity, $\mathbb{O}_{ij}(\mathbf{x}, \mathbf{y}) = \mathbb{O}_{ji}(\mathbf{y}, \mathbf{x})$ for $\mathbb{O} = \{\mathbb{G}, \mathbb{C}\}$.

Inserting (15) and (16) into (14), the scattered field at x_{D} takes the form of a vector-matrix-vector product,

$$\left\{ \begin{array}{c} E_i^{\text{scat}}(\mathbf{x}_{\text{D}}) \\ \\ H_i^{\text{scat}}(\mathbf{x}_{\text{D}}) \end{array} \right\} = (i\omega p_0) \cdot \frac{1}{Z_0} \underbrace{\left\{ \begin{array}{c} ikZ_0 Z^r g_a(\mathbf{x}_{\text{D}}, \hat{\mathbf{n}}_i) \\ -ikZ_0 c_a(\mathbf{x}_{\text{D}}, \hat{\mathbf{n}}_i) \end{array} \right\}^T}_{\equiv (\mathbf{r}^{\text{E}}_{i\text{D}})_a} \Big(W_{ab} \Big) \underbrace{\left\{ \begin{array}{c} ikZ_0 Z^r g_b(\mathbf{x}_{\text{S}}, \hat{\mathbf{n}}_j) \\ -ikZ_0 c_b(\mathbf{x}_{\text{S}}, \hat{\mathbf{n}}_j) \end{array} \right\}}_{\equiv (\mathbf{r}^{\text{E}}_{j\text{S}})_b} \tag{17}$$

and the scattering part of the electric DGF reads

$$\mathcal{G}^{\text{E}}_{ij}(\mathbf{x}_{\text{D}}, \mathbf{x}_{\text{S}}) = \frac{E_i^{\text{scat}}}{(ikZ_0 Z^r)(-i\omega p_0)} = -\frac{1}{ikZ_0^2 Z^r} \Big(\mathbf{r}^{\text{E}}_{i\text{D}} \cdot \mathbf{W} \cdot \mathbf{r}^{\text{E}}_{j\text{S}} \Big) \tag{18}$$

I think of the vectors $\mathbf{r}^{\text{E}}_{i\text{D}}$ and $\mathbf{r}^{\text{E}}_{j\text{S}}$ as "reduced-field" vectors; their dot product with a vector of surface-current coefficients yields the i, j components of the scattered electric fields at $x^{\text{D,S}}$.

VMVP formula for $\boldsymbol{\mathcal{G}}^{\text{M}}$

Computing the magnetic Green's function entails the following modifications:

- The incident fields now arise from a point magnetic source of strength m_0. This changes equation (11) to read

$$\left\{ \begin{array}{c} E_\ell^{\text{inc}}(\mathbf{x}) \\ \\ H_\ell^{\text{inc}}(\mathbf{x}) \end{array} \right\} = -i\omega m_0 \left\{ \begin{array}{c} \Gamma^{\text{EM}}_{\ell j}(\mathbf{x}, \mathbf{x}_{\text{S}}) \\ \\ \Gamma^{\text{MM}}_{\ell j}(\mathbf{x}, \mathbf{x}_{\text{S}}) \end{array} \right\} = (-i\omega m_0) \left\{ \begin{array}{r} ik\mathbb{C}_{\ell j}(\mathbf{x}, \mathbf{x}_{\text{S}}) \\ \\ \frac{ik}{Z_0 Z^r} \mathbb{G}_{\ell j}(\mathbf{x}, \mathbf{x}_{\text{S}}) \end{array} \right\}$$

- The quantity I want to compute is the scattered magnetic field. This replaces equation (14) with

$$H_i^{\text{scat}}(\mathbf{x}_{\text{D}}) = \int \begin{Bmatrix} \Gamma_{i\ell}^{\text{ME}}(\mathbf{x}_{\text{D}}, \mathbf{x}) \\ \Gamma_{i\ell}^{\text{MM}}(\mathbf{x}_{\text{D}}, \mathbf{x}) \end{Bmatrix}^T \begin{Bmatrix} K_\ell(\mathbf{x}) \\ N_\ell(\mathbf{x}) \end{Bmatrix} d\mathbf{x} \tag{19}$$

$$= \sum_a \begin{Bmatrix} -ikc_a(\mathbf{x}_{\text{D}}, \hat{\mathbf{n}}_i) \\ -\frac{ik}{Z^r} g_a(\mathbf{x}_{\text{D}}, \hat{\mathbf{n}}_i) \end{Bmatrix}^T \begin{Bmatrix} k_a \\ n_a \end{Bmatrix} \tag{20}$$

The expression analogous to (17) for the scattered magnetic field due to a magnetic source then reads

$$H_i^{\text{scat}} = +\frac{1}{Z_0} \underbrace{\begin{pmatrix} -ikc_a(\mathbf{x}_{\text{D}}, \hat{\mathbf{n}}_i) \\ -\frac{1}{ikZ^r} g_a(\mathbf{x}_{\text{D}}, \hat{\mathbf{n}}_i) \end{pmatrix}^T}_{\equiv(\mathbf{r}_{i\text{D}}^{\text{H}})_a} \begin{pmatrix} W_{ab} \end{pmatrix} \underbrace{\begin{pmatrix} -ikc_b(\mathbf{x}_{\text{S}}, \hat{\mathbf{n}}_j) \\ -\frac{1}{ikZ^r} g_b(\mathbf{x}_{\text{S}}, \hat{\mathbf{n}}_j) \end{pmatrix}}_{\equiv(\mathbf{r}_{j\text{S}}^{\text{H}})_b}$$

so the scattering part of the magnetic DGF reads

$$\mathcal{G}_{ij}^{\text{H}}(\mathbf{x}_{\text{D}}, \mathbf{x}_{\text{S}}) = +\frac{Z_0 Z^r}{ik(-i\omega m_0)} H_i^{\text{scat}} = +\frac{Z^r}{ik}\Big(\mathbf{r}_{i\text{D}}^{\text{H}} \cdot \mathbf{W} \cdot \mathbf{r}_{j\text{S}}^{\text{H}}\Big). \tag{21}$$

4.2 The periodic case

In the derivation of equations (18) and (21), we used the reciprocity of the homogeneous Green's functions, i.e.

$$\mathbb{K}_{ij}(\mathbf{x}, \mathbf{y}) = \mathbb{K}_{ji}(\mathbf{y}, \mathbf{x}).$$

For this periodic Green's function this statement takes the modified form

$$\overline{\mathbb{K}}_{ij}(\mathbf{x}, \mathbf{y}; \mathbf{k}_{\text{B}}) = \overline{\mathbb{K}}_{ji}(\mathbf{y}, \mathbf{x}; -\mathbf{k}_{\text{B}}).$$

Thus the periodic version of (18) reads

$$\overline{\mathcal{G}}_{ij}^{\text{E}}(\mathbf{x}_{\text{D}}, \mathbf{x}_{\text{S}}; \mathbf{k}_{\text{B}}) = -\frac{1}{ikZ_0^2 Z^r}\Big(\mathbf{r}_{i\text{D}}^{\text{E}}(\mathbf{k}_{\text{B}}) \cdot \mathbf{W}(\mathbf{k}_{\text{B}}) \cdot \mathbf{r}_{j\text{S}}^{\text{E}}(-\mathbf{k}_{\text{B}})\Big) \tag{22}$$

and the periodic version of (21) is similar.

5 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 (10) 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

$$\begin{aligned}
\mathbf{E}^{\text{ED}}(\mathbf{x};\mathbf{x}_0,\mathbf{p}_0) &= \frac{|\mathbf{p}_0|}{\epsilon_0\epsilon^r}\cdot\frac{e^{ikr}}{4\pi r^3}\cdot\Big[f_1(ikr)\hat{\mathbf{p}}_\mathbf{0} + f_2(ikr)(\hat{\mathbf{r}}\cdot\hat{\mathbf{p}}_\mathbf{0})\hat{\mathbf{r}}\Big] \\
\mathbf{H}^{\text{ED}}(\mathbf{x};\mathbf{x}_0,\mathbf{p}_0) &= \frac{1}{Z_0 Z^r}\cdot\frac{|\mathbf{p}_0|}{\epsilon_0\epsilon^r}\cdot\frac{e^{ikr}}{4\pi r^3}\cdot\Big[f_3(ikr)(\hat{\mathbf{r}}\times\hat{\mathbf{p}}_\mathbf{0})\Big]
\end{aligned}$$

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

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

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,

$$\mathbf{J}(\mathbf{x}) = -i\omega\mathbf{p}_0\delta(\mathbf{x}-\mathbf{x}_0) \tag{23}$$

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:

$$\begin{aligned}
E_i(\mathbf{x}) &= \int \Gamma^{\text{EE}}_{ij}(\mathbf{x},\mathbf{x}')J_j(\mathbf{x}')d\mathbf{x}' \\
&= -i\omega\Gamma^{\text{EE}}_{ij}(\mathbf{x},\mathbf{x}_0)p_{0j} \\
&= (-i\omega)(ikZ_0Z^r)G_{ij}(\mathbf{x},\mathbf{x}_0)p_{0j} \\
&= +k^2\cdot\frac{|\mathbf{p}_0|}{\epsilon_0\epsilon^r}\cdot G_{ij}(\mathbf{x},\mathbf{x}_0)\hat{p}_{0j}
\end{aligned} \tag{24a}$$

$$\begin{aligned}
H_i(\mathbf{x}) &= \int \Gamma^{\text{ME}}_{ij}(\mathbf{x},\mathbf{x}')J_j(\mathbf{x}')d\mathbf{x}' \\
&= -i\omega\Gamma^{\text{ME}}_{ij}(\mathbf{x},\mathbf{x}_0)p_{0j} \\
&= (-i\omega)(-ik)C_{ij}(\mathbf{x},\mathbf{x}_0)p_{0j} \\
&= -\frac{k^2}{Z_0Z^r}\cdot\frac{|\mathbf{p}|}{\epsilon_0\epsilon^r}\cdot C_{ij}(\mathbf{x},\mathbf{x}_0)\hat{p}_{0j}
\end{aligned} \tag{24b}$$

where the **G** and **C** dyadics are related to the scalar Helmholtz Green's function according to

$$G_{ij}(\mathbf{r}) = \Big[\delta_{ij} + \frac{1}{k^2}\partial_i\partial_j\Big]G_0(\mathbf{r}), \qquad C_{ij}(\mathbf{r}) = \frac{1}{ik}\varepsilon_{ijk}\partial_k G_0(\mathbf{r}). \tag{25}$$

Note that the **E** and **H** fields due to an electric current distribution **J** are

$$\mathbf{E}(\mathbf{x}) = ikZ_0\int \mathbf{G}(\mathbf{x}-\mathbf{x}')\cdot\mathbf{J}(\mathbf{x}'), \qquad \mathbf{H}(\mathbf{x}) = -ik\int \mathbf{C}(\mathbf{x}-\mathbf{x}')\cdot\mathbf{J}(\mathbf{x}'). \tag{26}$$

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 (24) and (25), but replace the non-periodic scalar Green's function G_0 with its Bloch-periodic version,

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

Then the components of the fields of an electric dipole array, equation (8), read

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

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:

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

Applying (25), we obtain the 2D Fourier expansion of the dyadic Green's functions:

$$\mathbf{G}(\boldsymbol{\rho}, z) = \int_{\mathbb{R}^2}\frac{d\mathbf{k}}{(2\pi)^2}\mathbf{g}(\boldsymbol{\rho}, z;\mathbf{k}), \qquad \mathbf{C}(\boldsymbol{\rho}, z) = \int_{\mathbb{R}^2}\frac{d\mathbf{k}}{(2\pi)^2}\mathbf{c}(\boldsymbol{\rho}, z;\mathbf{k}), \tag{27}$$

$$\mathbf{g}(\boldsymbol{\rho}, z;\mathbf{k}) = \left(\frac{i}{2k_0^2 k_z}\right)\begin{pmatrix} k_0^2 - k_x^2 & -k_x k_y & \mp k_z k_x \\ -k_y k_x & k_0^2 - k_y^2 & \mp k_z k_y \\ \mp k_x k_z & \mp k_y k_z & k_0^2 - k_z^2 \end{pmatrix} e^{i\mathbf{k}\cdot\boldsymbol{\rho}}e^{ik_z|z|} \tag{28a}$$

$$\mathbf{c}(\boldsymbol{\rho}, z;\mathbf{k}) = \left(\frac{i}{2k_0 k_z}\right)\begin{pmatrix} 0 & \pm k_z & -k_y \\ \mp k_z & 0 & k_x \\ k_y & -k_x & 0 \end{pmatrix} e^{i\mathbf{k}\cdot\boldsymbol{\rho}}e^{ik_z|z|} \tag{28b}$$

where the $\pm$ sign is sign(z). Now reinterpret the infinite integrals over the entire k_x, k_y plane in (27) as finite integrals over just the Brillouin zone;

$$\mathbf{G}(\boldsymbol{\rho}, z) = \int_0^{\Gamma_x} dk_x \int_0^{\Gamma_y} dk_y \, \frac{d\mathbf{k}}{(2\pi)^2} \overline{\mathbf{g}}(\boldsymbol{\rho}, z; \mathbf{k}), \qquad \mathbf{C}(\boldsymbol{\rho}, z) = \int_0^{\Gamma_x} dk_x \int_0^{\Gamma_y} dk_y \, \frac{d\mathbf{k}}{(2\pi)^2} \overline{\mathbf{c}}(\boldsymbol{\rho}, z; \mathbf{k}), \tag{29}$$

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

If I think of (29) as equations of the form (10), 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

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

B Analytical formulas for scattering part of DGFs above a homogeneous half space

For testing purposes it is very convenient to have analytical formulas for the DGFs above a half space with spatially homogeneous permittivity and permeability ϵ, μ.[2] These formulas are implemented in SCUFF-LDOS and may be accessed by adding the command-line option `--HalfSpace MyMaterial` (where `MyMaterial` is a SCUFF-EM material designation like `Gold` or `CONST_EPS_10+1I`).

B.1 2D integrals over the entire q plane

The expressions in this section are actually not useful for practical computations (the integrals converge too slowly), but I quote them here as a springboard for the alternative expressions of the following subsections.

$$\boldsymbol{\mathcal{G}}^E(\boldsymbol{\rho}, z; \boldsymbol{\rho}', z') = \int_{\mathbb{R}^2} \widetilde{\boldsymbol{\mathcal{G}}}^{\mathrm{E}}(\mathbf{q})\, d\mathbf{q} \tag{30a}$$

$$\boldsymbol{\mathcal{G}}^M(\boldsymbol{\rho}, z; \boldsymbol{\rho}', z') = \int_{\mathbb{R}^2} \widetilde{\boldsymbol{\mathcal{G}}}^{\mathrm{M}}(\mathbf{q})\, d\mathbf{q} \tag{30b}$$

$$\widetilde{\boldsymbol{\mathcal{G}}}^{\mathrm{E}}(\mathbf{q}) = \frac{i}{8\pi^2 q_z} e^{i\mathbf{q}\cdot(\boldsymbol{\rho}-\boldsymbol{\rho}') - q_z(z+z')} \Big\{ r_{\mathrm{TE}} \mathbf{M}^{\mathrm{TE}} + r_{\mathrm{TM}} \mathbf{M}^{\mathrm{TM}} \Big\} \tag{31a}$$

$$\widetilde{\boldsymbol{\mathcal{G}}}^{\mathrm{M}}(\mathbf{q}) = \frac{i}{8\pi^2 q_z} e^{i\mathbf{q}\cdot(\boldsymbol{\rho}-\boldsymbol{\rho}') - q_z(z+z')} \Big\{ r_{\mathrm{TM}} \mathbf{M}^{\mathrm{TE}} + r_{\mathrm{TE}} \mathbf{M}^{\mathrm{TM}} \Big\} \tag{31b}$$

[2] In compiling these formulas I referred to these references:

- H. Safari et al., "Van der Waals potentials of paramagnetic atoms," *Phys. Rev. A* **78** 062901 (2008).
- S. Scheel et al., "Macroscopic Quantum Electrodynamics—Concepts and Applications," *Acta Physica Slovaca* **58** 675 (2008).

$$\mathbf{M}^{\mathrm{TE}} \equiv \left(\begin{array}{c} -\widehat{q}_y \\ \widehat{q}_x \\ 0 \end{array}\right)\left(\begin{array}{c} -\widehat{q}_y \\ \widehat{q}_x \\ 0 \end{array}\right)^T$$

$$= \left(\begin{array}{ccc} \sin^2\theta & -\cos\theta\sin\theta & 0 \\ -\cos\theta\sin\theta & \cos^2\theta & 0 \\ 0 & 0 & 0 \end{array}\right)$$

$$\mathbf{M}^{\mathrm{TM}} \equiv \frac{1}{k_0^2}\left(\begin{array}{c} -q_z\widehat{q}_x \\ -q_z\widehat{q}_y \\ q \end{array}\right)\left(\begin{array}{c} -q_z\widehat{q}_x \\ -q_z\widehat{q}_y \\ q \end{array}\right)^T$$

$$= \frac{1}{k_0^2}\left(\begin{array}{ccc} q_z^2\cos^2\theta & q_z^2\sin\theta\cos\theta & -qq_z\cos\theta \\ q_z^2\sin\theta\cos\theta & q_z^2\sin^2\theta & -qq_z\sin\theta \\ -qq_z\cos\theta & -qq_z\sin\theta & q^2 \end{array}\right)$$

$$q \equiv |\mathbf{q}|, \qquad q_z \equiv \sqrt{q^2-k^2}, \qquad q_z' \equiv \sqrt{q^2-\epsilon\mu k^2},$$

$$r_{\mathrm{TE}} \equiv \frac{\mu q_z - q_z'}{\mu q_z + q_z'}, \qquad r_{\mathrm{TM}} \equiv \frac{\epsilon q_z - q_z'}{\epsilon q_z + q_z'}.$$

B.2 2D integrals over the Brillouin zone

For comparison with SCUFF-LDOS it is convenient to recast the infinite 2D integrals in (30) as integrals over a Brillouin zone:[3]

$$\boldsymbol{\mathcal{G}}^E(\boldsymbol{\rho},z;\boldsymbol{\rho}',z') = \int_{\mathrm{BZ}} \widehat{\boldsymbol{\mathcal{G}}}^{\mathrm{E}}(\mathbf{q})\,d\mathbf{q} \tag{32a}$$

$$\boldsymbol{\mathcal{G}}^M(\boldsymbol{\rho},z;\boldsymbol{\rho}',z') = \int_{\mathrm{BZ}} \widehat{\boldsymbol{\mathcal{G}}}^{\mathrm{M}}(\mathbf{q})\,d\mathbf{q} \tag{32b}$$

$$\widehat{\boldsymbol{\mathcal{G}}}^{\mathrm{E}}(\mathbf{k}_{\mathrm{B}}) = \sum_{\boldsymbol{\Gamma}} \widetilde{\boldsymbol{\mathcal{G}}}^{\mathrm{E}}(\mathbf{k}_{\mathrm{B}}+\boldsymbol{\Gamma}), \tag{33a}$$

$$\widehat{\boldsymbol{\mathcal{G}}}^{\mathrm{M}}(\mathbf{k}_{\mathrm{B}}) = \sum_{\boldsymbol{\Gamma}} \widetilde{\boldsymbol{\mathcal{G}}}^{\mathrm{M}}(\mathbf{k}_{\mathrm{B}}+\boldsymbol{\Gamma}) \tag{33b}$$

The quantities $\widehat{\boldsymbol{\mathcal{G}}}(\mathbf{k}_{\mathrm{B}})$ may be directly compared to the Brillouin-zone integrand values reported by SCUFF-LDOS in the `.byOmegakBloch` output file.

[3] Since the geometry in question has continuous translational symmetry, this can be the Brillouin zone for *any* lattice we like. In SCUFF-LDOS the lattice is defined by the geometry in the `.scuffgeo` file. This is why the `--geometry` command-line option must be specified for `--HalfSpace` calculations, even though the discretized geometry is otherwise not referenced.

B.3 1D integrals over |q|

The Brillouin-zone-resolved integrand values of the previous section are useful for checking the predictions of SCUFF-LDOS for individual Brillouin-zone points. However, if our goal is actually to evaluate the full **q** integrals to get the total DGFs at a given frequency, it is more efficient instead to write the **q**-plane integrals (30) in polar coordinates and integrate out the angular variable, leaving a 1D integral over the radial variable. This is effected by using the following table of integrals:

$$\int_0^{2\pi} e^{i(qx\cos\theta+qy\cos\theta)} \left\{\begin{array}{c} 1 \\ \cos\theta \\ \sin\theta \\ \cos^2\theta \\ \cos\theta\sin\theta \\ \sin^2\theta \end{array}\right\} = 2\pi \left\{\begin{array}{c} J_0(q\rho) \\ iJ_1(q\rho)\widehat{x} \\ iJ_1(q\rho)\widehat{y} \\ \Big[J_0(q\rho)-\frac{2}{q\rho}J_1(q\rho)-J_2(q\rho)\Big]\frac{\widehat{x}^2}{2}+\frac{J_1(q\rho)}{q\rho} \\ \Big[J_0(q\rho)-\frac{2}{q\rho}J_1(q\rho)-J_2(q\rho)\Big]\frac{\widehat{x}\widehat{y}}{2} \\ \Big[J_0(q\rho)-\frac{2}{q\rho}J_1(q\rho)-J_2(q\rho)\Big]\frac{\widehat{y}^2}{2}+\frac{J_1(q\rho)}{q\rho} \end{array}\right\}$$

the 2D integrals (30) can be reduced to 1D integrals:

$$\boldsymbol{\mathcal{G}}^{\mathrm{E}} = \frac{i}{4\pi}\int_0^\infty \frac{qdq}{q_z} e^{-q_z(z+z')} \Big\{ r_{\mathrm{TE}}\widetilde{\mathbf{M}}^{\mathrm{TE}} + r_{\mathrm{TM}}\widetilde{\mathbf{M}}^{\mathrm{TM}} \Big\} \tag{34}$$

$$\boldsymbol{\mathcal{G}}^{\mathrm{E}} = \frac{i}{4\pi}\int_0^\infty \frac{qdq}{q_z} e^{-q_z(z+z')} \Big\{ r_{\mathrm{TM}}\widetilde{\mathbf{M}}^{\mathrm{TE}} + r_{\mathrm{TE}}\widetilde{\mathbf{M}}^{\mathrm{TM}} \Big\} \tag{35}$$

where $\widetilde{\mathbf{M}}$ is the matrix $\mathbf{M}$ defined above with all θ factors replaced by the corresponding entry in the Bessel-function table above.

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

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

$$I = \int_{\mathbb{R}^2} d^2\mathbf{q}\, Q(\mathbf{q}).$$

Examples include equations (30). To rewrite such integrals in a form that facilitates comparison with SCUFF-LDOS calculations, it is convenient to recast them as Brillouin-zone integrations:

$$I = \int_{\mathrm{BZ}} d^2\mathbf{k}_{\mathrm{B}}\, \overline{Q}(\mathbf{k}_{\mathrm{B}}),$$

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

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

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