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

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Contents

1   Homogeneous Green's functions

Before doing anything we recall our notation and conventions for dyadic Green's functions. In a homogeneous material region with relative permittivity and permeability $\{\epsilon^r, \mu^r\}$, electric and magnetic volume currents $\mathbf{J}, \mathbf{M}$ give rise to electric and magnetic fields $\mathbf{E}, \mathbf{H}$ according to

$$
\left\{ \begin{array}{c} E_i(\mathbf{x}) \\ H_i(\mathbf{x}) \end{array} \right\} = \int \left(\begin{array}{cc} \Gamma_{ij}^{\mathrm{EE}}(\mathbf{x}, \mathbf{x}') & \Gamma_{ij}^{\mathrm{EM}}(\mathbf{x}, \mathbf{x}') \\ \Gamma_{ij}^{\mathrm{ME}}(\mathbf{x}, \mathbf{x}') & \Gamma_{ij}^{\mathrm{MM}}(\mathbf{x}, \mathbf{x}') \end{array} \right) \left(\begin{array}{c} J_i(\mathbf{x}) \\ M_i(\mathbf{x}) \end{array} \right) dV
$$

where

$$\mathbf{\Gamma}^{\mathrm{EE}} = ik Z_0 Z^r \mathbb{G} \tag{1a}$$

$$\mathbf{\Gamma}^{\mathrm{EM}} = ik \mathbb{C} \tag{1b}$$

$$\mathbf{\Gamma}^{\mathrm{ME}} = -ik \mathbb{C} \tag{1c}$$

$$\mathbf{\Gamma}^{\mathrm{MM}} = \frac{ik}{Z_0 Z^r} \mathbb{G} \tag{1d}$$

where $k = \sqrt{\epsilon^r \mu^r} \cdot \omega$ is the photon wavenumber in the medium, $Z^r = \sqrt{\frac{\mu^r}{\epsilon^r}}$ 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

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

$$\mathbb{C}_{ij}(k, \mathbf{r}) = \frac{e^{ikr}}{4\pi (ik) r^3} \varepsilon_{ijk} r_k. \tag{2b}$$

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

In the presence of scatterers, the scattering parts of the electric and magnetic dyadic Green's functions (DGFs) are

$$
\mathcal{G}^{\mathrm{E}}_{ij}(\omega;\mathbf{x},\mathbf{x}') \equiv \frac{1}{ikZ_0 Z^r}
\begin{pmatrix}
i\text{-component of scattered }\mathbf{E}\text{-field at }\mathbf{x}\text{ due to a unit-}\\
\text{strength }j\text{-directed point }\textbf{electric}\text{ dipole radiator at}\\
\mathbf{x}', \text{ all quantities having time dependence} \sim e^{-i\omega t}
\end{pmatrix}
$$

$$
\mathcal{G}^{\mathrm{M}}_{ij}(\omega;\mathbf{x},\mathbf{x}') \equiv \frac{Z_0 Z^r}{ik}
\begin{pmatrix}
i\text{-component of scattered }\mathbf{H}\text{-field at }\mathbf{x}\text{ due to a unit-}\\
\text{strength }j\text{-directed point }\textbf{magnetic}\text{ dipole radiator}\\
\text{at }\mathbf{x}', \text{ all quantities having time dependence} \sim e^{-i\omega t}
\end{pmatrix}
$$

Note that the prefactors in the definitions here are the reciprocals of those in (1a,d), and that $\boldsymbol{\mathcal{G}}^{\mathrm{E,M}}$ both 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]

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

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 $\mathbf{s}^{\mathrm{S}}$:

$$
\mathbf{E}^{\mathrm{inc}}(\mathbf{x}) = \mathbf{E}^{\mathrm{ED}}\Big(\mathbf{x}; \{\mathbf{x}_{\mathrm{S}}, \hat{\mathbf{x}}_j\}\Big), \qquad \mathbf{H}^{\mathrm{inc}}(\mathbf{x}) = \mathbf{H}^{\mathrm{ED}}\Big(\mathbf{x}; \{\mathbf{x}_{\mathrm{S}}, \hat{\mathbf{x}}_j\}\Big) \tag{3}
$$

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 (3) 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 $ikZ_0 Z_r$, 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.

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[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)

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

$$Q(\mathbf{x} + \mathbf{L}) = e^{i\mathbf{k}_{\mathrm{B}} \cdot \mathbf{L}} Q(\mathbf{x}) \tag{4}$$

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

The fields of a point dipole, equation (3), do *not* satisfy (4), 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,

$$\mathbf{E}^{\mathrm{EDA}}\Big(\mathbf{x}; \{\mathbf{x}_0, \mathbf{p}_0, \mathbf{k}_{\mathrm{B}}\}\Big) = \sum_{\mathbf{L}} e^{i\mathbf{k}_{\mathrm{B}} \cdot \mathbf{L}} \, \mathbf{E}^{\mathrm{ED}}\Big(\mathbf{x}; \{\mathbf{x}_0 + \mathbf{L}, \mathbf{p}_0\}\Big), \tag{5a}$$

$$\mathbf{H}^{\mathrm{EDA}}\Big(\mathbf{x}; \{\mathbf{x}_0, \mathbf{p}_0, \mathbf{k}_{\mathrm{B}}\}\Big) = \sum_{\mathbf{L}} e^{i\mathbf{k}_{\mathrm{B}} \cdot \mathbf{L}} \, \mathbf{H}^{\mathrm{ED}}\Big(\mathbf{x}; \{\mathbf{x}_0 + \mathbf{L}, \mathbf{p}_0\}\Big), \tag{5b}$$

(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),

$$\overline{\mathcal{G}_{ij}^{\mathrm{E}}}(\mathbf{x}, \mathbf{x}', \mathbf{k}_{\mathrm{B}}) \equiv \sum_{\mathbf{L}} e^{i\mathbf{k}_{\mathrm{B}} \cdot \mathbf{L}} \mathcal{G}_{ij}^{\mathrm{E}}(\mathbf{x}, \mathbf{x}' + \mathbf{L}), \tag{6}$$

with $\overline{\mathcal{G}_{ij}^{\mathrm{M}}}$ 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]

$$\mathcal{G}_{ij}^{\mathrm{E}}(\mathbf{x}, \mathbf{x}') = \frac{1}{\mathcal{V}_{\mathrm{BZ}}} \int_{\mathrm{BZ}} \overline{\mathcal{G}_{ij}^{\mathrm{E}}}(\mathbf{x}, \mathbf{x}', \mathbf{k}_{\mathrm{B}}) \, d\mathbf{k}_{\mathrm{B}} \tag{7}$$

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

Reciprocity of homogeneous Green's functions

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

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

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[2]To derive these equations, multiply both sides of (6) 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 $\mathcal{V}_{\mathrm{BZ}} = 4\pi^2/(L_x L_y)$]. Setting $\mathbf{L}' = 0$ recovers (7).

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

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

Evaluation of BZ integrals

The SCUFF-EM API offers a routine for computing the integrand of (7) 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.

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 $\boldsymbol{\Gamma}_1 = \left(\frac{2\pi}{L_x}\right) \hat{\mathbf{x}}, \boldsymbol{\Gamma}_2 = \left(\frac{2\pi}{L_y}\right) \hat{\mathbf{y}}$, and Brillouin-zone integrals take the form

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

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 $\mathcal{G}^{\text{E}}$

Consider first the electric DGF $\mathcal{G}^{\text{E}}_{ij}(\mathbf{x}_{\text{D}}, \mathbf{x}_{\text{S}})$, 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 $\mathbf{x}_{\text{S}}$:

$$
\left\{ \begin{array}{c} E^{\text{inc}}_\ell(\mathbf{x}) \\ H^{\text{inc}}_\ell(\mathbf{x}) \end{array} \right\} = -i\omega p_0 \left\{ \begin{array}{c} \Gamma^{\text{EE}}_{\ell j}(\mathbf{x}, \mathbf{x}_{\text{S}}) \\ \Gamma^{\text{ME}}_{\ell j}(\mathbf{x}, \mathbf{x}_{\text{S}}) \end{array} \right\} = (-i\omega p_0) \left\{ \begin{array}{c} ikZ_0 Z^r \mathbb{G}_{\ell j}(\mathbf{x}, \mathbf{x}_{\text{S}}) \\ -ik\mathbb{C}_{\ell j}(\mathbf{x}, \mathbf{x}_{\text{S}}) \end{array} \right\}
$$
$$(8)$$

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

$$
E^{\text{scat}}_i(\mathbf{x}_{\text{D}}) = \int \left\{ \begin{array}{c} \Gamma^{\text{EE}}_{i\ell}(\mathbf{x}_{\text{D}}, \mathbf{x}) \\ \Gamma^{\text{EM}}_{i\ell}(\mathbf{x}_{\text{D}}, \mathbf{x}) \end{array} \right\}^T \left\{ \begin{array}{c} K_\ell(\mathbf{x}) \\ N_\ell(\mathbf{x}) \end{array} \right\} d\mathbf{x}
\tag{9}
$$

$$
= \int \left\{ \begin{array}{c} ikZ_0 Z^r \mathbb{G}_{i\ell}(\mathbf{x}_{\text{D}}, \mathbf{x}) \\ +ik\mathbb{C}_{i\ell}(\mathbf{x}_{\text{D}}, \mathbf{x}) \end{array} \right\}^T \left\{ \begin{array}{c} K_\ell(\mathbf{x}) \\ N_\ell(\mathbf{x}) \end{array} \right\} d\mathbf{x}
\tag{10}
$$

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

$$
= \sum_a \left\{ \begin{array}{c} ikZ_0 Z^r g_a(\mathbf{x}_{\text{D}}, \hat{\mathbf{n}}_i) \\ -ikZ_0 c_a(\mathbf{x}_{\text{D}}, \hat{\mathbf{n}}_i) \end{array} \right\}^T \left\{ \begin{array}{c} k_a \\ n_a \end{array} \right\}
\tag{11}
$$

where I defined

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

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

$$
\left(\begin{array}{c} k_a \\ n_a \end{array} \right) = -W_{ab} \left(\begin{array}{c} e_b \\ h_b \end{array} \right).
\tag{12}
$$

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

$$
e_b \equiv \frac{1}{Z_0}\langle \mathbf{b}_m | \mathbf{E}^{\mathrm{inc}} \rangle = (-i\omega p_0)(ikZ^r) \underbrace{\int b_{b\ell}(\mathbf{x})\mathbb{G}_{\ell j}(\mathbf{x}, \mathbf{x}_{\mathrm{S}})\, dx}_{g_b(\mathbf{x}_{\mathrm{S}}, \hat{\mathbf{n}}_j)}
$$

$$
= (-i\omega p_0)(ikZ^r)g_b(\mathbf{x}_{\mathrm{S}}, \hat{\mathbf{n}}_j) \tag{13a}
$$

$$
h_b \equiv \quad \langle \mathbf{b}_m | \mathbf{H}^{\mathrm{inc}} \rangle = (-i\omega p_0)(ik)\underbrace{\left[-\int b_{b\ell}(\mathbf{x})\mathbb{C}_{\ell j}(\mathbf{x}, \mathbf{x}_{\mathrm{S}})\, dx \right]}_{-c_b(\mathbf{x}_{\mathrm{S}}, \hat{\mathbf{n}}_j)}
$$

$$
= -(-i\omega p_0)(ik)c_b(\mathbf{x}_{\mathrm{S}}, \hat{\mathbf{n}}_j). \tag{13b}
$$

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 (12) and (13) into (11), the scattered field at x_{D} takes the form of a vector-matrix-vector product,

$$
\left\{ \begin{array}{c} E_i^{\mathrm{scat}}(\mathbf{x}_{\mathrm{D}}) \\ H_i^{\mathrm{scat}}(\mathbf{x}_{\mathrm{D}}) \end{array} \right\} = (i\omega p_0) \cdot \frac{1}{Z_0} \underbrace{\left\{ \begin{array}{c} ikZ_0Z^r g_a(\mathbf{x}_{\mathrm{D}}, \hat{\mathbf{n}}_i) \\ -ikZ_0 c_a(\mathbf{x}_{\mathrm{D}}, \hat{\mathbf{n}}_i) \end{array} \right\}^T}_{\equiv (\mathbf{r}_{i\mathrm{D}}^{\mathrm{E}})_a} \left(W_{ab} \right) \underbrace{\left\{ \begin{array}{c} ikZ_0Z^r g_b(\mathbf{x}_{\mathrm{S}}, \hat{\mathbf{n}}_j) \\ -ikZ_0 c_b(\mathbf{x}_{\mathrm{S}}, \hat{\mathbf{n}}_j) \end{array} \right\}}_{\equiv (\mathbf{r}_{j\mathrm{S}}^{\mathrm{E}})_b}
$$

$$
\tag{14}
$$

and the scattering part of the electric DGF reads

$$
\mathcal{G}_{ij}^{\mathrm{E}}(\mathbf{x}_{\mathrm{D}}, \mathbf{x}_{\mathrm{S}}) = \frac{E_i^{\mathrm{scat}}}{(ikZ_0Z^r)(-i\omega p_0)} = -\frac{1}{ikZ_0^2 Z^r}\left(\mathbf{r}_{i\mathrm{D}}^{\mathrm{E}} \cdot \mathbf{W} \cdot \mathbf{r}_{j\mathrm{S}}^{\mathrm{E}} \right) \tag{15}
$$

I think of the vectors $\mathbf{r}_{i\mathrm{D}}^{\mathrm{E}}$ and $\mathbf{r}_{j\mathrm{S}}^{\mathrm{E}}$ 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 $x^{\mathrm{D,S}}$.

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

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 (8) to read

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

- The quantity I want to compute is the scattered magnetic field. This

replaces equation (11) with

$$H_i^{\text{scat}}(\mathbf{x}_{\text{D}}) = \int \left\{ \begin{array}{c} \Gamma_{i\ell}^{\text{ME}}(\mathbf{x}_{\text{D}}, \mathbf{x}) \\ \Gamma_{i\ell}^{\text{MM}}(\mathbf{x}_{\text{D}}, \mathbf{x}) \end{array} \right\}^T \left\{ \begin{array}{c} K_\ell(\mathbf{x}) \\ N_\ell(\mathbf{x}) \end{array} \right\} d\mathbf{x} \qquad (16)$$

$$= \sum_a \left\{ \begin{array}{c} -ik c_a(\mathbf{x}_{\text{D}}, \hat{\mathbf{n}}_i) \\ -\frac{ik}{Z^r} g_a(\mathbf{x}_{\text{D}}, \hat{\mathbf{n}}_i) \end{array} \right\}^T \left\{ \begin{array}{c} k_a \\ n_a \end{array} \right\} \qquad (17)$$

The expression analogous to (14) for the scattered magnetic field due to a magnetic source then reads

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

so the scattering part of the magnetic DGF reads

$$\mathcal{G}_{ij}^{\text{H}}(\mathbf{x}_{\text{D}}, \mathbf{x}_{\text{S}}) = +\frac{Z_0 Z^r}{ik(-i\omega m_0)} H_i^{\text{scat}} = +\frac{Z^r}{ik}\left(\mathbf{r}_{i\text{D}}^{\text{H}} \cdot \mathbf{W} \cdot \mathbf{r}_{j\text{S}}^{\text{H}} \right). \qquad (18)$$

4.2 The periodic case

In the derivation of equations (15) and (18), 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 (15) reads

$$\overline{\mathcal{G}}_{ij}^{\text{E}}(\mathbf{x}_{\text{D}}, \mathbf{x}_{\text{S}}; \mathbf{k}_{\text{B}}) = -\frac{1}{ikZ_0^2 Z^r}\left(\mathbf{r}_{i\text{D}}^{\text{E}}(\mathbf{k}_{\text{B}}) \cdot \mathbf{W}(\mathbf{k}_{\text{B}}) \cdot \mathbf{r}_{j\text{S}}^{\text{E}}(-\mathbf{k}_{\text{B}}) \right) \qquad (19)$$

and the periodic version of (18) is similar.

5   API Routines for computing dyadic Green's functions

The SCUFF-EM API routine that computes the quantity $\overline{\mathcal{G}}_{ij}^{\mathrm{E}}(\mathbf{x}, \mathbf{x}', k^{\mathrm{B}})$ in equation (7) is

```
        void RWGGeometry::GetDyadicGFs(double XEval[3], double XSource[3],
                                       cdouble Omega, double kBloch[2],
                                       HMatrix *M, HVector *KN,
-2-4pt-2-4pt                          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,
-2-4pt-2-4pt                          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

$$\mathbf{E}^{\text{ED}}(\mathbf{x}; \mathbf{x}_0, \mathbf{p}_0) = \frac{|\mathbf{p}_0|}{\epsilon_0 \epsilon^r} \cdot \frac{e^{ikr}}{4\pi r^3} \cdot \left[f_1(ikr)\hat{\mathbf{p}}_0 + f_2(ikr)(\hat{\mathbf{r}} \cdot \hat{\mathbf{p}}_0)\hat{\mathbf{r}} \right]$$

$$\mathbf{H}^{\text{ED}}(\mathbf{x}; \mathbf{x}_0, \mathbf{p}_0) = \frac{1}{Z_0 Z^r} \cdot \frac{|\mathbf{p}_0|}{\epsilon_0 \epsilon^r} \cdot \frac{e^{ikr}}{4\pi r^3} \cdot \left[f_3(ikr)(\hat{\mathbf{r}} \times \hat{\mathbf{p}}_0) \right]$$

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

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

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,

$$\mathbf{J}(\mathbf{x}) = -i\omega \mathbf{p}_0 \delta(\mathbf{x} - \mathbf{x}_0) \tag{20}$$

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:

$$\begin{aligned} E_i(\mathbf{x}) &= \int \Gamma_{ij}^{\text{EE}}(\mathbf{x}, \mathbf{x}') J_j(\mathbf{x}') d\mathbf{x}' \\ &= -i\omega \Gamma_{ij}^{\text{EE}}(\mathbf{x}, \mathbf{x}_0) p_{0j} \\ &= (-i\omega)(ik Z_0 Z^r) G_{ij}(\mathbf{x}, \mathbf{x}_0) p_{0j} \\ &= +k^2 \cdot \frac{|\mathbf{p}_0|}{\epsilon_0 \epsilon^r} \cdot G_{ij}(\mathbf{x}, \mathbf{x}_0)\hat{p}_{0j} \end{aligned} \tag{21a}$$

$$\begin{aligned} H_i(\mathbf{x}) &= \int \Gamma_{ij}^{\text{ME}}(\mathbf{x}, \mathbf{x}') J_j(\mathbf{x}') d\mathbf{x}' \\ &= -i\omega \Gamma_{ij}^{\text{ME}}(\mathbf{x}, \mathbf{x}_0) p_{0j} \\ &= (-i\omega)(-ik) C_{ij}(\mathbf{x}, \mathbf{x}_0) p_{0j} \\ &= -\frac{k^2}{Z_0 Z^r} \cdot \frac{|\mathbf{p}|}{\epsilon_0 \epsilon^r} \cdot C_{ij}(\mathbf{x}, \mathbf{x}_0)\hat{p}_{0j} \end{aligned} \tag{21b}$$

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

$$G_{ij}(\mathbf{r}) = \left[\delta_{ij} + \frac{1}{k^2}\partial_i\partial_j\right]G_0(\mathbf{r}), \qquad C_{ij}(\mathbf{r}) = \frac{1}{ik}\varepsilon_{ijk}\partial_k G_0(\mathbf{r}). \qquad (22)$$

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

$$\mathbf{E}(\mathbf{x}) = ikZ_0\int \mathbf{G}(\mathbf{x} - \mathbf{x}')\cdot\mathbf{J}(\mathbf{x}'), \qquad \mathbf{H}(\mathbf{x}) = -ik\int \mathbf{C}(\mathbf{x} - \mathbf{x}')\cdot\mathbf{J}(\mathbf{x}'). \qquad (23)$$

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 (21) and (22), 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 (5), read

$$E_i^{\text{EDA}}(\mathbf{x}) = k^2\cdot\frac{|\mathbf{p}_0|}{\epsilon_0\epsilon^r}\left[\delta_{ij} + \frac{1}{k^2}\partial_i\partial_j\right]\overline{G}_0(\mathbf{x} - \mathbf{x}')\hat{p}_{0j}$$

$$H_i^{\text{EDA}}(\mathbf{x}) = \frac{ik}{Z_0 Z^r}\cdot\frac{|\mathbf{p}_0|}{\epsilon_0\epsilon^r}\cdot\epsilon_{ijk}\partial_k\overline{G}_0(\mathbf{x} - \mathbf{x}')\hat{p}_{0j}.$$

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

$$\mathbf{G}(\boldsymbol{\rho}, z) = \int_{\mathbb{R}^2}\frac{d\mathbf{k}}{(2\pi)^2}\mathbf{g}(\boldsymbol{\rho}, z; \mathbf{k}), \qquad \mathbf{C}(\boldsymbol{\rho}, z) = \int_{\mathbb{R}^2}\frac{d\mathbf{k}}{(2\pi)^2}\mathbf{c}(\boldsymbol{\rho}, z; \mathbf{k}), \qquad (24)$$

$$\mathbf{g}(\boldsymbol{\rho}, z; \mathbf{k}) = \left(\frac{i}{2k_0^2 k_z}\right)\begin{pmatrix} k_0^2 - k_x^2 & -k_x k_y & \mp k_z k_x \\ -k_y k_x & k_0^2 - k_y^2 & \mp k_z k_y \\ \mp k_x k_z & \mp k_y k_z & k_0^2 - k_z^2 \end{pmatrix}e^{i\mathbf{k}\cdot\boldsymbol{\rho}}e^{ik_z|z|} \qquad (25a)$$

$$\mathbf{c}(\boldsymbol{\rho}, z; \mathbf{k}) = \left(\frac{i}{2k_0 k_z}\right)\begin{pmatrix} 0 & \pm k_z & -k_y \\ \mp k_z & 0 & k_x \\ k_y & -k_x & 0 \end{pmatrix}e^{i\mathbf{k}\cdot\boldsymbol{\rho}}e^{ik_z|z|} \qquad (25b)$$

where the $\pm$ sign is sign(z). Now reinterpret the infinite integrals over the entire k_x, k_y plane in (24) as finite integrals over just the Brillouin zone;

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

$$(26)$$

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

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

If I think of (26) as equations of the form (7), 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

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

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.[3] 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.

$$\boldsymbol{\mathcal{G}}^E(\boldsymbol{\rho}, z; \boldsymbol{\rho}', z') = \int_{\mathbb{R}^2} \widetilde{\boldsymbol{\mathcal{G}}}^{\mathrm{E}}(\mathbf{q}) \, d\mathbf{q} \tag{27a}$$

$$\boldsymbol{\mathcal{G}}^M(\boldsymbol{\rho}, z; \boldsymbol{\rho}', z') = \int_{\mathbb{R}^2} \widetilde{\boldsymbol{\mathcal{G}}}^{\mathrm{M}}(\mathbf{q}) \, d\mathbf{q} \tag{27b}$$

$$\widetilde{\boldsymbol{\mathcal{G}}}^{\mathrm{E}}(\mathbf{q}) = \frac{i}{8\pi^2 q_z} e^{i\mathbf{q}\cdot(\boldsymbol{\rho}-\boldsymbol{\rho}')-q_z(z+z')} \left\{ r_{\mathrm{TE}}\mathbf{M}^{\mathrm{TE}} + r_{\mathrm{TM}}\mathbf{M}^{\mathrm{TM}} \right\} \tag{28a}$$

$$\widetilde{\boldsymbol{\mathcal{G}}}^{\mathrm{M}}(\mathbf{q}) = \frac{i}{8\pi^2 q_z} e^{i\mathbf{q}\cdot(\boldsymbol{\rho}-\boldsymbol{\rho}')-q_z(z+z')} \left\{ r_{\mathrm{TM}}\mathbf{M}^{\mathrm{TE}} + r_{\mathrm{TE}}\mathbf{M}^{\mathrm{TM}} \right\} \tag{28b}$$

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[3]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).

$$\mathbf{M}^{\mathrm{TE}} \equiv \begin{pmatrix} -\widehat{q}_y \\ \widehat{q}_x \\ 0 \end{pmatrix} \begin{pmatrix} -\widehat{q}_y \\ \widehat{q}_x \\ 0 \end{pmatrix}^T$$

$$= \begin{pmatrix} \sin^2 \theta & -\cos \theta \sin \theta & 0 \\ -\cos \theta \sin \theta & \cos^2 \theta & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\mathbf{M}^{\mathrm{TM}} \equiv \frac{1}{k_0^2} \begin{pmatrix} -q_z \widehat{q}_x \\ -q_z \widehat{q}_y \\ q \end{pmatrix} \begin{pmatrix} -q_z \widehat{q}_x \\ -q_z \widehat{q}_y \\ q \end{pmatrix}^T$$

$$= \frac{1}{k_0^2} \begin{pmatrix} q_z^2 \cos^2 \theta & q_z^2 \sin \theta \cos \theta & -q q_z \cos \theta \\ q_z^2 \sin \theta \cos \theta & q_z^2 \sin^2 \theta & -q q_z \sin \theta \\ -q q_z \cos \theta & -q q_z \sin \theta & q^2 \end{pmatrix}$$

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

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

B.2 2D integrals over the Brillouin zone

For comparison with SCUFF-LDOS it is convenient to recast the infinite 2D integrals in (27) as integrals over a Brillouin zone:[4]

$$\boldsymbol{\mathcal{G}}^E(\boldsymbol{\rho}, z; \boldsymbol{\rho}', z') = \int_{\mathrm{BZ}} \widehat{\boldsymbol{\mathcal{G}}}^{\mathrm{E}}(\mathbf{q}) \, d\mathbf{q} \tag{29a}$$

$$\boldsymbol{\mathcal{G}}^M(\boldsymbol{\rho}, z; \boldsymbol{\rho}', z') = \int_{\mathrm{BZ}} \widehat{\boldsymbol{\mathcal{G}}}^{\mathrm{M}}(\mathbf{q}) \, d\mathbf{q} \tag{29b}$$

$$\widehat{\boldsymbol{\mathcal{G}}}^{\mathrm{E}}(\mathbf{k}_{\mathrm{B}}) = \sum_{\boldsymbol{\Gamma}} \widetilde{\boldsymbol{\mathcal{G}}}^{\mathrm{E}}(\mathbf{k}_{\mathrm{B}} + \boldsymbol{\Gamma}), \tag{30a}$$

$$\widehat{\boldsymbol{\mathcal{G}}}^{\mathrm{M}}(\mathbf{k}_{\mathrm{B}}) = \sum_{\boldsymbol{\Gamma}} \widetilde{\boldsymbol{\mathcal{G}}}^{\mathrm{M}}(\mathbf{k}_{\mathrm{B}} + \boldsymbol{\Gamma}) \tag{30b}$$

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.

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[4]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 $|\mathbf{q}|$

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 $\mathbf{q}$ integrals to get the total DGFs at a given frequency, it is more efficient instead to write the $\mathbf{q}$-plane integrals (27) 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:

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

the 2D integrals (27) can be reduced to 1D integrals:

$$\boldsymbol{\mathcal{G}}^{\mathrm{E}} = \frac{i}{4\pi} \int_0^\infty \frac{qdq}{q_z} e^{-q_z(z+z')} \left\{ r_{\mathrm{TE}}\widetilde{\mathbf{M}}^{\mathrm{TE}} + r_{\mathrm{TM}}\widetilde{\mathbf{M}}^{\mathrm{TM}} \right\} \tag{31}$$

$$\boldsymbol{\mathcal{G}}^{\mathrm{E}} = \frac{i}{4\pi} \int_0^\infty \frac{qdq}{q_z} e^{-q_z(z+z')} \left\{ r_{\mathrm{TM}}\widetilde{\mathbf{M}}^{\mathrm{TE}} + r_{\mathrm{TE}}\widetilde{\mathbf{M}}^{\mathrm{TM}} \right\} \tag{32}$$

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

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

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

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

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).