

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

Homer Reid

September 27, 2014

Contents

| | | |
|----------|---------------------------------------------------------------------------------------|-----------|
| 1 | Notation and conventions | 2 |
| 2 | Scattering Green's functions and LDOS in the non-periodic case | 4 |
| 3 | Extension to the periodic case | 5 |
| 4 | Vector-matrix-vector product formula for dyadic Green's functions | 7 |
| 4.1 | The non-periodic case | 7 |
| 4.2 | The periodic case | 9 |
| 5 | API Routines for computing dyadic Green's functions | 10 |
| A | Fields of a phased array of point dipole radiators | 11 |
| B | Analytical formulas for scattering part of DGFs above a homogeneous half space | 14 |
| B.1 | 2D integrals over the entire \mathbf{q} plane | 14 |
| B.2 | 2D integrals over the Brillouin zone | 15 |
| B.3 | 1D integrals over $ \mathbf{q} $ | 16 |
| C | Rewriting infinite 2D k-integrals as Brillouin-zone integrals | 17 |

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 $\mathbf{\Gamma} = \begin{pmatrix} \mathbf{\Gamma}_{\text{ME}}^{\text{EE}} & \mathbf{\Gamma}_{\text{MM}}^{\text{EM}} \\ \mathbf{\Gamma}_{\text{ME}}^{\text{ME}} & \mathbf{\Gamma}_{\text{MM}}^{\text{EM}} \end{pmatrix}$ 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} :

$$\begin{pmatrix} E_i(\mathbf{x}) \\ H_i(\mathbf{x}) \end{pmatrix} = \int \begin{pmatrix} \Gamma_{ij}^{\text{EE}}(\omega; \mathbf{x}; \mathbf{x}') & \Gamma_{ij}^{\text{EM}}(\omega; \mathbf{x}; \mathbf{x}') \\ \Gamma_{ij}^{\text{ME}}(\omega; \mathbf{x}; \mathbf{x}') & \Gamma_{ij}^{\text{MM}}(\omega; \mathbf{x}; \mathbf{x}') \end{pmatrix} \begin{pmatrix} J_j(\mathbf{x}') \\ M_j(\mathbf{x}') \end{pmatrix} dV,$$

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:

$$\mathbf{\Gamma} = \mathbf{\Gamma}^0 + \mathbf{\Gamma}^{\text{scat}} \quad (1)$$

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.

Homogenous DGFs

In a homogeneous material region with relative permittivity and permeability $\{\epsilon^r, \mu^r\}$, the four quadrants of the 6x6 tensor $\mathbf{\Gamma}^0$ may be expressed in terms of two 3×3 tensors \mathbb{G}, \mathbb{C} :

$$\mathbf{\Gamma}^{0, \text{EE}} = ikZ_0Z^r\mathbb{G} \quad (2a)$$

$$\mathbf{\Gamma}^{0, \text{EM}} = ik\mathbb{C} \quad (2b)$$

$$\mathbf{\Gamma}^{0, \text{ME}} = -ik\mathbb{C} \quad (2c)$$

$$\mathbf{\Gamma}^{0, \text{MM}} = \frac{ik}{Z_0Z^r}\mathbb{G} \quad (2d)$$

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

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

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

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

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

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

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

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

LDOS from DGFs

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

$$\rho^{\text{E}}(\omega; \mathbf{r}) = \left(\frac{k}{\pi c} \right) \cdot \left[\frac{1}{ikZ_0Z_r} \text{Tr Im } \mathbf{\Gamma}^{\text{EE}}(\omega; \mathbf{r}, \mathbf{r}) \right] \quad (5a)$$

$$\rho^{\text{M}}(\omega; \mathbf{r}) = \left(\frac{k}{\pi c} \right) \cdot \left[\frac{Z_0Z_r}{ik} \text{Tr Im } \mathbf{\Gamma}^{\text{MM}}(\mathbf{r}, \mathbf{r}) \right] \quad (5b)$$

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 $\text{Tr Im } \mathbb{G}$), 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:

$$\begin{aligned}\mathcal{G}_{ij}^{\text{E}}(\omega; \mathbf{x}, \mathbf{x}') &\equiv \frac{1}{ikZ_0Z_r} \mathbf{\Gamma}_{ij}^{\text{EE,scat}}(\omega; \mathbf{x}, \mathbf{x}') \\ &= \frac{1}{ikZ_0Z_r} \left(\begin{array}{l} i\text{-component of scattered } \mathbf{E}\text{-field at } \mathbf{x} \text{ due to a unit-} \\ \text{strength } j\text{-directed point } \mathbf{electric} \text{ dipole radiator at} \\ \mathbf{x}', \text{ all quantities having time dependence } \sim e^{-i\omega t} \end{array} \right) \\ \mathcal{G}_{ij}^{\text{M}}(\omega; \mathbf{x}, \mathbf{x}') &\equiv \frac{Z_0Z_r}{ik} \mathbf{\Gamma}_{ij}^{\text{MM,scat}}(\omega; \mathbf{x}, \mathbf{x}') \\ &= \frac{Z_0Z_r}{ik} \left(\begin{array}{l} i\text{-component of scattered } \mathbf{H}\text{-field at } \mathbf{x} \text{ due to a unit-} \\ \text{strength } j\text{-directed point } \mathbf{magnetic} \text{ dipole radiator} \\ \text{at } \mathbf{x}', \text{ all quantities having time dependence } \sim e^{-i\omega t} \end{array} \right)\end{aligned}$$

Like \mathbb{G} , the tensors $\mathcal{G}^{\text{E,M}}$ 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

$$\rho_{\text{scat}}^{\text{E}}(\omega; \mathbf{x}) \equiv \frac{k}{\pi c} \text{Tr Im } \mathcal{G}^{\text{E}}(\omega; \mathbf{x}, \mathbf{x}), \quad \rho_{\text{scat}}^{\text{m}}(\omega; \mathbf{x}) \equiv \frac{k}{\pi c} \text{Tr Im } \mathcal{G}^{\text{M}}(\omega; \mathbf{x}, \mathbf{x}).$$

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

$$\mathbf{E}^{\text{inc}}(\mathbf{x}) = \mathbf{E}^{\text{ED}}(\mathbf{x}; \{\mathbf{x}_s, \hat{\mathbf{x}}_j\}), \quad \mathbf{H}^{\text{inc}}(\mathbf{x}) = \mathbf{H}^{\text{ED}}(\mathbf{x}; \{\mathbf{x}_s, \hat{\mathbf{x}}_j\}) \quad (6)$$

where $\{\mathbf{E}, \mathbf{H}\}^{\text{ED}}(\mathbf{x}; \{\mathbf{x}_0, \mathbf{p}_0\})$ 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 (6) and compute the scattered—not total!—fields at the evaluation point \mathbf{x}_D . The three components of the \mathbf{E} -field at \mathbf{x}_D , divided by ikZ_0Z_r , yield the three vertical entries of the j th column of the 3×3 matrix $\mathcal{G}^{\text{E}}(\omega; \mathbf{x}_D, \mathbf{x}_s)$. Calculating \mathcal{G}^{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

$$Q(\mathbf{x} + \mathbf{L}) = e^{i\mathbf{k}_B \cdot \mathbf{L}} Q(\mathbf{x}) \quad (7)$$

where \mathbf{L} is any lattice vector and \mathbf{k}_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,

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

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

(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),

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

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

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

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

Reciprocity of homogeneous Green’s functions

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

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

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

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

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

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

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

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}_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

$$\frac{1}{V_{\text{BZ}}} \int_{\text{BZ}} f(\mathbf{k}_B) d\mathbf{k}_B = 4 \int_0^{1/2} du_1 \int_0^{1/2} du_2 f(u_1 \mathbf{\Gamma}_1 + u_2 \mathbf{\Gamma}_2)$$

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}^E

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

$$\begin{pmatrix} E_\ell^{\text{inc}}(\mathbf{x}) \\ H_\ell^{\text{inc}}(\mathbf{x}) \end{pmatrix} = -i\omega p_0 \begin{pmatrix} \Gamma_{\ell j}^{\text{EE}}(\mathbf{x}, \mathbf{x}_S) \\ \Gamma_{\ell j}^{\text{ME}}(\mathbf{x}, \mathbf{x}_S) \end{pmatrix} = (-i\omega p_0) \begin{pmatrix} ikZ_0 Z^r \mathbb{G}_{\ell j}(\mathbf{x}, \mathbf{x}_S) \\ -ik\mathbb{C}_{\ell j}(\mathbf{x}, \mathbf{x}_S) \end{pmatrix} \quad (11)$$

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

$$E_i^{\text{scat}}(\mathbf{x}_D) = \int \begin{pmatrix} \Gamma_{i\ell}^{\text{EE}}(\mathbf{x}_D, \mathbf{x}) \\ \Gamma_{i\ell}^{\text{EM}}(\mathbf{x}_D, \mathbf{x}) \end{pmatrix}^T \begin{pmatrix} K_\ell(\mathbf{x}) \\ N_\ell(\mathbf{x}) \end{pmatrix} d\mathbf{x} \quad (12)$$

$$= \int \begin{pmatrix} ikZ_0 Z^r \mathbb{G}_{i\ell}(\mathbf{x}_D, \mathbf{x}) \\ +ik\mathbb{C}_{i\ell}(\mathbf{x}_D, \mathbf{x}) \end{pmatrix}^T \begin{pmatrix} K_\ell(\mathbf{x}) \\ N_\ell(\mathbf{x}) \end{pmatrix} d\mathbf{x} \quad (13)$$

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

$$= \sum_a \begin{pmatrix} ikZ_0 Z^r g_a(\mathbf{x}_D, \hat{\mathbf{n}}_i) \\ -ikZ_0 c_a(\mathbf{x}_D, \hat{\mathbf{n}}_i) \end{pmatrix}^T \begin{pmatrix} k_a \\ n_a \end{pmatrix} \quad (14)$$

where I defined

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

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

$$\begin{pmatrix} k_a \\ n_a \end{pmatrix} = -W_{ab} \begin{pmatrix} e_b \\ h_b \end{pmatrix}. \quad (15)$$

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

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

$$\begin{aligned} h_b &\equiv \left\langle \mathbf{b}_m \middle| \mathbf{H}^{\text{inc}} \right\rangle = (-i\omega p_0)(ik) \underbrace{\left[- \int b_{b\ell}(\mathbf{x}) \mathbb{C}_{\ell j}(\mathbf{x}, \mathbf{x}_s) dx \right]}_{-c_b(\mathbf{x}_s, \hat{\mathbf{n}}_j)} \\ &= -(-i\omega p_0)(ik) c_b(\mathbf{x}_s, \hat{\mathbf{n}}_j). \end{aligned} \quad (16b)$$

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,

$$\begin{Bmatrix} E_i^{\text{scat}}(\mathbf{x}_D) \\ H_i^{\text{scat}}(\mathbf{x}_D) \end{Bmatrix} = (i\omega p_0) \cdot \frac{1}{Z_0} \underbrace{\begin{Bmatrix} ikZ_0 Z^r g_a(\mathbf{x}_D, \hat{\mathbf{n}}_i) \\ -ikZ_0 c_a(\mathbf{x}_D, \hat{\mathbf{n}}_i) \end{Bmatrix}^T}_{\equiv (\mathbf{r}_{iD}^E)_a} \left(W_{ab} \right) \underbrace{\begin{Bmatrix} ikZ_0 Z^r g_b(\mathbf{x}_s, \hat{\mathbf{n}}_j) \\ -ikZ_0 c_b(\mathbf{x}_s, \hat{\mathbf{n}}_j) \end{Bmatrix}}_{\equiv (\mathbf{r}_{jS}^E)_b} \quad (17)$$

and the scattering part of the electric DGF reads

$$\mathcal{G}_{ij}^E(\mathbf{x}_D, \mathbf{x}_s) = \frac{E_i^{\text{scat}}}{(ikZ_0 Z^r)(-i\omega p_0)} = -\frac{1}{ikZ_0^2 Z^r} \left(\mathbf{r}_{iD}^E \cdot \mathbf{W} \cdot \mathbf{r}_{jS}^E \right) \quad (18)$$

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

VMVP formula for \mathcal{G}^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

$$\begin{Bmatrix} E_\ell^{\text{inc}}(\mathbf{x}) \\ H_\ell^{\text{inc}}(\mathbf{x}) \end{Bmatrix} = -i\omega m_0 \begin{Bmatrix} \Gamma_{\ell j}^{\text{EM}}(\mathbf{x}, \mathbf{x}_s) \\ \Gamma_{\ell j}^{\text{MM}}(\mathbf{x}, \mathbf{x}_s) \end{Bmatrix} = (-i\omega m_0) \begin{Bmatrix} ik\mathbb{C}_{\ell j}(\mathbf{x}, \mathbf{x}_s) \\ \frac{ik}{Z_0 Z^r} \mathbb{G}_{\ell j}(\mathbf{x}, \mathbf{x}_s) \end{Bmatrix}$$

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

replaces equation (14) with

$$H_i^{\text{scat}}(\mathbf{x}_D) = \int \left\{ \begin{array}{c} \Gamma_{i\ell}^{\text{ME}}(\mathbf{x}_D, \mathbf{x}) \\ \Gamma_{i\ell}^{\text{MM}}(\mathbf{x}_D, \mathbf{x}) \end{array} \right\}^T \left\{ \begin{array}{c} K_\ell(\mathbf{x}) \\ N_\ell(\mathbf{x}) \end{array} \right\} d\mathbf{x} \quad (19)$$

$$= \sum_a \left\{ \begin{array}{c} -ikc_a(\mathbf{x}_D, \hat{\mathbf{n}}_i) \\ -\frac{ik}{Z^r} g_a(\mathbf{x}_D, \hat{\mathbf{n}}_i) \end{array} \right\}^T \left\{ \begin{array}{c} k_a \\ n_a \end{array} \right\} \quad (20)$$

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

$$H_i^{\text{scat}} = + \frac{1}{Z_0} \underbrace{\left(\begin{array}{c} -ikc_a(\mathbf{x}_D, \hat{\mathbf{n}}_i) \\ -\frac{1}{ikZ^r} g_a(\mathbf{x}_D, \hat{\mathbf{n}}_i) \end{array} \right)^T}_{\equiv (\mathbf{r}_{iD}^H)_a} \left(W_{ab} \right) \underbrace{\left(\begin{array}{c} -ikc_b(\mathbf{x}_S, \hat{\mathbf{n}}_j) \\ -\frac{1}{ikZ^r} g_b(\mathbf{x}_S, \hat{\mathbf{n}}_j) \end{array} \right)}_{\equiv (\mathbf{r}_{jS}^H)_b}$$

so the scattering part of the magnetic DGF reads

$$\mathcal{G}_{ij}^H(\mathbf{x}_D, \mathbf{x}_S) = + \frac{Z_0 Z^r}{ik(-i\omega m_0)} H_i^{\text{scat}} = + \frac{Z^r}{ik} \left(\mathbf{r}_{iD}^H \cdot \mathbf{W} \cdot \mathbf{r}_{jS}^H \right). \quad (21)$$

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

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

Thus the periodic version of (18) reads

$$\overline{\mathcal{G}}_{ij}^E(\mathbf{x}_D, \mathbf{x}_S; \mathbf{k}_B) = -\frac{1}{ikZ_0^2 Z^r} \left(\mathbf{r}_{iD}^E(\mathbf{k}_B) \cdot \mathbf{W}(\mathbf{k}_B) \cdot \mathbf{r}_{jS}^E(-\mathbf{k}_B) \right) \quad (22)$$

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 $\overline{\mathcal{G}}_{ij}^E(\mathbf{x}, \mathbf{x}', k^B)$ 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

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

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

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,

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

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:

$$\begin{aligned}E_i(\mathbf{x}) &= \int \Gamma_{ij}^{\text{EE}}(\mathbf{x}, \mathbf{x}') J_j(\mathbf{x}') d\mathbf{x}' \\ &= -i\omega \Gamma_{ij}^{\text{EE}}(\mathbf{x}, \mathbf{x}_0) p_{0j} \\ &= (-i\omega)(ik Z_0 Z^r) G_{ij}(\mathbf{x}, \mathbf{x}_0) p_{0j} \\ &= +k^2 \cdot \frac{|\mathbf{p}_0|}{\epsilon_0 \epsilon^r} \cdot G_{ij}(\mathbf{x}, \mathbf{x}_0) \hat{p}_{0j} \quad (24a)\end{aligned}$$

$$\begin{aligned}H_i(\mathbf{x}) &= \int \Gamma_{ij}^{\text{ME}}(\mathbf{x}, \mathbf{x}') J_j(\mathbf{x}') d\mathbf{x}' \\ &= -i\omega \Gamma_{ij}^{\text{ME}}(\mathbf{x}, \mathbf{x}_0) p_{0j} \\ &= (-i\omega)(-ik) C_{ij}(\mathbf{x}, \mathbf{x}_0) p_{0j} \\ &= -\frac{k^2}{Z_0 Z^r} \cdot \frac{|\mathbf{p}|}{\epsilon_0 \epsilon^r} \cdot C_{ij}(\mathbf{x}, \mathbf{x}_0) \hat{p}_{0j} \quad (24b)\end{aligned}$$

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

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

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

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

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,

$$G_0(\mathbf{x} - \mathbf{x}') \longrightarrow \overline{G}_0(\mathbf{x}, \mathbf{x}'; \mathbf{k}_B) \equiv \sum_{\mathbf{L}} e^{i\mathbf{k}_B \cdot \mathbf{L}} G_0(\mathbf{x} - \mathbf{x}' - \mathbf{L}).$$

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

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

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

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 the non-periodic scalar Green's function:

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

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

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

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

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

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

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

$$\begin{aligned} \bar{\mathbf{g}}(\boldsymbol{\rho}, z; k_x, k_y) &= \sum_{n_x, n_y=-\infty}^{\infty} \mathbf{g}(\boldsymbol{\rho}, z; k_x + n_x \Gamma_x, k_y + n_y \Gamma_y), \\ \bar{\mathbf{c}}(\boldsymbol{\rho}, z; k_x, k_y) &= \sum_{n_x, n_y=-\infty}^{\infty} \mathbf{c}(\boldsymbol{\rho}, z; k_x + n_x \Gamma_x, k_y + n_y \Gamma_y). \end{aligned}$$

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

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

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 .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 \mathbf{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.

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

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

$$\tilde{\mathcal{G}}^E(\mathbf{q}) = \frac{i}{8\pi^2 q_z} e^{i\mathbf{q} \cdot (\boldsymbol{\rho} - \boldsymbol{\rho}') - q_z(z+z')} \left\{ r_{\text{TE}} \mathbf{M}^{\text{TE}} + r_{\text{TM}} \mathbf{M}^{\text{TM}} \right\} \quad (31a)$$

$$\tilde{\mathcal{G}}^M(\mathbf{q}) = \frac{i}{8\pi^2 q_z} e^{i\mathbf{q} \cdot (\boldsymbol{\rho} - \boldsymbol{\rho}') - q_z(z+z')} \left\{ r_{\text{TM}} \mathbf{M}^{\text{TE}} + r_{\text{TE}} \mathbf{M}^{\text{TM}} \right\} \quad (31b)$$

²In 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).

$$\begin{aligned}
\mathbf{M}^{\text{TE}} &\equiv \begin{pmatrix} -\hat{q}_y \\ \hat{q}_x \\ 0 \end{pmatrix} \begin{pmatrix} -\hat{q}_y \\ \hat{q}_x \\ 0 \end{pmatrix}^T \\
&= \begin{pmatrix} \sin^2 \theta & -\cos \theta \sin \theta & 0 \\ -\cos \theta \sin \theta & \cos^2 \theta & 0 \\ 0 & 0 & 0 \end{pmatrix} \\
\mathbf{M}^{\text{TM}} &\equiv \frac{1}{k_0^2} \begin{pmatrix} -q_z \hat{q}_x \\ -q_z \hat{q}_y \\ q \end{pmatrix} \begin{pmatrix} -q_z \hat{q}_x \\ -q_z \hat{q}_y \\ q \end{pmatrix}^T \\
&= \frac{1}{k_0^2} \begin{pmatrix} q_z^2 \cos^2 \theta & q_z^2 \sin \theta \cos \theta & -qq_z \cos \theta \\ q_z^2 \sin \theta \cos \theta & q_z^2 \sin^2 \theta & -qq_z \sin \theta \\ -qq_z \cos \theta & -qq_z \sin \theta & q^2 \end{pmatrix} \\
q &\equiv |\mathbf{q}|, \quad q_z \equiv \sqrt{q^2 - k^2}, \quad q'_z \equiv \sqrt{q^2 - \epsilon \mu k^2}, \\
r_{\text{TE}} &\equiv \frac{\mu q_z - q'_z}{\mu q_z + q'_z}, \quad r_{\text{TM}} \equiv \frac{\epsilon q_z - q'_z}{\epsilon q_z + q'_z}.
\end{aligned}$$

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

$$\mathcal{G}^E(\rho, z; \rho', z') = \int_{\text{BZ}} \hat{\mathcal{G}}^E(\mathbf{q}) d\mathbf{q} \quad (32a)$$

$$\mathcal{G}^M(\rho, z; \rho', z') = \int_{\text{BZ}} \hat{\mathcal{G}}^M(\mathbf{q}) d\mathbf{q} \quad (32b)$$

$$\hat{\mathcal{G}}^E(\mathbf{k}_B) = \sum_{\Gamma} \tilde{\mathcal{G}}^E(\mathbf{k}_B + \Gamma), \quad (33a)$$

$$\hat{\mathcal{G}}^M(\mathbf{k}_B) = \sum_{\Gamma} \tilde{\mathcal{G}}^M(\mathbf{k}_B + \Gamma) \quad (33b)$$

The quantities $\hat{\mathcal{G}}(\mathbf{k}_B)$ may be directly compared to the Brillouin-zone integrand values reported by SCUFF-LDOS in the `.byOmegaBloch` output file.

³Since 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 (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:

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

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

$$\mathcal{G}^E = \frac{i}{4\pi} \int_0^\infty \frac{q dq}{q_z} e^{-q_z(z+z')} \left\{ r_{TE} \widetilde{\mathbf{M}}^{TE} + r_{TM} \widetilde{\mathbf{M}}^{TM} \right\} \quad (34)$$

$$\mathcal{G}^E = \frac{i}{4\pi} \int_0^\infty \frac{q dq}{q_z} e^{-q_z(z+z')} \left\{ r_{TM} \widetilde{\mathbf{M}}^{TE} + r_{TE} \widetilde{\mathbf{M}}^{TM} \right\} \quad (35)$$

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 \mathbf{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:

$$I = \int_{\text{BZ}} d^2\mathbf{k}_B \bar{Q}(\mathbf{k}_B),$$

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

$$\bar{Q}(\mathbf{k}_B) = \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} Q(\mathbf{k}_B + n_1\mathbf{\Gamma}_1 + n_2\mathbf{\Gamma}_2)$$

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).