Calculation of Reflection and Transmission Coefficients in SCUFF-TRANSMISSION

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Contents

1 The Setup

SCUFF-TRANSMISSION considers geometries with 2D periodicity, i.e. the structure consists of a unit-cell geometry of finite extent in the z direction that is infinitely periodically replicated in both the x and y directions. The structure is illuminated either from below (the default) or from above by a plane wave with propagation vector $\mathbf{k}$ confined to the xz plane.

Working at angular frequency ω, let the free-space wavelength be $k_0 = \frac{\omega}{c}$, and let the relative permittivity and permeability of the lowermost and uppermost regions in the geometry be $\epsilon_{\text{L,U}}$ and $\mu_{\text{L,U}}$. The wavenumber and relative wave impedance in the uppermost and lowermost regions are

$$\begin{aligned} k_{\text{L}} &= \sqrt{\epsilon_{\text{L}}\mu_{\text{L}}} \cdot k_0, \qquad & Z_{\text{L}} &= \sqrt{\frac{\mu_{\text{L}}}{\epsilon_{\text{L}}}} \\ k_{\text{U}} &= \sqrt{\epsilon_{\text{U}}\mu_{\text{U}}} \cdot k_0, \qquad & Z_{\text{U}} &= \sqrt{\frac{\mu_{\text{U}}}{\epsilon_{\text{U}}}}. \end{aligned}$$

I will refer to region from which the planewave originates (either the uppermost or lowermost homogeneous region in the SCUFF-EM geometry) as the "source" region. The region into which the planewave eventually emanates is the "destination" region.

In what follows, I will use the symbols $\mathbf{k}, Z$ and $\mathbf{k}', Z'$ respectively to denote the wavevectors and relative wave impedances in the source and destination regions. Then I have

$$\begin{array}{lll} \text{wave incident from below:} & \{|\mathbf{k}|, Z\} = \{k, Z\}_{\text{L}}, & \{|\mathbf{k}'|, Z'\} = \{k, Z\}_{\text{U}} \\ \text{wave incident from above:} & \{|\mathbf{k}|, Z\} = \{k, Z\}_{\text{U}}, & \{|\mathbf{k}'|, Z'\} = \{k, Z\}_{\text{L}}. \end{array}$$

I will take $\mathbf{k}$ to live in the xz plane (i.e. $\mathbf{k}$ has no y component, $k_y = 0$) and I will let θ be the angle of incidence. Thus the incident wavevector is

$$\begin{array}{ll} \text{wave incident from below:} & \mathbf{k} = k\sin\theta\,\hat{\mathbf{x}} + k\cos\theta\,\hat{\mathbf{z}} \\ \text{wave incident from above:} & \mathbf{k} = k\sin\theta\,\hat{\mathbf{x}} - k\cos\theta\,\hat{\mathbf{z}} \end{array}$$

The transmitted wavevector is

$$\begin{array}{ll} \text{wave incident from below:} & \mathbf{k}' = k'\sin\theta'\,\hat{\mathbf{x}} + k'\cos\theta'\,\hat{\mathbf{z}} \\ \text{wave incident from above:} & \mathbf{k}' = k'\sin\theta'\,\hat{\mathbf{x}} - k'\cos\theta'\,\hat{\mathbf{z}} \end{array}$$

The incident and transmitted angles are related by

$$k'\sin\theta' = k\sin\theta.$$

For a general vector $\mathbf{v}$, I will define $\hat{\mathbf{v}} = \mathbf{v}/|\mathbf{v}|$ to be a unit vector in the direction of $\mathbf{v}$.

Definition of scattering coefficients

The incident, reflected, and transmitted fields may be written in the form

$$\begin{aligned}
\mathbf{E}^{\text{inc}}(\mathbf{x}) &= E_0\boldsymbol{\epsilon}_0^{\text{inc}} e^{i(k_x x \pm k_z z)} & \mathbf{H}^{\text{inc}}(\mathbf{x}) &= H_0\overline{\boldsymbol{\epsilon}}_0^{\text{inc}} e^{i(k_x x \pm k_z z)} \\
\mathbf{E}^{\text{refl}}(\mathbf{x}) &= rE_0\boldsymbol{\epsilon}_0^{\text{refl}} e^{i(k_x x \mp k_z z)} & \mathbf{H}^{\text{refl}}(\mathbf{x}) &= rH_0\overline{\boldsymbol{\epsilon}}_0^{\text{refl}} e^{i(k_x x \mp k_z z)} \\
\mathbf{E}^{\text{trans}}(\mathbf{x}) &= tE_0\boldsymbol{\epsilon}_0^{\text{trans}} e^{i(k_x x \pm k_z' z)} & \mathbf{H}^{\text{trans}}(\mathbf{x}) &= tH_0'\,\overline{\boldsymbol{\epsilon}}_0^{\text{trans}}\, e^{i(k_x x \pm k_z' z)}
\end{aligned} \tag{1}$$

where E_0 is the incident field magnitude, $\boldsymbol{\epsilon}_0^{\text{inc}}$ is the incident-field polarization vector, $\pm$ is positive (negative) if the wave is incident from below (above), and

$$H_0 \equiv \frac{i|\mathbf{k}|E_0}{ZZ_0}, \qquad H_0' \equiv \frac{i|\mathbf{k}|E_0}{Z'Z_0}, \qquad \overline{\boldsymbol{\epsilon}} = \hat{\mathbf{k}} \times \boldsymbol{\epsilon}, \qquad \boldsymbol{\epsilon} = -\hat{\mathbf{k}} \times \overline{\boldsymbol{\epsilon}}.$$

Equations (1) define the reflection and transmission coefficients r and t computed by SCUFF-TRANSMISSION.

2 Scattering coefficients from surface currents

Next we consider an extended structure described by Bloch-periodic boundary conditions, i.e. all fields and currents satisfy

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

where $\mathbf{Q}$ is a field ($\mathbf{E}$ or $\mathbf{H}$) or a surface current ($\mathbf{K}$ or $\mathbf{N}$) and the Bloch wavevector is[1]

$$\mathbf{k}_{\mathrm{B}} = k\sin\theta\,\hat{\mathbf{x}} = k'\sin\theta'\,\hat{\mathbf{x}}.$$

For plane waves like (1), equation (2) actually holds for any arbitrary vector $\mathbf{L}$; for our purposes we will only need to use it for certain special vectors $\mathbf{L}$ determined by the structure of the lattice in our PBC geometry. We will derive expressions for the plane-wave reflection and transmission coefficients in terms of the surface-current distribution in the unit cell of the structure.

Fields from surface currents

On the other hand, the scattered $\mathbf{E}$ fields in the source and destination regions may be obtained in the usual way from the surface-current distributions on the surfaces bounding those regions. For example, at points in the destination medium, the scattered (that is, transmitted) $\mathbf{E}$ field is given by

$$\begin{aligned}\mathbf{E}^{\mathrm{trans}}(\mathbf{x}) &= \oint_{\mathcal{S}} \Big\{\boldsymbol{\Gamma}^{\mathrm{EE}}(\mathbf{x},\mathbf{x}')\cdot\mathbf{K}(\mathbf{x}') + \boldsymbol{\Gamma}^{\mathrm{EM}}(\mathbf{x},\mathbf{x}')\cdot\mathbf{N}(\mathbf{x}')\Big\}d\mathbf{x}' \\ &= ik'\oint_{\mathcal{S}}\Big\{Z_0Z'\mathbf{G}(k';\mathbf{x},\mathbf{x}')\cdot\mathbf{K}(\mathbf{x}') + \mathbf{C}(k';\mathbf{x},\mathbf{x}')\cdot\mathbf{N}(\mathbf{x}')\Big\}d\mathbf{x}' \qquad (3)\end{aligned}$$

where $\mathcal{S}$ is the surface bounding the uppermost region and $\mathbf{G},\mathbf{C}$ are the homogeneous dyadic GFs. Using the Bloch periodicity of the surface currents, i.e.

$$\left\{\begin{array}{c}\mathbf{K}(\mathbf{x}+\mathbf{L})\\ \mathbf{N}(\mathbf{x}+\mathbf{L})\end{array}\right\} = e^{i\mathbf{k}_{\mathrm{B}}\cdot\mathbf{L}}\left\{\begin{array}{c}\mathbf{K}(\mathbf{x})\\ \mathbf{N}(\mathbf{x})\end{array}\right\}$$

we can restrict the surface integral in (3) to just the lattice unit cell:

$$\mathbf{E}^{\mathrm{trans}}(\mathbf{x}) = ik'\int_{\mathrm{UC}}\Big\{Z_0Z'\overline{\mathbf{G}}(k';\mathbf{x},\mathbf{x}')\cdot\mathbf{K}(\mathbf{x}') + \overline{\mathbf{C}}(k';\mathbf{x},\mathbf{x}')\cdot\mathbf{N}(\mathbf{x}')\Big\}\,d\mathbf{x}' \tag{4}$$

where the periodic Green's functions are

$$\left\{\begin{array}{c}\overline{\mathbf{G}}(\mathbf{x},\mathbf{x}')\\ \overline{\mathbf{C}}(\mathbf{x},\mathbf{x}')\end{array}\right\} \equiv \sum_{\mathbf{L}} e^{i\mathbf{k}_{\mathrm{B}}\cdot\mathbf{L}}\left\{\begin{array}{c}\mathbf{G}(\mathbf{x},\mathbf{x}'+\mathbf{L})\\ \mathbf{C}(\mathbf{x},\mathbf{x}'+\mathbf{L})\end{array}\right\} \tag{5}$$

[1] Recall our conventions that **(a)** the propagation vector lives in the xy plane, **(b)** unprimed (primed) quantities refer to quantities in the source (destination) region.

I now invoke the following representation of the dyadic Green's functions (Chew, 1995): for $z > z'$,

$$\mathbf{G}(k;\boldsymbol{\rho},z;\boldsymbol{\rho}',z') = \int \frac{d\mathbf{q}}{(2\pi)^2}\,\widetilde{\mathbf{G}}^{\pm}(k;\mathbf{q})e^{i\mathbf{q}\cdot(\boldsymbol{\rho}-\boldsymbol{\rho}')}e^{\pm iq_z(z-z')} \tag{6a}$$

$$\mathbf{C}(k;\boldsymbol{\rho},z;\boldsymbol{\rho}',z') = \int \frac{d\mathbf{q}}{(2\pi)^2}\,\widetilde{\mathbf{C}}^{\pm}(k;\mathbf{q})e^{i\mathbf{q}\cdot(\boldsymbol{\rho}-\boldsymbol{\rho}')}e^{\pm iq_z(z-z')} \tag{6b}$$

where $\mathbf{q} = (q_x, q_y)$ is a two-dimensional Fourier wavevector, $d\mathbf{q} = dq_x dq_y$, $q_z = \sqrt{k^2 - |\mathbf{q}|^2}$, $\pm = \text{sign}(z - z')$, and

$$\widetilde{\mathbf{G}}^{\pm}(k;\mathbf{q}) = \frac{i}{2q_z}\left[\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \frac{1}{k^2}\begin{pmatrix} q_x^2 & q_xq_y & \pm q_xq_z \\ q_yq_x & q_y^2 & \pm q_yq_z \\ \pm q_zq_x & \pm q_zq_y & q_z^2 \end{pmatrix}\right]$$

$$\widetilde{\mathbf{C}}^{\pm}(k;\mathbf{q}) = \frac{i}{2q_zk}\begin{pmatrix} 0 & \pm q_z & -q_y \\ -\pm q_z & 0 & q_x \\ q_y & -q_x & 0 \end{pmatrix}.$$

Inserting (6) into (5), I obtain, for the periodic version of e.g. the $\mathbf{G}$ kernel,

$$\begin{aligned}\overline{\mathbf{G}}(k;\boldsymbol{\rho},z;\boldsymbol{\rho}',z) &= \int \frac{d\mathbf{q}}{(2\pi)^2}\widetilde{\mathbf{G}}^{\pm}(k;\mathbf{q})e^{i\mathbf{q}\cdot(\boldsymbol{\rho}-\boldsymbol{\rho}')}e^{\pm iq_z(z-z')}\underbrace{\sum_{\mathbf{L}} e^{i(\mathbf{k}_{\mathrm{B}}-\mathbf{q})\cdot\mathbf{L}}}_{\mathcal{V}_{\mathrm{BZ}}\sum_{\boldsymbol{\Gamma}}\delta(\mathbf{q}-\mathbf{k}-\boldsymbol{\Gamma})} \\ &= \mathcal{V}_{\mathrm{UC}}^{-1}\sum_{\mathbf{q}=\mathbf{k}_{\mathrm{B}}+\boldsymbol{\Gamma}}\widetilde{\mathbf{G}}^{\pm}(k;\mathbf{q})e^{i\mathbf{q}\cdot(\boldsymbol{\rho}-\boldsymbol{\rho}')}e^{\pm iq_z(z-z')}\end{aligned}$$

where the sum over $\boldsymbol{\Gamma}$ runs over reciprocal lattice vectors; the prefactor $\mathcal{V}_{\mathrm{BZ}}$, the volume of the Brillouin zone, is related to the unit-cell volume by $\mathcal{V}_{\mathrm{BZ}} = 4\pi^2/V_{\mathrm{UC}}$ for a 2D square lattice. Similarly, we find

$$\overline{\mathbf{C}}(k;\boldsymbol{\rho},z;\boldsymbol{\rho}',z) = \mathcal{V}_{\mathrm{UC}}^{-1}\sum_{\mathbf{q}=\mathbf{k}_{\mathrm{B}}+\boldsymbol{\Gamma}}\widetilde{\mathbf{C}}^{\pm}(k;\mathbf{q})e^{i\mathbf{q}\cdot(\boldsymbol{\rho}-\boldsymbol{\rho}')}e^{\pm iq_z(z-z')}.$$

Keeping only the $\boldsymbol{\Gamma} = 0$ term in these sums, the scattered $\mathbf{E}$-fields in the uppermost and lowermost regions are thus

$$\mathbf{E}^{\text{upper}}(\mathbf{x}) = e^{i(k_{\mathrm{Ux}}x+k_{\mathrm{Uz}}z)}\Big[ik_{\mathrm{U}}Z_0Z_{\mathrm{U}}\widetilde{\mathbf{G}}^{+}(k_{\mathrm{U}};\mathbf{k}_{\mathrm{B}})\widetilde{\mathbf{K}}_{\mathrm{U}}(\mathbf{k}_{\mathrm{B}}) + ik_{\mathrm{U}}\widetilde{\mathbf{C}}^{+}(k_{\mathrm{U}};\mathbf{k}_{\mathrm{B}})\widetilde{\mathbf{N}}(\mathbf{k}_{\mathrm{B}})\Big] \tag{7}$$

$$\mathbf{E}^{\text{lower}}(\mathbf{x}) = e^{i(k_{\mathrm{Lx}}x-k_{\mathrm{Lz}}z)}\Big[ik_{\mathrm{L}}Z_0Z_{\mathrm{U}}\widetilde{\mathbf{G}}^{-}(k_{\mathrm{L}};\mathbf{k}_{\mathrm{B}})\widetilde{\mathbf{K}}(\mathbf{k}_{\mathrm{B}}) + ik_{\mathrm{L}}\widetilde{\mathbf{C}}^{-}(k_{\mathrm{L}};\mathbf{k}_{\mathrm{B}})\widetilde{\mathbf{N}}(\mathbf{k}_{\mathrm{B}})\Big] \tag{8}$$

where e.g. $\widetilde{\mathbf{K}}_{\mathrm{U}}$ is something like the two-dimensional Fourier transform of the surface currents on the boundary of the uppermost region $\mathcal{R}_{\mathrm{U}}$:

$$\widetilde{\mathbf{K}}_{\mathrm{U}}(\mathbf{k}_{\mathrm{B}}) \equiv \frac{1}{\mathcal{V}_{\mathrm{UC}}}\int_{\partial\mathcal{R}_{\mathrm{U}}}\mathbf{K}(\boldsymbol{\rho}',z')e^{-i\mathbf{k}_{\mathrm{B}}\cdot\boldsymbol{\rho}'-iq_z|z'|}d\mathbf{x}', \qquad q_z^2 = k_{\mathrm{U}}^2 - |\mathbf{k}_{\mathrm{B}}|^2.$$

with $\widetilde{\mathbf{K}}_{\mathrm{L}}$ and $\widetilde{\mathbf{N}}_{\mathrm{U,L}}$ defined similarly.

Comparing this to (1c), we see that the transmission and reflection coefficients for the polarization defined by polarization vector $\boldsymbol{\epsilon}$ are given by

$$\left\{ \begin{array}{c} t \\ r \end{array} \right\} = ik_{\mathrm{U}} Z_0 Z_{\mathrm{U}} \boldsymbol{\epsilon}^\dagger \widetilde{\mathbf{G}}^+(k_{\mathrm{U}}, \mathbf{k}_{\mathrm{B}}) \widetilde{\mathbf{K}}_{\mathrm{U}}(\mathbf{k}_{\mathrm{B}}) + ik_{\mathrm{U}} \boldsymbol{\epsilon}^\dagger \widetilde{\mathbf{C}}^+(k_{\mathrm{U}}, \mathbf{k}_{\mathrm{B}}) \widetilde{\mathbf{N}}(\mathbf{k}_{\mathrm{B}}) \tag{9}$$

$$\left\{ \begin{array}{c} r \\ t \end{array} \right\} = ik_{\mathrm{L}} Z_0 Z_{\mathrm{L}} \boldsymbol{\epsilon}^\dagger \widetilde{\mathbf{G}}^+(k_{\mathrm{L}}, \mathbf{k}_{\mathrm{B}}) \widetilde{\mathbf{K}}_{\mathrm{L}}(\mathbf{k}_{\mathrm{B}}) + ik_{\mathrm{L}} \boldsymbol{\epsilon}^\dagger \widetilde{\mathbf{C}}^+(k_{\mathrm{L}}, \mathbf{k}_{\mathrm{B}}) \widetilde{\mathbf{N}}(\mathbf{k}_{\mathrm{B}}) \tag{10}$$

The expressions on the RHS compute the upper (lower) quantities on the LHS for the case in which the plane wave is incident from below (above).

The $\widetilde{\mathbf{K}}$ and $\widetilde{\mathbf{N}}$ quantities are given by sums of contributions from individual basis functions; for example,

$$\widetilde{\mathbf{K}}_{\mathrm{U}}(\mathbf{q}) = \frac{1}{\mathcal{V}_{\mathrm{UC}}} \sum_{\mathbf{b}_\alpha \in \partial \mathcal{R}_{\mathrm{U}}} k_\alpha \widetilde{\mathbf{b}_\alpha}(\mathbf{q}), \qquad \widetilde{\mathbf{N}}_{\mathrm{U}}(\mathbf{q}) = -\frac{Z_0}{\mathcal{V}_{\mathrm{UC}}} \sum_{\mathbf{b}_\alpha \in \partial \mathcal{R}_{\mathrm{U}}} n_\alpha \widetilde{\mathbf{b}_\alpha}(\mathbf{q})$$

where the sums are over all RWG basis functions that live on surfaces bounding the uppermost medium and $\{k_\alpha, n_\alpha\}$ are the surface-current coefficients obtained as the solution to the SCUFF-EM scattering problem.

2.1 Computation of $\widetilde{\mathbf{b}}(\mathbf{q})$

For RWG functions the quantity $\widetilde{\mathbf{b}}(\mathbf{q})$ may be evaluated in closed form:

$$\begin{aligned}
\widetilde{\mathbf{b}_\alpha}(\mathbf{q}) &\equiv \int_{\sup\, \mathbf{b}_\alpha} \mathbf{b}_\alpha(\mathbf{x}) e^{-i\mathbf{q}\cdot\mathbf{x}}\, d\mathbf{x} \\
&= \ell_\alpha \int_0^1 du \int_0^u dv \left\{ e^{-i\mathbf{q}\cdot[\mathbf{Q}^+ + u\mathbf{A}^+ + v\mathbf{B}]} \Big(u\mathbf{A}^+ + v\mathbf{B} \Big) \right. \\
&\qquad\qquad \left. - e^{-i\mathbf{q}\cdot[\mathbf{Q}^- + u\mathbf{A}^- + v\mathbf{B}]} \Big(u\mathbf{A}^- + v\mathbf{B} \Big) \right\} \\
&= \ell_\alpha \left\{ e^{-i\mathbf{q}\cdot\mathbf{Q}^+} \Big[f_1\big(\mathbf{q}\cdot\mathbf{A}^+, \mathbf{q}\cdot\mathbf{B}\big)\mathbf{A}^+ + f_2\big(\mathbf{q}\cdot\mathbf{A}^+, \mathbf{q}\cdot\mathbf{B}\big)\mathbf{B} \Big] \right. \\
&\qquad \left. - e^{-i\mathbf{q}\cdot\mathbf{Q}^-} \Big[f_1\big(\mathbf{q}\cdot\mathbf{A}^-, \mathbf{q}\cdot\mathbf{B}\big)\mathbf{A}^- + f_2\big(\mathbf{q}\cdot\mathbf{A}^-, \mathbf{q}\cdot\mathbf{B}\big)\mathbf{B} \Big] \right\}
\end{aligned}$$

where

$$\begin{aligned}
f_1(x,y) &= \int_0^1 \int_0^u u e^{-i(ux+vy)}\, dv\, du \\
f_2(x,y) &= \int_0^1 \int_0^u v e^{-i(ux+vy)}\, dv\, du.
\end{aligned}$$