Calculation of Reflection and Transmission Coefficients in SCUFF-TRANSMISSION

Homer Reid

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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, refractive index, and relative wave impedance in the uppermost and lowermost regions are

$$k_{\text{L}} = n_{\text{L}} \cdot k_0, \qquad n_{\text{L}} \equiv \sqrt{\epsilon_{\text{L}}\mu_{\text{L}}}, \qquad Z_{\text{L}} = \sqrt{\frac{\mu_{\text{L}}}{\epsilon_{\text{L}}}}$$

$$k_{\text{U}} = n_{\text{U}} \cdot k_0, \qquad n_{\text{U}} \equiv \sqrt{\epsilon_{\text{U}}\mu_{\text{U}}}, \qquad Z_{\text{U}} = \sqrt{\frac{\mu_{\text{U}}}{\epsilon_{\text{U}}}}.$$

I will refer to region from which the planewave originates (either the uppermost or lowermost homogeneous region in the SCUFF-EM geometry) as the "incident" region. The region into which the planewave eventually emanates is the "transmitted" region. I will use the sub/superscripts I, T to denote these quantities; thus the wavenumber and relative wave impedance in the incident and transmitted regions are

$$\Big\{k_{\text{I}}, Z_{\text{I}}, k_{\text{T}}, Z_{\text{T}}\Big\} = \begin{cases} \big\{k_{\text{L}}, Z_{\text{L}}, k_{\text{U}}, Z_{\text{U}}\big\}, & \text{wave incident from below} \\ \big\{k_{\text{U}}, Z_{\text{U}}, k_{\text{L}}, Z_{\text{L}}\big\}, & \text{wave incident from above} \end{cases}$$

In what follows, I will use the symbols $\mathbf{k}^{\text{I}}, \mathbf{k}^{\text{R}}, \mathbf{k}^{\text{T}}$ respectively to denote the propagation vectors of the incident, reflected, and transmitted waves. I will take these vectors always to live in the xz plane (i.e. $\mathbf{k}$ has no y component, $k_y = 0$). I will let θ_{I} and θ_{T} be the angles of incidence and transmission (the angles between the incident and transmitted wavevector and the z axis).

$$\text{wave incident from below:} \qquad \mathbf{k}^{\text{I}} = k_{\text{L}}\Big[\sin\theta_{\text{I}}\,\hat{\mathbf{x}} + \cos\theta_{\text{I}}\,\hat{\mathbf{z}}\Big]$$

$$\text{wave incident from above:} \qquad \mathbf{k}^{\text{I}} = k_{\text{U}}\Big[\sin\theta_{\text{I}}\,\hat{\mathbf{x}} - \cos\theta_{\text{I}}\,\hat{\mathbf{z}}\Big]$$

The reflected wavevector is

$$\text{wave incident from below:} \qquad \mathbf{k}^{\text{R}} = k_{\text{L}}\Big[\sin\theta_{\text{I}}\,\hat{\mathbf{x}} - \cos\theta_{\text{I}}\,\hat{\mathbf{z}}\Big]$$

$$\text{wave incident from above:} \qquad \mathbf{k}^{\text{R}} = k_{\text{L}}\Big[\sin\theta_{\text{I}}\,\hat{\mathbf{x}} + \cos\theta_{\text{I}}\,\hat{\mathbf{z}}\Big]$$

The transmitted wavevector is

$$\text{wave incident from below:} \qquad \mathbf{k}^{\text{T}} = k_{\text{U}}\Big[\sin\theta_{\text{T}}\,\hat{\mathbf{x}} + \cos\theta_{\text{T}}\,\hat{\mathbf{z}}\Big]$$

$$\text{wave incident from above:} \qquad \mathbf{k}^{\text{T}} = k_{\text{L}}\Big[\sin\theta_{\text{T}}\,\hat{\mathbf{x}} - \cos\theta_{\text{T}}\,\hat{\mathbf{z}}\Big]$$

The incident and transmitted angles are related by

$$n_{\text{I}} \sin\theta_{\text{I}} = n_{\text{T}} \sin\theta_{\text{T}}.$$

For a general vector $\mathbf{v}$, I will define $\widehat{\mathbf{v}} = \mathbf{v}/|\mathbf{v}|$ 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

$$\begin{aligned}
\mathbf{E}^{\text{I}}(\mathbf{x}) &= E_0 \boldsymbol{\epsilon}^{\text{I}} e^{i\mathbf{k}^{\text{I}}\cdot\mathbf{x}} & \mathbf{H}^{\text{I}}(\mathbf{x}) &= H_0 \overline{\boldsymbol{\epsilon}}^{\text{I}} e^{i\mathbf{k}^{\text{I}}\cdot\mathbf{x}} l \\
\mathbf{E}^{\text{R}}(\mathbf{x}) &= r E_0 \boldsymbol{\epsilon}^{\text{R}} e^{i\mathbf{k}^{\text{R}}\cdot\mathbf{x}} & \mathbf{H}^{\text{R}}(\mathbf{x}) &= r H_0 \overline{\boldsymbol{\epsilon}}^{\text{R}} e^{i\mathbf{k}^{\text{R}}\cdot\mathbf{x}} \\
\mathbf{E}^{\text{T}}(\mathbf{x}) &= t E_0 \boldsymbol{\epsilon}^{\text{T}} e^{i\mathbf{k}^{\text{T}}\cdot\mathbf{x}} & \mathbf{H}^{\text{T}}(\mathbf{x}) &= t H_0' \overline{\boldsymbol{\epsilon}}^{\text{T}}, e^{i\mathbf{k}^{\text{T}}\cdot\mathbf{x}}
\end{aligned} \tag{1}$$

where E_0 is the incident field magnitude, $\boldsymbol{\epsilon}^{\text{I,R,T}}$ are $\mathbf{E}$-field polarization vectors, $\overline{\boldsymbol{\epsilon}}^{\text{I,R,T}}$ are $\mathbf{H}$-field polarization vectors, and we have

$$H_0 \equiv \frac{i|\mathbf{k}|E_0}{Z_{\text{I}} Z_0}, \qquad H_0' \equiv \frac{i|\mathbf{k}|E_0}{Z_{\text{T}} Z_0}, \qquad \overline{\boldsymbol{\epsilon}} \equiv \widehat{\mathbf{k}} \times \boldsymbol{\epsilon}, \qquad \boldsymbol{\epsilon} = -\widehat{\mathbf{k}} \times \overline{\boldsymbol{\epsilon}}.$$

The polarization vectors are given by

$$\begin{aligned}
&\text{for the TE case:} \qquad \boldsymbol{\epsilon}^{\text{I}}_{\text{TE}} = \boldsymbol{\epsilon}^{\text{R}}_{\text{TE}} = \boldsymbol{\epsilon}^{\text{T}}_{\text{TE}} = \hat{\mathbf{y}}, \qquad \overline{\boldsymbol{\epsilon}}^{\text{I,R,T}}_{\text{TE}} = \widehat{\mathbf{k}^{\text{I,R,T}}} \times \hat{\mathbf{y}} \\
&\text{for the TM case:} \qquad \overline{\boldsymbol{\epsilon}}^{\text{I}}_{\text{TM}} = \overline{\boldsymbol{\epsilon}}^{\text{R}}_{\text{TM}} = \overline{\boldsymbol{\epsilon}}^{\text{T}}_{\text{TM}} = \hat{\mathbf{y}} \qquad \boldsymbol{\epsilon}^{\text{I,R,T}}_{\text{TM}} = -\widehat{\mathbf{k}^{\text{I,R,T}}} \times \hat{\mathbf{y}}
\end{aligned}$$

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]

$$\mathbf{k}_\mathrm{B} = k_\mathrm{I}\sin\theta_\mathrm{I}\,\hat{\mathbf{x}} = k_\mathrm{T}\sin\theta_\mathrm{T}\,\hat{\mathbf{x}}.$$

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 incident and transmitted 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 transmitted medium, the scattered (that is, transmitted) $\mathbf{E}$ field is given by

$$\begin{aligned}\mathbf{E}^\mathrm{T}(\mathbf{x}) &= \oint_{\mathcal{S}_\mathrm{T}} \Big\{\mathbf{\Gamma}^{\mathrm{EE;T}}(\mathbf{x},\mathbf{x}')\cdot\mathbf{K}(\mathbf{x}') + \mathbf{\Gamma}^{\mathrm{EM;T}}(\mathbf{x},\mathbf{x}')\cdot\mathbf{N}(\mathbf{x}')\Big\} d\mathbf{x}' \\ &= ik_\mathrm{T}\oint_{\mathcal{S}} \Big\{Z_0 Z_\mathrm{T}\mathbf{G}(k_\mathrm{T};\mathbf{x},\mathbf{x}')\cdot\mathbf{K}(\mathbf{x}') + \mathbf{C}(k_\mathrm{T};\mathbf{x},\mathbf{x}')\cdot\mathbf{N}(\mathbf{x}')\Big\} d\mathbf{x}' \end{aligned} \tag{3}$$

where $\mathcal{S}_\mathrm{T}$ is the surface bounding the transmitted region and $\mathbf{G},\mathbf{C}$ are the homogeneous dyadic GFs for that region. 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:

$$\mathbf{E}^\mathrm{T}(\mathbf{x}) = ik_\mathrm{T}\int_{\mathrm{UC}} \Big\{Z_0 Z_\mathrm{T}\overline{\mathbf{G}}(k_\mathrm{T};\mathbf{x},\mathbf{x}')\cdot\mathbf{K}(\mathbf{x}') + \overline{\mathbf{C}}(k_\mathrm{T};\mathbf{x},\mathbf{x}')\cdot\mathbf{N}(\mathbf{x}')\Big\} d\mathbf{x}' \tag{4}$$

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 convention that the propagation vector lives in the xy plane.

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

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

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

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

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

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

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

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

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

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

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

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

with $\widetilde{\mathbf{K}}_{\text{L}}$ and $\widetilde{\mathbf{N}}_{\text{U,L}}$ 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

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

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

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,

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

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:

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

where

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