

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  $\omega$ , 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  $\epsilon_{L,U}$  and  $\mu_{L,U}$ . The wavenumber, refractive index, and relative wave impedance in the uppermost and lowermost regions are

$$\begin{aligned} k_L &= n_L \cdot k_0, & n_L &\equiv \sqrt{\epsilon_L \mu_L}, & Z_L &= \sqrt{\frac{\mu_L}{\epsilon_L}} \\ k_U &= n_U \cdot k_0, & n_U &\equiv \sqrt{\epsilon_U \mu_U}, & Z_U &= \sqrt{\frac{\mu_U}{\epsilon_U}}. \end{aligned}$$

I will refer to region from which the planewave originates (either the uppermost or lowermost homogeneous region in the SCUFF-EM geometry) as the “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

$$\left\{ k_I, Z_I, k_T, Z_T \right\} = \begin{cases} \{k_L, Z_L, k_U, Z_U\}, & \text{wave incident from below} \\ \{k_U, Z_U, k_L, Z_L\}, & \text{wave incident from above} \end{cases}$$

In what follows, I will use the symbols  $\mathbf{k}^I, \mathbf{k}^R, \mathbf{k}^T$  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  $\theta_I$  and  $\theta_T$  be the angles of incidence and transmission (the angles between the incident and transmitted wavevector and the  $z$  axis).

$$\text{wave incident from below:} \quad \mathbf{k}^I = k_L \left[ \sin \theta_I \hat{\mathbf{x}} + \cos \theta_I \hat{\mathbf{z}} \right]$$

$$\text{wave incident from above:} \quad \mathbf{k}^I = k_U \left[ \sin \theta_I \hat{\mathbf{x}} - \cos \theta_I \hat{\mathbf{z}} \right]$$

The reflected wavevector is

$$\text{wave incident from below:} \quad \mathbf{k}^R = k_L \left[ \sin \theta_I \hat{\mathbf{x}} - \cos \theta_I \hat{\mathbf{z}} \right]$$

$$\text{wave incident from above:} \quad \mathbf{k}^R = k_L \left[ \sin \theta_I \hat{\mathbf{x}} + \cos \theta_I \hat{\mathbf{z}} \right]$$

The transmitted wavevector is

$$\text{wave incident from below:} \quad \mathbf{k}^T = k_U \left[ \sin \theta_T \hat{\mathbf{x}} + \cos \theta_T \hat{\mathbf{z}} \right]$$

$$\text{wave incident from above:} \quad \mathbf{k}^T = k_L \left[ \sin \theta_T \hat{\mathbf{x}} - \cos \theta_T \hat{\mathbf{z}} \right]$$

The incident and transmitted angles are related by

$$n_i \sin \theta_i = n_T \sin \theta_T.$$

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

$$\begin{aligned} \mathbf{E}^I(\mathbf{x}) &= E_0 \boldsymbol{\epsilon}^I e^{i\mathbf{k}^I \cdot \mathbf{x}} & \mathbf{H}^I(\mathbf{x}) &= H_0 \bar{\boldsymbol{\epsilon}}^I e^{i\mathbf{k}^I \cdot \mathbf{x}} \\ \mathbf{E}^R(\mathbf{x}) &= r E_0 \boldsymbol{\epsilon}^R e^{i\mathbf{k}^R \cdot \mathbf{x}} & \mathbf{H}^R(\mathbf{x}) &= r H_0 \bar{\boldsymbol{\epsilon}}^R e^{i\mathbf{k}^R \cdot \mathbf{x}} \\ \mathbf{E}^T(\mathbf{x}) &= t E_0 \boldsymbol{\epsilon}^T e^{i\mathbf{k}^T \cdot \mathbf{x}} & \mathbf{H}^T(\mathbf{x}) &= t H'_0 \bar{\boldsymbol{\epsilon}}^T e^{i\mathbf{k}^T \cdot \mathbf{x}} \end{aligned} \quad (1)$$

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

$$H_0 \equiv \frac{i|\mathbf{k}|E_0}{Z_1 Z_0}, \quad H'_0 \equiv \frac{i|\mathbf{k}|E_0}{Z_T Z_0}, \quad \bar{\boldsymbol{\epsilon}} \equiv \hat{\mathbf{k}} \times \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} = -\hat{\mathbf{k}} \times \bar{\boldsymbol{\epsilon}}.$$

The polarization vectors are given by

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

Equations (??) 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

$$\mathbf{Q}(\mathbf{x} + \mathbf{L}) = e^{i\mathbf{k}_B \cdot \mathbf{L}} \mathbf{Q}(\mathbf{x}) \quad (2)$$

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<sup>1</sup>

$$\mathbf{k}_B = k_I \sin \theta_I \hat{\mathbf{x}} = k_T \sin \theta_T \hat{\mathbf{x}}.$$

For plane waves like (??), equation (??) 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

$$\begin{aligned} \mathbf{E}^T(\mathbf{x}) &= \oint_{\mathcal{S}_T} \left\{ \mathbf{\Gamma}^{\text{EE};T}(\mathbf{x}, \mathbf{x}') \cdot \mathbf{K}(\mathbf{x}') + \mathbf{\Gamma}^{\text{EM};T}(\mathbf{x}, \mathbf{x}') \cdot \mathbf{N}(\mathbf{x}') \right\} d\mathbf{x}' \\ &= ik_T \oint_{\mathcal{S}} \left\{ Z_0 Z_T \mathbf{G}(k_T; \mathbf{x}, \mathbf{x}') \cdot \mathbf{K}(\mathbf{x}') + \mathbf{C}(k_T; \mathbf{x}, \mathbf{x}') \cdot \mathbf{N}(\mathbf{x}') \right\} d\mathbf{x}' \quad (3) \end{aligned}$$

where  $\mathcal{S}_T$  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.

$$\begin{Bmatrix} \mathbf{K}(\mathbf{x} + \mathbf{L}) \\ \mathbf{N}(\mathbf{x} + \mathbf{L}) \end{Bmatrix} = e^{i\mathbf{k}_B \cdot \mathbf{L}} \begin{Bmatrix} \mathbf{K}(\mathbf{x}) \\ \mathbf{N}(\mathbf{x}) \end{Bmatrix}$$

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

$$\mathbf{E}^T(\mathbf{x}) = ik_T \int_{\text{UC}} \left\{ Z_0 Z_T \overline{\mathbf{G}}(k_T; \mathbf{x}, \mathbf{x}') \cdot \mathbf{K}(\mathbf{x}') + \overline{\mathbf{C}}(k_T; \mathbf{x}, \mathbf{x}') \cdot \mathbf{N}(\mathbf{x}') \right\} d\mathbf{x}' \quad (4)$$

where the periodic Green's functions are

$$\begin{Bmatrix} \overline{\mathbf{G}}(\mathbf{x}, \mathbf{x}') \\ \overline{\mathbf{C}}(\mathbf{x}, \mathbf{x}') \end{Bmatrix} \equiv \sum_{\mathbf{L}} e^{i\mathbf{k}_B \cdot \mathbf{L}} \begin{Bmatrix} \mathbf{G}(\mathbf{x}, \mathbf{x}' + \mathbf{L}) \\ \mathbf{C}(\mathbf{x}, \mathbf{x}' + \mathbf{L}) \end{Bmatrix} \quad (5)$$

<sup>1</sup>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  $z > z'$ ,

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

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

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

$$\tilde{\mathbf{G}}^\pm(k; \mathbf{q}) = \frac{i}{2q_z} \left[ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \frac{1}{k^2} \begin{pmatrix} q_x^2 & q_x q_y & \pm q_x q_z \\ q_y q_x & q_y^2 & \pm q_y q_z \\ \pm q_z q_x & \pm q_z q_y & q_z^2 \end{pmatrix} \right]$$

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

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

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

where the sum over  $\mathbf{\Gamma}$  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

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

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

$$\mathbf{E}^{\text{upper}}(\mathbf{x}) = e^{i(k_{\text{U}x}x + k_{\text{U}z}z)} \left[ ik_{\text{U}} Z_0 Z_{\text{U}} \tilde{\mathbf{G}}^+(k_{\text{U}}; \mathbf{k}_B) \tilde{\mathbf{K}}_{\text{U}}(\mathbf{k}_B) + ik_{\text{U}} \tilde{\mathbf{C}}^+(k_{\text{U}}; \mathbf{k}_B) \tilde{\mathbf{N}}(\mathbf{k}_B) \right] \quad (7)$$

$$\mathbf{E}^{\text{lower}}(\mathbf{x}) = e^{i(k_{\text{L}x}x - k_{\text{L}z}z)} \left[ ik_{\text{L}} Z_0 Z_{\text{U}} \tilde{\mathbf{G}}^-(k_{\text{L}}; \mathbf{k}_B) \tilde{\mathbf{K}}(\mathbf{k}_B) + ik_{\text{L}} \tilde{\mathbf{C}}^-(k_{\text{L}}; \mathbf{k}_B) \tilde{\mathbf{N}}(\mathbf{k}_B) \right] \quad (8)$$

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

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

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

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

$$\begin{Bmatrix} t \\ r \end{Bmatrix} = ik_U Z_0 Z_U \boldsymbol{\epsilon}^\dagger \tilde{\mathbf{G}}^+(k_U, \mathbf{k}_B) \tilde{\mathbf{K}}_U(\mathbf{k}_B) + ik_U \boldsymbol{\epsilon}^\dagger \tilde{\mathbf{C}}^+(k_U, \mathbf{k}_B) \tilde{\mathbf{N}}(\mathbf{k}_B) \quad (9)$$

$$\begin{Bmatrix} r \\ t \end{Bmatrix} = ik_L Z_0 Z_L \boldsymbol{\epsilon}^\dagger \tilde{\mathbf{G}}^-(k_L, \mathbf{k}_B) \tilde{\mathbf{K}}_L(\mathbf{k}_B) + ik_L \boldsymbol{\epsilon}^\dagger \tilde{\mathbf{C}}^-(k_L, \mathbf{k}_B) \tilde{\mathbf{N}}(\mathbf{k}_B) \quad (10)$$

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

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

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 $\tilde{\mathbf{b}}(\mathbf{q})$

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

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

where

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