Numerically solving integral equations of wave ensembles

Artur L. Gower[†]

[†]School of Mathematics, University of Manchester, Oxford Road, Manchester M13 9PL, UK

May 1, 2018

Abstract

Allows for a broad frequency range, and to easily test different statistical assumptions. Assumptions such as the pair-correlation and QCA.

Keywords: polydisperse, multiple scattering, Fredholm Integral equations, multi-species, effective waves, quasicrystalline approximation, statistical methods

1 Effective waves for uniformly distributed species

We consider a halfspace $x > 0$ filled with S types of inclusions (species) that are uniformly distributed. The fields are governed by the scalar wave equation:

$$\nabla^2 u + k^2 u = 0, \quad \text{(in the background material)} \tag{1}$$

$$\nabla^2 u + k_j^2 u = 0, \quad \text{(inside the } j\text{-th scatterer)}, \tag{2}$$

The background and species material properties are summarised in Table 1. The goal is to calculate how a medium with these scatterers, randomly uniformly distributed, reflects and transmits waves in an ensemble average sense.

For simplicity we will consider that all particles are cylindrical, though it is easy to extend the results to any smooth particle by using Waterman's T-matrixWaterman (1971); Varadan et al. (1978); Mishchenko et al. (1996).

Background properties:	wavenumber k	density ρ	sound speed c	
Specie properties:	number density $\mathfrak{n}_j$	density ρ_j	sound speed c_j	radius a_j
total number density $\mathfrak{n}$	effective wavenumber k_*	species min. distance $a_{j\ell} > a_j + a_\ell$		

Table 1: Summary of material properties and notation. The index j refers to properties of the j-th species. Note a typical choice for $a_{j\ell}$ is $a_{j\ell} = c(a_j + a_\ell)$, where $c = 1.01$.

2 Cylindrical species

We consider an incident wave

$$u_{\text{in}} = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \quad \text{with} \quad \mathbf{k}\cdot\mathbf{x} = kx\cos\theta_{\text{in}} + ky\sin\theta_{\text{in}}, \tag{3}$$

and angle of incidence θ_{in} from the x-axis, exciting a material occupying the halfspace $x > 0$.

Combining equations (3.6) and the quasicrystalline approximation (3.10) from (Gower et al., 2018), we arrive at

$$\sum_{n=-\infty}^{\infty} \int_{\mathcal{S}} \int_{\substack{x_2>0 \\ \|\mathbf{x}_1-\mathbf{x}_2\|>a_{12}}} \mathcal{A}_n(k\mathbf{x}_2, \mathbf{s}_2) F_{n-m}(k\mathbf{x}_2 - k\mathbf{x}_1, k) d\mathbf{x}_2 d\mathbf{s}_2^n$$

$$+ \mathcal{A}_m(k\mathbf{x}_1, \mathbf{s}_1) + \mathrm{e}^{\mathrm{i}\mathbf{x}_1\cdot\mathbf{k}} \mathrm{e}^{\mathrm{i}m(\pi/2-\theta_{\text{in}})} = 0, \quad \text{for} \quad x_1 > 0, \quad (4)$$

where

$$d\mathbf{s}_2^n = \mathfrak{n} Z_n(\mathbf{s}_2) p(\mathbf{s}_2) d\mathbf{s}_2, \quad (5)$$

$$F_n(\mathbf{X}, k) = (-1)^n \mathrm{e}^{\mathrm{i}n\Theta} H_n(R)(1 + g(R/k; \mathbf{s}_1, \mathbf{s}_2)), \quad (6)$$

with (R, Θ) being the polar coordinates of $\mathbf{X} = (X, Y)$, $p(\mathbf{s}_1)$ is the probability density function of picking a species in $\mathcal{S}$ and we assumed statistical independence $p(\mathbf{s}_1, \mathbf{s}_2) = p(\mathbf{s}_1)p(\mathbf{s}_2)$. Note we included k in the argument of $\mathcal{A}_m$ for convenience, as later we will non-dimensionalise. The function $g(R; \mathbf{s}_1, \mathbf{s}_2)$ is the pair-correlation, assuming R is the distance between two particles, one centred of type $\mathbf{s}_1$ and another of type $\mathbf{s}_2$. If we were to use whole correction, then $g(R; \mathbf{s}_1, \mathbf{s}_2) = 0$. For most random systems we expect that rapidly $g(R; \mathbf{s}_1, \mathbf{s}_2) \to 0$ as $R \to \infty$, so we will assume

$$g(R; \mathbf{s}_1, \mathbf{s}_2) = 0, \quad \text{for} \quad R > \bar{a}_{12}. \quad (7)$$

In terms of the notation from (Gower et al., 2018):

$$|\mathcal{R}_N|p(\mathbf{\Lambda}_2|\mathbf{\Lambda}_1) = |\mathcal{R}_N|^2\frac{p(\mathbf{\Lambda}_1,\mathbf{\Lambda}_2)}{p(\mathbf{s}_1)} = |\mathcal{R}_N|^2 p(\mathbf{s}_2)p(\mathbf{x}_1,\mathbf{x}_2|\mathbf{s}_1,\mathbf{s}_2)$$
$$= p(\mathbf{s}_2)(1+g(\|\mathbf{x}_1-\mathbf{x}_2\|;\mathbf{s}_1,\mathbf{s}_2)). \quad (8)$$

For computational efficiency, we will change variables to

$$X = k\mathbf{x}_2 - k\mathbf{x}_1, \quad (x,y) = (kx_1, ky_1), \quad (9)$$

We also borrow equation (4.1) from (Gower et al., 2018) to substitute

$$\mathcal{A}_m(kx_1, ky_1, \mathbf{s}) = \mathcal{A}_m(kx_1,\mathbf{s})\mathrm{e}^{\mathrm{i}ky_1\sin\theta_{\mathrm{in}}},$$

which is due to the symmetry of (4). Substituting the above into (4), we can rewrite the integrated term:

$$\int_{\substack{x_2>0\\ \|\mathbf{x}_2-\mathbf{x}_1\|>a_{12}}} \mathcal{A}_n(kx_2,\mathbf{s}_2)\mathrm{e}^{\mathrm{i}y_2k\sin\theta_{\mathrm{in}}}F_{n-m}(k\mathbf{x}_2-k\mathbf{x}_1,k)d\mathbf{x}_2 =$$
$$\frac{\mathrm{e}^{\mathrm{i}y\sin\theta_{\mathrm{in}}}}{k^2}\int_{X>-x}\mathcal{A}_n(X+x,\mathbf{s}_2)\int_{Y^2>k^2a_{12}^2-X^2}\mathrm{e}^{\mathrm{i}Y\sin\theta_{\mathrm{in}}}F_{n-m}(\mathbf{X},k)dY dX,$$

then we split the integral on the right in the form

$$\int_{Y^2>k^2a_{12}^2-X^2}\mathrm{e}^{\mathrm{i}Y\sin\theta_{\mathrm{in}}}F_{n-m}(\mathbf{X},k)dY = \chi_{\{|X|<ka_{12}\}}B_{n-m}(X,k) + \chi_{\{|X|>ka_{12}\}}S_{n-m}(X,k),$$

where by using (7), equation (B.3) from Gower et al. (2018),

$$S_n(X,k) = \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}Y\sin\theta_{\mathrm{in}}} F_n(\mathbf{X},k)dY = G_n(X,k) + \frac{2}{\cos\theta_{\mathrm{in}}} \begin{cases} \mathrm{i}^n \mathrm{e}^{-\mathrm{i}n\theta_{\mathrm{in}}} \mathrm{e}^{\mathrm{i}X\cos\theta_{\mathrm{in}}} & X \geq 0, \\ (-\mathrm{i})^n \mathrm{e}^{\mathrm{i}n\theta_{\mathrm{in}}} \mathrm{e}^{-\mathrm{i}X\cos\theta_{\mathrm{in}}} & X < 0, \end{cases} \tag{10}$$

with

$$\begin{aligned} G_n(X,k) &= (-1)^n \int_{-\sqrt{k^2\bar{a}_{12}^2 - X^2}}^{\sqrt{k^2\bar{a}_{12}^2 - X^2}} \mathrm{e}^{\mathrm{i}Y\sin\theta_{\mathrm{in}}} \mathrm{e}^{\mathrm{i}n\Theta} H_n(R) g(R/k;\mathbf{s}_1,\mathbf{s}_2)dY \\ &= 2(-1)^n \int_0^{\sqrt{k^2\bar{a}_{12}^2 - X^2}} \cos\left(Y\sin\theta_{\mathrm{in}} + n\Theta\right) H_n(R) g(R/k;\mathbf{s}_1,\mathbf{s}_2)dY \end{aligned} \tag{11}$$

The term

$$\begin{aligned} B_n(X,k) &= \int_{-\infty}^{\infty} \chi_{\{Y^2 > k^2 a_{12}^2 - X^2\}} \mathrm{e}^{\mathrm{i}Y\sin\theta_{\mathrm{in}}} F_n(\mathbf{X},k)dY \\ &= 2(-1)^n \int_{\sqrt{k^2 a_{12}^2 - X^2}}^{\infty} \cos\left(Y\sin\theta_{\mathrm{in}} + n\Theta\right) H_n(R)(1 + g(R/k;\mathbf{s}_1,\mathbf{s}_2))dY. \end{aligned} \tag{12}$$

It is difficult to numerically integrate the above because the integrand tends to zero very slowly as Y increases. To numerically integrate the above we use

$$\cos\left(Y\sin\theta_{\mathrm{in}} + n\Theta\right) = \cos((n\pi)/2 + Y\sin(\theta_{\mathrm{in}})) + \mathcal{O}(X/Y), \tag{13}$$

$$H_n(R) = -(-1)^{3/4} \mathrm{e}^{-\mathrm{i}n\pi/2} \sqrt{\frac{2}{\pi Y}} + \mathcal{O}(X^{3/2}/Y^{3/2}), \tag{14}$$

which we use to rewrite

$$B_n(X,k) = 2(-1)^n \int_{\sqrt{k^2 a_{12}^2 - X^2}}^{Y_1} \cos\left(Y \sin\theta_{\rm in} + n\Theta\right) H_n(R)(1 + g(R/k; \mathbf{s}_1, \mathbf{s}_2))dY$$
$$+ \frac{1+\mathrm{i}}{\sqrt{\pi Y_1}\cos(\theta_{\rm in})^2} \mathrm{e}^{\mathrm{i}Y_1(1-\sin(\theta_{\rm in}))} \left[1 + (-1)^n \mathrm{e}^{2\mathrm{i}Y_1 \sin(\theta_{\rm in})}(1 - \sin(\theta_{\rm in})) + \sin(\theta_{\rm in})\right] + \mathcal{O}(X/Y), \tag{15}$$

where we assumed that $g(R/k; \mathbf{s}_1, \mathbf{s}_2) = 0$ for $Y > Y_1$.

Written in full the governing equation (4) now becomes

$$\sum_{n=-\infty}^{\infty} \int_{\mathcal{S}} \int_{X>0} \mathcal{A}_n(X, \mathbf{s}_2) K(X - x, k) dX d\mathbf{s}_2^n$$
$$+ k^2 \mathcal{A}_m(x, \mathbf{s}_1) + k^2 \mathrm{e}^{\mathrm{i}x\cos\theta_{\rm in}} \mathrm{e}^{\mathrm{i}m(\pi/2 - \theta_{\rm in})} = 0, \quad \text{for} \quad x_1 > 0, \tag{16}$$

where I swapped the integration variable $X \to X - x$. where

$$K(X - x, k) = \chi_{\{|X-x| > ka_{12}\}} S_{n-m}(X - x, k) + \chi_{\{|X-x| < ka_{12}\}} B_{n-m}(X - x, k). \tag{17}$$

Numerically it is better to substitute in the above to reach

To start, by solving the single species and consider only whole correction pair-correlation. After trying methods based on Chebyshev and function approximation, I've decided they are too computationally intense. For this reason I'm going with a simpler discretisation: let $\mathcal{A}_n^j = \mathcal{A}_n(x^j)$ where $x^j = jh$ for $j = 0, \ldots, N$. A regular spaced mesh is best because of the convolution. With analogous notation for the other fields, let the vectors:

$$\boldsymbol{\mathcal{A}}_n = (\mathcal{A}_n^j)_j, \quad \boldsymbol{S}_n = (S_n^j)_j, \quad \boldsymbol{B}_n = (B_n^j)_j, \quad \boldsymbol{b}_n = -k^2(\mathrm{e}^{\mathrm{i}x^j\cos\theta_{\rm in}} \mathrm{e}^{\mathrm{i}n(\pi/2-\theta_{\rm in})})_j. \tag{18}$$

$$\sum_{n=-\infty}^{\infty}\int_{X>0}\mathcal{A}_n(X)S_{n-m}(X-x)dX d\mathbf{s}_2^n$$

$$+\sum_{n=-\infty}^{\infty}\int_{\substack{|X-x|<ka_{12}\\X>0}}\mathcal{A}_n(X)(B_{n-m}(X-x,k)-S_{n-m}(X-x))dX d\mathbf{s}_2^n$$

$$+k^2\mathcal{A}_m(x)+k^2\mathrm{e}^{\mathrm{i}x\cos\theta_{\mathrm{in}}}\mathrm{e}^{\mathrm{i}m(\pi/2-\theta_{\mathrm{in}})}=0,\quad \text{for}\quad x_1>0, \tag{19}$$

$$\mathfrak{n}\sum_{n,j\geq 0}Z_n\sigma_j\left(S_{n-m}^{j-\ell}+(B_{n-m}^{j-\ell}-S_{n-m}^{j-\ell})\chi_{\{|j-\ell|\leq p\}}\right)\mathcal{A}_n^j+k^2\mathcal{A}_m^\ell=b_m^\ell, \tag{20}$$

for $\ell>0$, where $p=\lfloor ka_{12}/h\rfloor$, and σ_j repesents the discrete integral. In matrix form,

$$\mathfrak{n}\sum_n Z_n(\boldsymbol{P}_{n-m}+\boldsymbol{Q}_{n-m})\boldsymbol{\mathcal{A}}_n+k^2\boldsymbol{I}\boldsymbol{\mathcal{A}}_m=\boldsymbol{b}_m, \tag{21}$$

where we used the matrices:

$$P_n^{\ell j}=\sigma_j S_n^{j-\ell},\quad Q_n^{\ell j}=\sigma_j(B_n^{j-\ell}-S_n^{j-\ell})\chi_{\{|j-\ell|\leq p\}}, \tag{22}$$

where $j,\ell=0,1,\ldots,N$. Finally in block-matrix form: $\boldsymbol{M}\boldsymbol{\mathcal{A}}=\boldsymbol{b}$, where

$$\boldsymbol{M}_{mn}=\mathfrak{n}Z_n(\boldsymbol{P}_{n-m}+\boldsymbol{Q}_{n-m})+k^2\delta_{mn}\boldsymbol{I}, \tag{23}$$

$$\boldsymbol{\mathcal{A}}=[\boldsymbol{\mathcal{A}}_{-M},\boldsymbol{\mathcal{A}}_{1-M},\cdots,\boldsymbol{\mathcal{A}}_{M-1},\boldsymbol{\mathcal{A}}_M]^T, \tag{24}$$

$$\boldsymbol{b}=[\boldsymbol{b}_{-M},\boldsymbol{b}_{1-M},\cdots,\boldsymbol{b}_{M-1},\boldsymbol{b}_M]^T. \tag{25}$$

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