Coupled Electric and Magnetic Dipoles Method for Scattering Calculations and its Implementation in Julia.

Augustin Muster (based on the notes of Luis. S. Froufe-Pérez)

November 2022

Abstract

In this document the derivation of a discrete electric and magnetic dipoles approximation method is developed as well as the computation of the scattering, absorption and extinction cross section for a group of electric and magnetic dipoles. After, this, the implementation in julia of this method is discussed. Full documentation on the package can be fount at ....

Contents

Part I
Electric DDA: Theory

1 DDA method description

1.1 Lattice and polarisabilities

Let us consider a solid of volume V discretized in N dipoles on a cubic lattice (of lattice parameter d) with dielectric tensor $\varepsilon(\boldsymbol{r})$ in a homogoneous medium with dielectric constant $\varepsilon_h$such that

$$V = Nd^3. \tag{1}$$

Each dipole is associated with his position $\boldsymbol{r_n}$, $n = 1, ..., N$and his quaisitatic polarisability tensor defined by

$$\boldsymbol{\alpha}_{n0} = (\epsilon(\boldsymbol{r_n}) - \epsilon_h I)((\epsilon(\boldsymbol{r_n}) - \epsilon_h I) + \boldsymbol{L_n^{-1}}\epsilon_h)^{-1}\boldsymbol{L_n^{-1}}V_n, \tag{2}$$

where $\boldsymbol{I}$ ˆis the identy matrix, $V_n = d^3$ is the volume of a discretization unit and $\boldsymbol{L_n}$is the depolarisation tensor defined as

$$[\boldsymbol{L}_n]_{ij} = \delta_{ij}\frac{1}{3} \tag{3}$$

for a cube. A radiative correction of the polarisability has to be taken into account. With this correction, the polarisability tensor $\boldsymbol{\alpha}_n$ now reads7

$$\boldsymbol{\alpha}_n = \left(\boldsymbol{\alpha}_{n0}^{-1} - i\frac{k^3}{6\pi}\right)^{-1}, \tag{4}$$

where k is the wavenumber of the incident wave.

1.2 Scattering

Let us consider that the solid is illuminated by an inciedent field $\boldsymbol{E}_0(\boldsymbol{r})$ the field $\boldsymbol{E}_{exc}(\boldsymbol{r}_n)$ extiting the nth dipole is equal to the incident field plus the contribution of the other dipoles, i.e.

$$\boldsymbol{E}_{exc}(\boldsymbol{r}_n) = \boldsymbol{E}_0(\boldsymbol{r}_n) + k^2 \sum_{m \neq n}^{N} \boldsymbol{G}(\boldsymbol{r}_n, \boldsymbol{r}_m)\boldsymbol{\alpha}_m \boldsymbol{E}_{exc}(\boldsymbol{r}_m), \tag{5}$$

where $\boldsymbol{G}(\boldsymbol{r}_n, \boldsymbol{r}_m)$ is the green tensor which reads

$$\boldsymbol{G}(\boldsymbol{r}_n, \boldsymbol{r}_m) = \frac{\exp(ikR)}{4\pi R}\left(\left(1 + \frac{i}{kR} - \frac{1}{k^2R^2}\right)\boldsymbol{I} - \left(1 + \frac{3i}{kR} - \frac{3}{k^2R^2}\right)\frac{\boldsymbol{R}\otimes\boldsymbol{R}}{R^2}\right), \tag{6}$$

with $\boldsymbol{R} = \boldsymbol{r}_n - \boldsymbol{r}_m$, $R = |\boldsymbol{R}|$. This equation in then just a big system of 3N linear equations that reads

$$\begin{bmatrix} \boldsymbol{I} & \dots & -k^2\boldsymbol{G}(\boldsymbol{r}_1, \boldsymbol{r}_N)\boldsymbol{\alpha} \\ \vdots & \ddots & \vdots \\ -k^2\boldsymbol{G}(\boldsymbol{r}_N, \boldsymbol{r}_1)1 & \dots & \boldsymbol{I} \end{bmatrix} \begin{bmatrix} \boldsymbol{E}_{exc}(\boldsymbol{r}_1) \\ \vdots \\ \boldsymbol{E}_{exc}(\boldsymbol{r}_N) \end{bmatrix} = \begin{bmatrix} \boldsymbol{E}_0(\boldsymbol{r}_1) \\ \vdots \\ \boldsymbol{E}_0(\boldsymbol{r}_N) \end{bmatrix} \tag{7}$$

that can be solved in order to get the $\boldsymbol{E}_{exc}(\boldsymbol{r}_n)$. Using this, the polarizations of each dipole can be computed using $\boldsymbol{P}_n = \boldsymbol{\alpha}_n\boldsymbol{E}_{exc}(\boldsymbol{r}_n)$

1.3 Cross sections calculations

Then, the extinction, absorbtion and scattering cross section $\sigma_{ext}, \sigma_{abs}, \sigma_{sca}$ (that follows $\sigma_{ext} = \sigma_{abs} + \sigma_{sca}$) can be comuted using (considerning that the incident field is a plane wave $\boldsymbol{E}_0(\boldsymbol{r}) = \boldsymbol{E}_0\exp(ikr)$))

$$\sigma_{ext} = \frac{k}{\epsilon_h|\boldsymbol{E}_o|^2}\sum_{n=1}^{N} Im(\boldsymbol{E}_0^*(\boldsymbol{r})\cdot\boldsymbol{P}_n) \tag{8}$$

$$\sigma_{sca} = \frac{k^3}{{\epsilon_h}^2|\boldsymbol{E}_o|^2}\sum_{n,m=1}^{N} \boldsymbol{P}_n^*\cdot Im(\boldsymbol{G}(\boldsymbol{r}_n, \boldsymbol{r}_m))\boldsymbol{P}_n \tag{9}$$

$$\sigma_{abs} = \frac{k}{{\epsilon_h}^2|\boldsymbol{E}_o|^2}\sum_{n=1}^{N} Im(\boldsymbol{P}_n\cdot(\boldsymbol{\alpha}_{n0}\boldsymbol{P}_n)^*) \tag{10}$$

Part II
Electric and Magnetic DDA: Theory

2 Induced dipoles and scattered fields

We consider dipolar electric and magnetic particles. For a particle placed at $\mathbf{r}_0$ the induced electric and magnetic dipoles are

$$\mathbf{p} = \epsilon_0\tilde{\alpha}_E\mathbf{E}_i(\mathbf{r}_0) \tag{11a}$$

$$\mathbf{m} = \tilde{\alpha}_M\tilde{\mathbf{H}}_i(\mathbf{r}_0) \tag{11b}$$

where $\mathbf{E}_i(\mathbf{r}_0)$ and $\tilde{\mathbf{H}}_i(\mathbf{r}_0)$ are respectively the exciting electric and magnetic fields at the particle's position.

The electromagnetic field generated by electric and magnetic dipoles is

$$\mathbf{E}(\mathbf{r}) = \frac{k^2}{\epsilon_0}\tilde{\mathbb{G}}_E(\mathbf{r}, \mathbf{r}_0)\mathbf{p} + iZk\tilde{\mathbb{G}}_M(\mathbf{r}, \mathbf{r}_0)\mathbf{m} \tag{12a}$$

$$\tilde{\mathbf{H}}(\mathbf{r}) = \frac{-i}{Z}\frac{k}{\epsilon_0}\tilde{\mathbb{G}}_M(\mathbf{r}, \mathbf{r}_0)\mathbf{p} + k^2\tilde{\mathbb{G}}_E(\mathbf{r}, \mathbf{r}_0)\mathbf{m} \tag{12b}$$

Then, the scattered fields are

$$\mathbf{E}_s(\mathbf{r}) = k^2 \tilde{\mathbb{G}}_E(\mathbf{r},\mathbf{r}_0)\,\tilde{\alpha}_E \mathbf{E}_i(\mathbf{r}_0) + iZk\tilde{\mathbb{G}}_M(\mathbf{r},\mathbf{r}_0)\,\tilde{\alpha}_M \tilde{\mathbf{H}}_i(\mathbf{r}_0) \tag{13a}$$

$$\tilde{\mathbf{H}}_s(\mathbf{r}) = \frac{-i}{Z} k\tilde{\mathbb{G}}_M(\mathbf{r},\mathbf{r}_0)\,\tilde{\alpha}_E \mathbf{E}_i(\mathbf{r}_0) + k^2\tilde{\mathbb{G}}_E(\mathbf{r},\mathbf{r}_0)\,\tilde{\alpha}_M \tilde{\mathbf{H}}_i(\mathbf{r}_0) \tag{13b}$$

Green's tensors are defined through the following expressions:

$$\tilde{\mathbb{G}}_E(\mathbf{r},\mathbf{r}_0) = \frac{e^{ikr}}{4\pi r}\left\{\frac{(kr)^2 + ikr - 1}{(kr)^2}\mathbb{I} + \frac{-(kr)^2 - 3ikr + 3}{(kr)^2}\mathbf{u}_r\mathbf{u}_r\right\} \tag{14a}$$

$$\tilde{\mathbb{G}}_M(\mathbf{r},\mathbf{r}_0) = \frac{e^{ikr}}{4\pi r} k\left(\frac{ikr-1}{kr}\right)\mathbf{u}_r\times \tag{14b}$$

where $r \equiv |\mathbf{r}-\mathbf{r}_0|$, and $\mathbf{u}_r \equiv (\mathbf{r}-\mathbf{r}_0)/r$.

For a spherical particle, the polarizabilities can be written as:

$$\tilde{\alpha}_E = i\left(\frac{k^3}{6\pi}\right)^{-1} a_1 \tag{15a}$$

$$\tilde{\alpha}_M = i\left(\frac{k^3}{6\pi}\right)^{-1} b_1 \tag{15b}$$

where a_1 and b_1 are the first two Mie coefficients of the expansion of the scattered fields. In principle it is also valid for multilayered spherical particles.

We use

$$Z = \sqrt{\frac{\mu_0\mu}{\epsilon_0\epsilon}}$$

$$k = \frac{\omega}{c}\sqrt{\epsilon\mu}$$

3 Renormalization of variables

We redefine the Green tensors as

$$\mathbb{G}_E(\mathbf{r},\mathbf{r}_0) = \frac{e^{ikr}}{kr}\left\{\frac{(kr)^2 + ikr - 1}{(kr)^2}\mathbb{I} + \frac{-(kr)^2 - 3ikr + 3}{(kr)^2}\mathbf{u}_r\mathbf{u}_r\right\} = \frac{4\pi}{k}\tilde{\mathbb{G}}_E(\mathbf{r},\mathbf{r}_0) \tag{16a}$$

$$\mathbb{G}_M(\mathbf{r},\mathbf{r}_0) = \frac{e^{ikr}}{kr}\left(\frac{ikr-1}{kr}\right)\mathbf{u}_r\times = \frac{4\pi}{k^2}\tilde{\mathbb{G}}_M(\mathbf{r},\mathbf{r}_0) \tag{16b}$$

Notice that the imaginary part of the electric Green's tensor with this normalization verifies

$$\mathrm{Im}\left\{\mathbb{G}_E(\mathbf{r},\mathbf{r}_0)\right\} = \frac{2}{3}\mathbb{I} \tag{17}$$

we also redefine the polarizabilities as

$$\alpha_E = \frac{k^3\tilde{\alpha}_E}{4\pi} = i\frac{3}{2}a_1 \tag{18a}$$

$$\alpha_E = \frac{k^3\tilde{\alpha}_M}{4\pi} = i\frac{3}{2}b_1 \tag{18b}$$

With this definition of the adimensional polarizabilities, the optical theorem reads:

$$\frac{2}{3}\left|\alpha_{E/M}\right|^2 = \mathrm{Im}\left(\alpha_{E/M}\right) \tag{19}$$

and we shall work with a renormalized magnetic field

$$\mathbf{H} = Z\tilde{\mathbf{H}} \tag{20}$$

with units of electric field.

With the above definitions, equation (13) can be written as

$$\mathbf{E}_s\left(\mathbf{r}\right) = \mathbb{G}_E\left(\mathbf{r},\mathbf{r}_0\right)\alpha_E\mathbf{E}_i\left(\mathbf{r}_0\right) + i\mathbb{G}_M\left(\mathbf{r},\mathbf{r}_0\right)\alpha_M\mathbf{H}_i\left(\mathbf{r}_0\right) \tag{21}$$

$$\mathbf{H}_s\left(\mathbf{r}\right) = -i\mathbb{G}_M\left(\mathbf{r},\mathbf{r}_0\right)\alpha_E\mathbf{E}_i\left(\mathbf{r}_0\right) + \mathbb{G}_E\left(\mathbf{r},\mathbf{r}_0\right)\alpha_M\mathbf{H}_i\left(\mathbf{r}_0\right) \tag{22}$$

With all the above definitions for adimensional quantities, the DDA equations can be written as

$$\mathbf{E}_i = \mathbf{E}_0\left(\mathbf{r}_i\right) + \sum_{j\neq i}\mathbb{G}_E\left(\mathbf{r}_i,\mathbf{r}_j\right)\alpha_E^{(j)}\mathbf{E}_j + i\mathbb{G}_M\left(\mathbf{r}_i,\mathbf{r}_j\right)\alpha_M^{(j)}\mathbf{H}_j \tag{23a}$$

$$\mathbf{H}_i = \mathbf{H}_0\left(\mathbf{r}_i\right) + \sum_{j\neq i} -i\mathbb{G}_M\left(\mathbf{r}_i,\mathbf{r}_j\right)\alpha_E^{(j)}\mathbf{E}_j + \mathbb{G}_E\left(\mathbf{r}_i,\mathbf{r}_j\right)\alpha_M^{(j)}\mathbf{H}_j \tag{23b}$$

where $\mathbf{E}_i$ and $\mathbf{H}_i$ are the total exciting fields acting on the $i-th$ particle, and $\alpha_{E/M}^{(i)}$ is the electric or magnetic polarizability of the $i-th$ particle.

For point sources, it is convenient to also introduce renormalization of variables. For an electric dipole $\tilde{\mathbf{p}}$, we have

$$\mathbf{E}\left(\mathbf{r}\right) = \frac{k^3}{4\pi\epsilon_0}\mathbb{G}_E\left(\mathbf{r},\mathbf{r}_0\right)\tilde{\mathbf{p}} \tag{24}$$

and

$$\mathbf{H}\left(\mathbf{r}\right) = -i\frac{k^3}{4\pi\epsilon_0}\mathbb{G}_M\left(\mathbf{r},\mathbf{r}_0\right)\tilde{\mathbf{p}} \tag{25}$$

hence, it is convenient to define a normalized electric dipole

$$\mathbf{p} \equiv \frac{k^3}{4\pi\epsilon_0}\tilde{\mathbf{p}} \tag{26}$$

i.e., we renormalize the electric dipole such that it has units of an electric field. with this, we have

$$\mathbf{E}\left(\mathbf{r}\right) = \mathbb{G}_E\left(\mathbf{r},\mathbf{r}_0\right)\mathbf{p} \tag{27a}$$

$$\mathbf{H}\left(\mathbf{r}\right) = -i\mathbb{G}_M\left(\mathbf{r},\mathbf{r}_0\right)\mathbf{p} \tag{27b}$$

Analogously, for a magnetic dipole $\tilde{\mathbf{m}}$, the renormalization (leading to a magnetic dipole with units of an elecric field) is

$$\mathbf{m} \equiv Z\frac{k^3}{4\pi}\tilde{\mathbf{m}} \tag{28}$$

and with this,

$$\mathbf{E}\left(\mathbf{r}\right) = i\mathbb{G}_M\left(\mathbf{r},\mathbf{r}_0\right)\mathbf{m} \tag{29a}$$

$$\mathbf{H}\left(\mathbf{r}\right) = \mathbb{G}_E\left(\mathbf{r},\mathbf{r}_0\right)\mathbf{m} \tag{29b}$$

If the incoming signal is a planewave $\mathbf{E}(\mathbf{r}) = \mathbf{E}_0 e^{i\mathbf{k}\cdot\mathbf{r}} = \mathbf{E}_0 e^{ik\mathbf{u}_k\cdot\mathbf{r}}$, the (renormalized) magnetic field can be written as.

$$\mathbf{H} = \mathbf{u}_k \times \mathbf{E}(\mathbf{r}) = \begin{pmatrix} \mathbf{u}_y\mathbf{E}_z - \mathbf{u}_z\mathbf{E}_y \\ \mathbf{u}_z\mathbf{E}_x - \mathbf{u}_x\mathbf{E}_z \\ \mathbf{u}_x\mathbf{E}_y - \mathbf{u}_y\mathbf{E}_x \end{pmatrix} \tag{30}$$

4 Cross sections, transmission and reflection coefficients.

The Poynting vector $\mathbf{S} = 1/2\mathrm{Re}\left\{\mathbf{E}\times\tilde{\mathbf{H}}\right\}$can be written, after renormalizing variables as

$$\mathbf{S} = 1/2\mathrm{Re}\left\{\mathbf{E}\times\mathbf{H}/Z^*\right\} \tag{31}$$

considering that

$$\tilde{\mathbf{H}} = \frac{-i}{\omega\mu_0\mu}\nabla\times\mathbf{E} = \frac{-i}{k}\nabla\times\mathbf{E} \tag{32}$$

we have for a planewave

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_0 e^{i\mathbf{k}\cdot\mathbf{r}} \tag{33}$$

an hence, the normalized magnetic field is

$$\mathbf{H} = \frac{\mathbf{k}}{|\mathbf{k}|}\times\mathbf{E}_0 e^{i\mathbf{k}\cdot\mathbf{r}} \tag{34}$$

Hence, for a plane wave we have (in a real material)

$$\mathbf{S} = \frac{1}{2Z}\left|\mathbf{E}_0\right|^2\frac{\mathbf{k}}{|\mathbf{k}|} \tag{35}$$

To obtain the scattering, absorption and extinction cross section, we separate the total electric and magnetic field in incoming and scattered components:

$$\mathbf{E}_t = \mathbf{E}_i + \mathbf{E}_s \tag{36a}$$

$$\mathbf{H}_t = \mathbf{H}_i + \mathbf{H}_s \tag{36b}$$

and hence, the Poynting vector can be written as (we assume a real material)

$$\begin{aligned}\mathbf{S} &= \frac{1}{2Z}\mathrm{Re}\left\{\mathbf{E}_t\times\mathbf{H}_t^*\right\} = \frac{1}{2Z}\mathrm{Re}\left\{(\mathbf{E}_i+\mathbf{E}_s)\times(\mathbf{H}_i^*+\mathbf{H}_s^*)\right\} \\ &= \frac{1}{2Z}\mathrm{Re}\left\{\mathbf{E}_i\times\mathbf{H}_i^*\right\} + \frac{1}{2Z}\mathrm{Re}\left\{\mathbf{E}_s\times\mathbf{H}_s^*\right\} + \frac{1}{2Z}\mathrm{Re}\left\{\mathbf{E}_i\times\mathbf{H}_s^* + \mathbf{E}_s\times\mathbf{H}_i^*\right\} \\ &\equiv \mathbf{S}_i + \mathbf{S}_s - \mathbf{S}_e \end{aligned} \tag{37}$$

where we have defined

$$\mathbf{S}_i \equiv \frac{1}{2Z}\mathrm{Re}\left\{\mathbf{E}_i\times\mathbf{H}_i^*\right\} \tag{38a}$$

$$\mathbf{S}_s \equiv \frac{1}{2Z}\mathrm{Re}\left\{\mathbf{E}_s\times\mathbf{H}_s^*\right\} \tag{38b}$$

$$\mathbf{S}_e \equiv \frac{-1}{2Z}\mathrm{Re}\left\{\mathbf{E}_i\times\mathbf{H}_s^* + \mathbf{E}_s\times\mathbf{H}_i^*\right\} \tag{38c}$$

respectively incoming, scattering and extinction components of the Poynting vector.

We shall assume that the incoming fields are planewaves in order to define scattering and extinction cross section.

In this case, we have

$$\int d\Omega\, \mathbf{S}_i \cdot \mathbf{u}_n = 0 \tag{39}$$

i.e., the surface integral of the incoming Poynting vector is null on a closed surface.

4.1 Scattering cross section (valid also for far field radiated power)

Scattering cross section is defined through the ratio of scattered power to incoming intensity:

$$\sigma_s \equiv \frac{P_{scatt}}{I_i} \tag{40}$$

and the scattered power can be defined using the integral of the scattered intensity in a spherical surface at infinity,

$$P_{scatt} = \lim_{R\to\infty} R^2 \int d\Omega\, \mathbf{S}_s \cdot \mathbf{u}_n \tag{41}$$

Considering that the scattered fields are the ones created by the induced dipoles in the system, we have

$$\mathbf{E}_s(\mathbf{r}) = \sum_i \mathbb{G}_E(\mathbf{r}, \mathbf{r}_i)\, \alpha_E^{(i)} \mathbf{E}_i + i\mathbb{G}_M(\mathbf{r}, \mathbf{r}_i)\, \alpha_M^{(i)} \mathbf{H}_i \tag{42a}$$

$$\mathbf{H}_s(\mathbf{r}) = \sum_i -i\mathbb{G}_M(\mathbf{r}, \mathbf{r}_i)\, \alpha_E^{(i)} \mathbf{E}_i + \mathbb{G}_E(\mathbf{r}, \mathbf{r}_i)\, \alpha_M^{(i)} \mathbf{H}_i \tag{42b}$$

We shall consider the asymptotic expansion of the fields at distances much larger to any of the dipoles than the wavelength. We consider the expansion

$$e^{ik(\mathbf{r}-\mathbf{r}_0)} \simeq e^{ikr} e^{-ik\mathbf{r}_o\cdot\mathbf{u}_r} \tag{43}$$

valid when

$$|\mathbf{r}| \gg |\mathbf{r}_0| \tag{44a}$$

$$k\,|\mathbf{r}| \gg 1 \tag{44b}$$

. We have defined

$$r \equiv |\mathbf{r}| \tag{45a}$$

$$\mathbf{u}_r \equiv \mathbf{r}/r \tag{45b}$$

All subsequent terms in the expansion (43) contain (integer) powers of $1/kr$, and hence will not contribute to integrals of the form (41).

With this, we have

$$\mathbb{G}_E(\mathbf{r}, \mathbf{r}_0) \simeq \frac{e^{ikr}}{kr} e^{-ik\mathbf{r}_o\cdot\mathbf{u}_r} (\mathbb{I} - \mathbf{u}_r\mathbf{u}_r) \tag{46a}$$

$$\mathbb{G}_M(\mathbf{r}, \mathbf{r}_0) \simeq i\frac{e^{ikr}}{kr} e^{-ik\mathbf{r}_o\cdot\mathbf{u}_r} \mathbf{u}_r \times \tag{46b}$$

With the above considerations, we can approximate the scattering poynting vector as

$$
\begin{aligned}
\mathbf{S}_s = \;& \frac{1}{2Z\left(kr\right)^2}\mathrm{Re}\left\{\sum_{i,j} e^{ik\mathbf{u}_r\cdot(\mathbf{r}_j-\mathbf{r}_i)}\left[\alpha_E^{(i)}\alpha_M^{(j)*}\left(\left(\mathbb{I}-\mathbf{u}_r\mathbf{u}_r\right)\mathbf{E}_i\right)\times\left(\left(\mathbb{I}-\mathbf{u}_r\mathbf{u}_r\right)\mathbf{H}_j^*\right)\right]\right\} \\
&+\frac{1}{2Z\left(kr\right)^2}\mathrm{Re}\left\{\sum_{i,j} e^{ik\mathbf{u}_r\cdot(\mathbf{r}_j-\mathbf{r}_i)}\left[\alpha_E^{(i)}\alpha_E^{(j)*}\left(\left(\mathbb{I}-\mathbf{u}_r\mathbf{u}_r\right)\mathbf{E}_i\right)\times\left(\mathbf{u}_r\times\mathbf{E}_j^*\right)\right]\right\} \\
&+\frac{1}{2Z\left(kr\right)^2}\mathrm{Re}\left\{\sum_{i,j} e^{ik\mathbf{u}_r\cdot(\mathbf{r}_j-\mathbf{r}_i)}\left[-\alpha_M^{(i)}\alpha_M^{(j)*}\left(\mathbf{u}_r\times\mathbf{H}_i\right)\times\left(\left(\mathbb{I}-\mathbf{u}_r\mathbf{u}_r\right)\mathbf{H}_j^*\right)\right]\right\} \\
&+\frac{1}{2Z\left(kr\right)^2}\mathrm{Re}\left\{\sum_{i,j} e^{ik\mathbf{u}_r\cdot(\mathbf{r}_j-\mathbf{r}_i)}\left[-\alpha_M^{(i)}\alpha_E^{(j)^*}\left(\mathbf{u}_r\times\mathbf{H}_i\right)\times\left(\mathbf{u}_r\times\mathbf{E}_j^*\right)\right]\right\}
\end{aligned}
\tag{47}
$$

We have to consider the scalar products (in the integrand of eq.(41)),

$$
\begin{aligned}
\mathbf{u}_r\cdot\left[\left(\left(\mathbb{I}-\mathbf{u}_r\mathbf{u}_r\right)\mathbf{E}_i\right)\times\left(\left(\mathbb{I}-\mathbf{u}_r\mathbf{u}_r\right)\mathbf{H}_j^*\right)\right] &= \mathbf{u}_r\cdot\left[\left(\mathbf{E}_i\times\mathbf{H}_j^*\right)-\mathbf{E}_i\times\mathbf{u}_r\left(\mathbf{u}_r\cdot\mathbf{H}_j^*\right)-\mathbf{u}_r\times\mathbf{H}_j^*\left(\mathbf{E}_i\cdot\mathbf{u}_r\right)\right] \\
&= \mathbf{u}_r\cdot\left(\mathbf{E}_i\times\mathbf{H}_j^*\right) && \text{(48a)} \\
\mathbf{u}_r\cdot\left[\left(\left(\mathbb{I}-\mathbf{u}_r\mathbf{u}_r\right)\mathbf{E}_i\right)\times\left(\mathbf{u}_r\times\mathbf{E}_j^*\right)\right] &= \mathbf{u}_r\cdot\left[\mathbf{E}_i\times\left(\mathbf{u}_r\times\mathbf{E}_j^*\right)\right]-\mathbf{u}_r\times\left[\mathbf{u}_r\times\left(\mathbf{u}_r\times\mathbf{E}_j^*\right)\right]\left(\mathbf{E}_i\cdot\mathbf{u}_r\right) = \\
&= \mathbf{u}_r\cdot\left[\mathbf{E}_i\times\left(\mathbf{u}_r\times\mathbf{E}_j^*\right)\right] \\
&= \mathbf{u}_r\cdot\left[\mathbf{u}_r\left(\mathbf{E}_i\cdot\mathbf{E}_j^*\right)-\mathbf{E}_j^*\left(\mathbf{u}_r\cdot\mathbf{E}_i\right)\right] \\
&= \left(\mathbf{E}_i\cdot\mathbf{E}_j^*\right)-\left(\mathbf{u}_r\cdot\mathbf{E}_i\right)\left(\mathbf{u}_r\cdot\mathbf{E}_j^*\right) && \text{(48b)} \\
\mathbf{u}_r\cdot\left[\left(\mathbf{u}_r\times\mathbf{H}_i\right)\times\left(\left(\mathbb{I}-\mathbf{u}_r\mathbf{u}_r\right)\mathbf{H}_j^*\right)\right] &= \mathbf{u}_r\cdot\left[\left(\mathbf{u}_r\times\mathbf{H}_i\right)\times\mathbf{H}_j^*\right] = \left(\mathbf{u}_r\cdot\mathbf{H}_i\right)\left(\mathbf{u}_r\cdot\mathbf{H}_j^*\right)-\left(\mathbf{H}_i\cdot\mathbf{H}_j^*\right) && \text{(48c)} \\
\mathbf{u}_r\cdot\left[\left(\mathbf{u}_r\times\mathbf{H}_i\right)\times\left(\mathbf{u}_r\times\mathbf{E}_j^*\right)\right] &= \mathbf{u}_r\cdot\left\{\mathbf{u}_r\left[\mathbf{u}_r\cdot\left(\mathbf{H}_i\times\mathbf{E}_j^*\right)\right]-\mathbf{E}_j^*\left[\mathbf{u}_r\cdot\left(\mathbf{H}_i\times\mathbf{u}_r\right)\right]\right\} \\
&= \mathbf{u}_r\cdot\left(\mathbf{H}_i\times\mathbf{E}_j^*\right) = -\left[\mathbf{u}_r\cdot\left(\mathbf{E}_j\times\mathbf{H}_i^*\right)\right]^* && \text{(48d)}
\end{aligned}
$$

To obtain the scattering cross section, we have to perform integrals of the form (for fixed $\mathbf{v}_i$, $\mathbf{w}$)

$$\int d\Omega\, e^{ik\mathbf{u}_r\cdot\mathbf{w}} \equiv I_0 \tag{49a}$$

$$\int d\Omega\, \mathbf{u}_r\cdot\mathbf{v}e^{ik\mathbf{u}_r\cdot\mathbf{w}} \equiv I_1 \tag{49b}$$

$$\int d\Omega\, \left(\mathbf{u}_r\cdot\mathbf{v}_1\right)\left(\mathbf{u}_r\cdot\mathbf{v}_2\right)e^{ik\mathbf{u}_r\cdot\mathbf{w}} \equiv I_2 \tag{49c}$$

We define the z axis along the vector $\mathbf{w}$ (which is real), hence, in polar coordinates,

$$\mathbf{u}_r = \begin{pmatrix} \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \end{pmatrix} \tag{50a}$$

$$d\Omega = d\phi d\theta \sin\theta \tag{50b}$$

$$k\mathbf{u}_r \cdot \mathbf{w} = kw\cos\theta \tag{50c}$$

$$\mathbf{u}_r \cdot \mathbf{v} = \sin\theta\cos\phi v_x + \sin\theta\sin\phi v_y + \cos\theta v_z \tag{50d}$$

$$\begin{aligned}(\mathbf{u}_r \cdot \mathbf{v}_1)(\mathbf{u}_r \cdot \mathbf{v}_2) = &\sin^2\theta\left[\cos^2\phi v_{1x}v_{2x} + \sin^2\phi v_{1y}v_{2y} + \sin\phi\cos\phi\,(v_{1x}v_{2y} + v_{1y}v_{2x})\right] \\ &+ \cos\theta\sin\theta\left[\cos\phi\,(v_{1x}v_{2z} + v_{1z}v_{2x}) + \sin\phi\,(v_{1y}v_{2z} + v_{1z}v_{2y})\right] \\ &+ \cos^2\theta v_{1z}v_{2z}\end{aligned} \tag{50e}$$

Then, we have

$$I_0 = \int d\Omega\, e^{ik\mathbf{u}_r\cdot\mathbf{w}} = 2\pi\int_0^\pi d\theta\,\sin\theta e^{ikw\cos\theta} = 2\pi\int_{-1}^1 dz\, e^{ikwz} = 4\pi i\frac{\sin(kw)}{kw} \tag{51}$$

and, considering eq.(50d)

$$\begin{aligned}I_1 &= \int d\Omega\,\mathbf{u}_r\cdot\mathbf{v}e^{ik\mathbf{u}_r\cdot\mathbf{w}} = \int_0^{2\pi} d\phi\int_0^\pi d\theta\,\left(\sin\theta\cos\phi v_x + \sin\theta\sin\phi v_y + \cos\theta v_z\right)\sin\theta e^{ikw\cos\theta} \\ &= 2\pi v_z\int_0^\pi d\theta\,\sin\theta\cos\theta e^{ikw\cos\theta} = 2\pi v_z\int_{-1}^1 dz\, ze^{ikwz} = 4\pi v_z i\left(\frac{\sin(kw)}{(kw)^2} - \frac{\cos(kw)}{(kw)}\right)\end{aligned} \tag{52}$$

and, considering eq.(50e) (we shall omit the explicit integration in ϕ).

$$\begin{aligned}I_2 &= \int d\Omega\,\left(\mathbf{u}_r\cdot\mathbf{v}_1\right)\left(\mathbf{u}_r\cdot\mathbf{v}_2\right)e^{ik\mathbf{u}_r\cdot\mathbf{w}} = 2\pi\int_0^\pi d\theta\,\left[\frac{1}{2}\sin^2\theta\,(v_{1x}v_{2x} + v_{1y}v_{2y}) + \cos^2\theta v_{1z}v_{2z}\right]\sin\theta e^{ikw\cos\theta} \\ &= 4\pi\left(v_{1z}v_{2z} - \frac{1}{2}v_{1x}v_{2x} - \frac{1}{2}v_{1y}v_{2y}\right)\left[\frac{(kw)^2 - 2}{(kw)^3}\sin(kw) + \frac{2}{(kw)^2}\cos(kw)\right] + 2\pi\frac{\sin(kw)}{kw}\left(v_{1x}v_{2x} + v_{1y}v_{2y}\right)\end{aligned} \tag{53}$$

Where we have considered the primitives

$$\int dx\, e^{i\alpha x} = \frac{e^{i\alpha x}}{i\alpha} \tag{54a}$$

$$\int dx\, xe^{i\alpha x} = \frac{e^{i\alpha x}}{\alpha^2}\left(1 - i\alpha x\right) \tag{54b}$$

$$\int dx\, x^2e^{i\alpha x} = \frac{e^{i\alpha x}}{\alpha^3}\left(2i + 2\alpha x - i\alpha^2x^2\right) \tag{54c}$$

Some of the above expression can be written in a different way if we take

$$\int_{-1}^1 dx\, e^{i\alpha x} = \mathrm{Im}\left\{\frac{2e^{i\alpha}}{\alpha}\right\} \tag{55a}$$

$$\int_{-1}^1 dx\, xe^{i\alpha x} = i\mathrm{Im}\left\{\frac{2e^{i\alpha}}{\alpha^2}\left(1 - i\alpha\right)\right\} \tag{55b}$$

$$\int_{-1}^1 dx\, x^2e^{i\alpha x} = \mathrm{Re}\left\{\frac{2e^{i\alpha}}{\alpha^3}\left(2i + 2\alpha - i\alpha^2\right)\right\} = \mathrm{Im}\left\{\frac{2e^{i\alpha}}{\alpha^3}\left(-2 + 2i\alpha + \alpha^2\right)\right\} \tag{55c}$$

If we define the projector in the subspace spanned by $\mathbf{w}$ as

$$\mathbb{P}_{\mathbf{w}} \equiv \frac{\mathbf{w}\mathbf{w}^t}{|\mathbf{w}|^2} \tag{56}$$

In the coordinate system where $\mathbf{u}_z \parallel \mathbf{w}$ we have

$$\begin{pmatrix} 0 \\ 0 \\ v_z \end{pmatrix} = \mathbb{P}_{\mathbf{w}}\mathbf{v} \tag{57}$$

also, in this coordinate system,

$$\begin{pmatrix} v_x \\ v_y \\ 0 \end{pmatrix} = (\mathbb{I} - \mathbb{P}_{\mathbf{w}})\,\mathbf{v} \tag{58}$$

And

$$v_{1x}v_{2x} + v_{1y}v_{2y} = \mathbf{v}_1^t\,(\mathbb{I} - \mathbb{P}_{\mathbf{w}})\,(\mathbb{I} - \mathbb{P}_{\mathbf{w}})\,\mathbf{v}_2 = \mathbf{v}_1^t\,(\mathbb{I} - \mathbb{P}_{\mathbf{w}})\,\mathbf{v}_2 \tag{59}$$

with this we can write

$$I_0 = \int d\Omega\, e^{ik\mathbf{u}_r\cdot\mathbf{w}} = 4\pi \mathrm{Im}\left\{\frac{e^{ikw}}{kw}\right\} \tag{60a}$$

$$I_1 = \int d\Omega\, \mathbf{u}_r\cdot\mathbf{v}e^{ik\mathbf{u}_r\cdot\mathbf{w}} = 4\pi i\frac{\mathbf{w}\cdot\mathbf{v}}{|\mathbf{w}|}\mathrm{Im}\left\{\frac{e^{ikw}}{(kw)^2}\,(1-ikw)\right\} \tag{60b}$$

$$\begin{aligned} I_2 =& \int d\Omega\,\left(\mathbf{u}_r\cdot\mathbf{v}_1\right)\left(\mathbf{u}_r\cdot\mathbf{v}_2\right)e^{ik\mathbf{u}_r\cdot\mathbf{w}} \\ =&4\pi\mathrm{Im}\left\{\frac{e^{ikw}}{(kw)^3}\,(1-ikw)\right\}\mathbf{v}_1^t\mathbf{v}_2 \\ &+ 4\pi\mathrm{Im}\left\{\frac{e^{ikw}}{(kw)^3}\left((kw)^2+3ikw-3\right)\right\}\mathbf{v}_1^t\mathbb{P}_{\mathbf{w}}\mathbf{v}_2 \end{aligned} \tag{60c}$$

Hence,

$$
\begin{aligned}
\int d\Omega\, \mathbf{S}_s \cdot \mathbf{u}_r =& \frac{1}{2Zk^2}\mathrm{Re}\left\{4\pi i\alpha_E^{(i)}\alpha_M^{(j)*}\left(\mathbf{E}_i \times \mathbf{H}_j^*\right)\cdot \mathbf{u}_{ji}\mathrm{Im}\left\{\frac{e^{ikr_{ji}}}{(kr_{ji})^2}\left(1-ikr_{ji}\right)\right\}\right\} \\
&+ \frac{1}{2Zk^2}\mathrm{Re}\left\{4\pi\alpha_E^{(i)}\alpha_E^{(j)*}\left(\mathbf{E}_i\cdot\mathbf{E}_j^*\right)\mathrm{Im}\left\{\frac{e^{ikr_{ji}}}{kr_{ji}}\right\}\right\} \\
&- \frac{1}{2Zk^2}\mathrm{Re}\left\{4\pi\alpha_E^{(i)}\alpha_E^{(j)*}\mathrm{Im}\left\{\frac{e^{ikr_{ji}}}{(kr_{ji})^3}\left(1-ikr_{ji}\right)\right\}\mathbf{E}_i^t\mathbf{E}_j\right\} \\
&- \frac{1}{2Zk^2}\mathrm{Re}\left\{4\pi\alpha_E^{(i)}\alpha_E^{(j)*}\mathrm{Im}\left\{\frac{e^{ikr_{ji}}}{(kr_{ji})^3}\left((kr_{ji})^2+3ikr_{ji}-3\right)\right\}\mathbf{E}_i^t\mathbb{P}_{\mathbf{r}_{ji}}\mathbf{E}_j^*\right\} \\
&+ \frac{1}{2Zk^2}\mathrm{Re}\left\{4\pi\alpha_M^{(i)}\alpha_M^{(j)*}\left(\mathbf{H}_i\cdot\mathbf{H}_j^*\right)\mathrm{Im}\left\{\frac{e^{ikr_{ji}}}{kr_{ji}}\right\}\right\} \\
&- \frac{1}{2Zk^2}\mathrm{Re}\left\{4\pi\alpha_M^{(i)}\alpha_M^{(j)*}\mathrm{Im}\left\{\frac{e^{ikr_{ji}}}{(kr_{ji})^3}\left(1-ikr_{ji}\right)\right\}\mathbf{H}_i^t\mathbf{H}_j\right\} \\
&- \frac{1}{2Zk^2}\mathrm{Re}\left\{4\pi\alpha_M^{(i)}\alpha_M^{(j)*}\mathrm{Im}\left\{\frac{e^{ikr_{ji}}}{(kr_{ji})^3}\left((kr_{ji})^3+3ikr_{ji}-3\right)\right\}\mathbf{H}_i^t\mathbb{P}_{\mathbf{r}_{ji}}\mathbf{H}_j^*\right\} \\
&- \frac{1}{2Zk^2}\mathrm{Re}\left\{4\pi i\alpha_M^{(i)}\alpha_E^{(j)*}\left(\mathbf{H}_i \times \mathbf{E}_j^*\right)\cdot \mathbf{u}_{ji}\mathrm{Im}\left\{\frac{e^{ikr_{ji}}}{(kr_{ji})^2}\left(1-ikr_{ji}\right)\right\}\right\} \qquad (61)
\end{aligned}
$$

where $\mathbf{r}_{ji} \equiv (\mathbf{r}_j - \mathbf{r}_i)$,$r_{ji} = |\mathbf{r}_j - \mathbf{r}_i|$, and $\mathbf{u}_{ji} \equiv \mathbf{r}_{ji}/r_{ji}$.

Considering that (with renormalized variables)

$$\mathbf{p}_i = \alpha_E^{(i)}\mathbf{E}_i \qquad (62a)$$

$$\mathbf{m}_i = \alpha_M^{(i)}\mathbf{H}_i \qquad (62b)$$

, and the form of the magnetic green tensor given by eq. (16b), and

$$\left(\mathbf{E}_i \times \mathbf{H}_j^*\right)\cdot\mathbf{u}_{ji} = -\mathbf{E}_i\cdot\left(\mathbf{u}_{ji}\times\mathbf{H}_j^*\right) = \mathbf{H}_j^*\cdot\left(\mathbf{u}_{ji}\times\mathbf{E}_i\right) \qquad (63)$$

we have

$$
\begin{aligned}
\mathrm{Re}\left\{i\alpha_E^{(i)}\alpha_M^{(j)*}\left(\mathbf{E}_i\times\mathbf{H}_j^*\right)\cdot\mathbf{u}_{ji}\mathrm{Im}\left\{\frac{e^{ikr_{ji}}}{kr_{ji}}\left(1-ikr_{ji}\right)\right\}\right\} &= -\mathrm{Im}\left\{\left(\mathbf{p}_i\times\mathbf{m}_j^*\right)\cdot\mathbf{u}_{ji}\mathrm{Im}\left\{\frac{e^{ikr_{ji}}}{kr_{ji}}\left(1-ikr_{ji}\right)\right\}\right\} \\
&= -\mathrm{Im}\left\{\mathbf{p}_i\cdot\mathrm{Im}\left\{\mathbb{G}_m\left(\mathbf{r}_j,\mathbf{r}_i\right)\right\}\mathbf{m}_j^*\right\} \qquad (64)
\end{aligned}
$$

Analogously we have

$$\mathrm{Re}\left\{i\alpha_M^{(i)}\alpha_E^{(j)*}\left(\mathbf{H}_i\times\mathbf{E}_j^*\right)\cdot\mathbf{u}_{ji}\mathrm{Im}\left\{\frac{e^{ikr_{ji}}}{kr_{ji}}\left(1-ikr_{ji}\right)\right\}\right\} = Im\left\{\mathbf{p}_j^*\cdot\mathrm{Im}\left\{\mathbb{G}_m\left(\mathbf{r}_j,\mathbf{r}_i\right)\right\}\mathbf{m}_i\right\} \qquad (65)$$

With this, the sum of the first and last terms of the R.H.S. of equation (61) can be written as

$$\begin{aligned}
&\frac{2\pi}{Zk^2}\sum_{i,j}\mathrm{Re}\left\{i\left[\left(\mathbf{p}_i\times\mathbf{m}_j^*\right)\cdot\mathbf{u}_{ji}-\left(\mathbf{m}_i\times\mathbf{p}_j^*\right)\cdot\mathbf{u}_{ji}\right]\mathrm{Im}\left\{\frac{e^{ikr_{ji}}}{kr_{ji}}\left(1-ikr_{ji}\right)\right\}\right\}\\
=&\frac{2\pi}{Zk^2}\sum_{i,j}-\mathrm{Im}\left\{\mathbf{p}_i\cdot\mathrm{Im}\left\{\mathbb{G}_m\left(\mathbf{r}_j,\mathbf{r}_i\right)\right\}\mathbf{m}_j^*-\mathrm{Im}\left\{\mathbf{p}_j^*\cdot\mathrm{Im}\left\{\mathbb{G}_m\left(\mathbf{r}_j,\mathbf{r}_i\right)\right\}\mathbf{m}_i\right\}\right\}\\
=&\frac{2\pi}{Zk^2}\sum_{i>j}-\mathrm{Im}\left\{\mathbf{p}_i\cdot\mathrm{Im}\left\{\mathbb{G}_m\left(\mathbf{r}_j,\mathbf{r}_i\right)\right\}\mathbf{m}_j^*-\mathbf{p}_j\cdot\mathrm{Im}\left\{\mathbb{G}_m\left(\mathbf{r}_j,\mathbf{r}_i\right)\right\}\mathbf{m}_i^*\right\}\\
&+\frac{2\pi}{Zk^2}\sum_{i>j}-\mathrm{Im}\left\{\mathbf{p}_j^*\cdot\mathrm{Im}\left\{\mathbb{G}_m\left(\mathbf{r}_j,\mathbf{r}_i\right)\right\}\mathbf{m}_i-\mathbf{p}_i^*\cdot\mathrm{Im}\left\{\mathbb{G}_m\left(\mathbf{r}_j,\mathbf{r}_i\right)\right\}\mathbf{m}_j\right\}=\\
=&\frac{4\pi}{Zk^2}\sum_{i>j}\mathrm{Im}\left\{-\mathbf{p}_i\cdot\mathrm{Im}\left\{\mathbb{G}_m\left(\mathbf{r}_j,\mathbf{r}_i\right)\right\}\mathbf{m}_j^*+\mathbf{p}_j\cdot\mathrm{Im}\left\{\mathbb{G}_m\left(\mathbf{r}_j,\mathbf{r}_i\right)\right\}\mathbf{m}_i^*\right\}
\end{aligned}\tag{66}$$

where we have considered that

$$\mathrm{Im}\left\{\mathbb{G}_m\left(\mathbf{r}_i,\mathbf{r}_i\right)\right\}=0\tag{67}$$

and that

$$\mathbb{G}_m\left(\mathbf{r}_j,\mathbf{r}_i\right)=-\mathbb{G}_m\left(\mathbf{r}_i,\mathbf{r}_j\right)\tag{68}$$

Regarding the terms proportional to $\alpha_E^{(i)}\alpha_E^{(j)*}$ in eq. (61) we have,

$$\begin{aligned}
&\left(\mathbf{p}_i\cdot\mathbf{p}_j^*\right)\mathrm{Im}\left\{\frac{e^{ikr_{ji}}}{kr_{ji}}\right\}-\mathrm{Im}\left\{\frac{e^{ikr_{ji}}}{\left(kr_{ji}\right)^3}\left(1-ikr_{ji}\right)\right\}\mathbf{p}_i^t\mathbf{p}_j^*-\mathrm{Im}\left\{\frac{e^{ikr_{ji}}}{\left(kr_{ji}\right)^3}\left(\left(kr_{ji}\right)^2+3ikr_{ji}-3\right)\right\}\mathbf{p}_i^t\mathbb{P}_{\mathbf{r}_{ji}}\mathbf{p}_j^*=\\
&=\mathbf{p}_i^t\mathrm{Im}\left\{\mathbb{G}_E\left(\mathbf{r}_i,\mathbf{r}_j\right)\right\}\mathbf{p}_j^*
\end{aligned}\tag{69}$$

Please notice that

$$\mathrm{Im}\left\{\mathbb{G}_E\left(\mathbf{r}_i,\mathbf{r}_j\right)\right\}=\frac{2}{3}\mathbb{I}\tag{70}$$

Collecting all previous results, we can write:

$$\begin{aligned}
\int d\Omega\,\mathbf{S}_s\cdot\mathbf{u}_r=&\frac{4\pi}{3Zk^2}\left[\sum_i\left|\mathbf{p}_i\right|^2+\sum_i\left|\mathbf{m}_i\right|^2\right]\\
&+\frac{4\pi}{Zk^2}\mathrm{Re}\left\{\sum_{i>j}\mathbf{p}_i^t\mathrm{Im}\left\{\mathbb{G}_E\left(\mathbf{r}_i,\mathbf{r}_j\right)\right\}\mathbf{p}_j^*+\mathbf{m}_i^t\mathrm{Im}\left\{\mathbb{G}_E\left(\mathbf{r}_i,\mathbf{r}_j\right)\right\}\mathbf{m}_j^*\right\}\\
&+\frac{4\pi}{Zk^2}\sum_{i>j}\mathrm{Im}\left\{-\mathbf{p}_j^*\cdot\mathrm{Im}\left\{\mathbb{G}_m\left(\mathbf{r}_j,\mathbf{r}_i\right)\right\}\mathbf{m}_i+\mathbf{p}_i^*\cdot\mathrm{Im}\left\{\mathbb{G}_m\left(\mathbf{r}_j,\mathbf{r}_i\right)\right\}\mathbf{m}_j\right\}
\end{aligned}\tag{71}$$

where the sum runs across all induced electric and magnetic dipoles resp.

Equation (71) can be trivially extended to obtain the power radiated in the far field by an electric of magnetic point source surrounded by electric and magnetic dipoles. We only need to extend the sum to the source dipole and, of course, include all induced dipoles.

4.2 Extinction cross section (incoming planewave).

While the scattering cross section can be expressed as a function of the induced electric and magnetic dipoles, the extinction cross section depend explicitly on the form of the incoming field.

We shall consider three main types of incoming fields: electric point dipole, magnetic point dipole and plane wave. The extinction cross section is meaningful for an incoming planewave. We shall use the asymptotic expansions for the fields and perform integrals by the stationary phase method.

$$\mathbb{G}_E(\mathbf{r},\mathbf{r}_0) \simeq \frac{e^{ikr}}{kr} e^{-ik\mathbf{r}_o\cdot\mathbf{u}_r} \left(\mathbb{I} - \mathbf{u}_r\mathbf{u}_r\right) \tag{72a}$$

$$\mathbb{G}_M(\mathbf{r},\mathbf{r}_0) \simeq i\frac{e^{ikr}}{kr} e^{-ik\mathbf{r}_o\cdot\mathbf{u}_r} \mathbf{u}_r\times \tag{72b}$$

And the incoming field

$$\mathbf{E}_i(\mathbf{r}) = \mathbf{E}_0 e^{ik\mathbf{u}_k\cdot\mathbf{r}} \tag{73a}$$

$$\mathbf{H}_i(\mathbf{r}) = \mathbf{H}_0 e^{ik\mathbf{u}_k\cdot\mathbf{r}} \tag{73b}$$

where

$$\mathbf{H}_0 = \mathbf{u}_k \times \mathbf{E}_0 = \begin{pmatrix} \mathbf{u}_y\mathbf{E}_{0z} - \mathbf{u}_z\mathbf{E}_{0y} \\ \mathbf{u}_z\mathbf{E}_{0x} - \mathbf{u}_x\mathbf{E}_{0z} \\ \mathbf{u}_x\mathbf{E}_{0y} - \mathbf{u}_y\mathbf{E}_{0x} \end{pmatrix} \tag{74}$$

with this,

$$\mathbf{E}_i \times \mathbf{H}_s^* = \sum_n \left\{ \left(\alpha_E^{(n)}\right)^* \mathbf{E}_0 \times \left(\mathbf{u}_r \times \mathbf{E}_n^*\right) + \left(\alpha_M^{(n)}\right)^* \left[\mathbf{E}_0 \times \mathbf{H}_n^* - \mathbf{E}_0 \times \mathbf{u}_r \left(\mathbf{u}_r \cdot \mathbf{H}_n^*\right)\right] \right\} \frac{e^{i(k\mathbf{u}_k\cdot\mathbf{r}-kr)}}{kr} e^{ik\mathbf{r}_n\cdot\mathbf{u}_r} \tag{75a}$$

$$\mathbf{E}_s \times \mathbf{H}_i^* = \sum_n \left\{ \alpha_E^{(n)} \left[\mathbf{E}_n \times \mathbf{H}_0^* - \mathbf{u}_r \times \mathbf{H}_0^* \left(\mathbf{u}_r \cdot \mathbf{E}_n\right)\right] - \alpha_M^{(n)} \left(\mathbf{u}_r \times \mathbf{H}_n\right) \times \mathbf{H}_0^* \right\} \frac{e^{i(kr-k\mathbf{u}_k\cdot\mathbf{r})}}{kr} e^{-ik\mathbf{r}_n\cdot\mathbf{u}_r} \tag{75b}$$

Now we have to take the limit $kr \to \infty$, but in this case we have to proceed in different way as we have done when calculating the scattering cross section.

We take the Z axis to be parallel to $\mathbf{u}_k$. In polar coordinates (being θ the polar angle) we have

$$k\mathbf{u}_k \cdot \mathbf{r} - kr = kr\left(\cos\theta - 1\right) = -2kr\sin^2\left(\frac{\theta}{2}\right) \tag{76}$$

Hence, we have integrals of the form

$$\int_0^{2\pi} d\phi \int_0^{\pi} d\theta\, \sin\theta e^{\pm 2ikr\sin^2\left(\frac{\theta}{2}\right)} f(\theta,\phi) \tag{77}$$

We notice that

$$\frac{\partial \sin^2\left(\frac{\theta}{2}\right)}{\partial\theta} = \sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\theta}{2}\right) = 0 \Rightarrow \theta = \begin{cases} \theta = 0 \\ \theta = \pi \end{cases} \tag{78}$$

Hence, in the limit $kr \to \infty$ only $\mathbf{u}_r = \pm\mathbf{u}_k$ shall contribute to the integral.

We hace to consider also that

$$\int_0^{\infty} dx\, x^n e^{ikrx^2} \propto \left(\frac{1}{kr}\right)^{\frac{n+1}{2}} \tag{79}$$

We have integrals of the form

$$r^2 \int_0^{2\pi} d\phi \int_0^{\pi} d\theta\, \sin\theta \frac{e^{\pm 2ikr \sin^2\left(\frac{\theta}{2}\right)}}{kr} f(\theta,\phi) \tag{80}$$

if we expand in power series

$$\sin(\theta)\; f(\theta,\phi) = \sum_{n=1}^{\infty} f_{n-1}(\phi)\, \theta^n \tag{81}$$

the only non-vanishing contribution in the limit $kr \to \infty$ is $n = 0$, i.e. considering only the value of $f(\theta,\phi)$ at the stationary points. In fact this result constitute the Jones' lemma (See Born&Wolf appendix XII for instance) which states that

$$\frac{1}{R}\int_{\Omega} d\Omega\, G(\mathbf{n})\, e^{-ikR(\mathbf{n}_0\cdot\mathbf{n})} = \frac{2\pi i}{k}\left[G(\mathbf{n}_0)\, e^{-ikr} - G(-\mathbf{n}_0)\, e^{ikr}\right] \tag{82}$$

where $\mathbf{n}_0$ is a fixed unitary vector, and $\mathbf{n}$ is the outwards normal of a sphere. The integration domain Ω is a sphere or radius R.

We have then to consider

$$\mathbf{u}_k\cdot(\mathbf{E}_0\times(\mathbf{u}_k\times\mathbf{E}_n^*)) = \mathbf{u}_k\cdot(\mathbf{u}_k(\mathbf{E}_0\cdot\mathbf{E}_n^*) - \mathbf{E}_n^*(\mathbf{u}_k\cdot\mathbf{E}_0)) = (\mathbf{E}_0\cdot\mathbf{E}_n^*) \tag{83a}$$

$$\mathbf{u}_k\cdot(\mathbf{E}_0\times\mathbf{H}_n^*) = \mathbf{H}_n^*\cdot(\mathbf{u}_k\times\mathbf{E}_0) = \mathbf{H}_n^*\cdot\mathbf{H}_0 \tag{83b}$$

$$\mathbf{u}_k\cdot(\mathbf{E}_0\times\mathbf{u}_k) = 0 \tag{83c}$$

$$\mathbf{u}_k\cdot(\mathbf{E}_n\times\mathbf{H}_0^*) = \mathbf{u}_k\cdot(\mathbf{E}_n\times(\mathbf{u}_k\times\mathbf{E}_o^*)) = \mathbf{u}_k\cdot(\mathbf{u}_k(\mathbf{E}_n\cdot\mathbf{E}_0^*) - \mathbf{E}_0^*(\mathbf{E}_n\cdot\mathbf{u}_k)) = \mathbf{E}_n\cdot\mathbf{E}_0^* \tag{83d}$$

$$\mathbf{u}_k\cdot(\mathbf{u}_k\times\mathbf{H}_0^*) = 0 \tag{83e}$$

$$\mathbf{u}_k\cdot((\mathbf{u}_k\times\mathbf{H}_n)\times\mathbf{H}_0^*) = \mathbf{u}_k\cdot(\mathbf{H}_n(\mathbf{u}_k\cdot\mathbf{H}_0^*) - \mathbf{u}_k(\mathbf{H}_n\cdot\mathbf{H}_0^*)) = -\mathbf{H}_n\cdot\mathbf{H}_0^* \tag{83f}$$

which are the **??** when $\mathbf{u}_r = \mathbf{u}_k$. Notice that eq.(83a) and eq.(83d) are the same, eq.(83c) and eq.(83e) do not contribute, and eq.(83b) and eq.(83f) are also the same.

If we change $\mathbf{u}_r = \mathbf{u}_k$ by $\mathbf{u}_r = -\mathbf{u}_k$ in equations **??** , we find analogous expression to the equations (83) but changing signs in eq.(83b) and eq.(83d) .

If we defines

$$A_n \equiv \alpha_E^{(n)}(\mathbf{E}_n\cdot\mathbf{E}_0^*) \tag{84a}$$

$$B_n \equiv \alpha_M^{(n)}(\mathbf{H}_n\cdot\mathbf{H}_0^*) \tag{84b}$$

Then, we have

$$\int d\Omega\, (\mathbf{E}_s\times\mathbf{H}_i^*)\cdot\mathbf{u}_r = \frac{2\pi i}{k^2}\sum_n\left[(A_n+B_n)\, e^{-ik\mathbf{r}_n\cdot\mathbf{u}_k} + (A_n-B_n)\, e^{ik\mathbf{r}_n\cdot\mathbf{u}_k} e^{2ikr}\right] \tag{85a}$$

$$\int d\Omega\, (\mathbf{E}_i\times\mathbf{H}_s^*)\cdot\mathbf{u}_r = \frac{-2\pi i}{k^2}\sum_n\left[(A_n^*+B_n^*)\, e^{ik\mathbf{r}_n\cdot\mathbf{u}_k} - (A_n^*-B_n^*)\, e^{-ik\mathbf{r}_n\cdot\mathbf{u}_k} e^{-2ikr}\right] \tag{85b}$$

Then the power associated to the extinction Poynting vector is

$$P_{ext} = \int d\Omega\, \mathbf{S}_{ext} \cdot \mathbf{u}_r = \frac{1}{2Z}\mathrm{Re}\left\{ \int d\Omega\, \left(-\mathbf{E}_s \times \mathbf{H}_i^* - \mathbf{E}_i \times \mathbf{H}_s^*\right) \cdot \mathbf{u}_r \right\} =$$

$$= \frac{2\pi}{Zk^2} \sum_n \mathrm{Im}\left\{ \left(\alpha_E^{(n)} \left(\mathbf{E}_n \cdot \mathbf{E}_0^*\right) + \alpha_M^{(n)} \left(\mathbf{H}_n \cdot \mathbf{H}_0^*\right) \right) e^{-ik\mathbf{r}_n \cdot \mathbf{u}_k} \right\} = \quad (86)$$

$$= \frac{2\pi}{Zk^2} \sum_n \mathrm{Im}\left\{ \left(\alpha_E^{(n)} \left(\mathbf{E}_n \cdot \mathbf{E}_0^*\left(\mathbf{r}_n\right)\right) + \alpha_M^{(n)} \left(\mathbf{H}_n \cdot \mathbf{H}_0^*\left(\mathbf{r}_n\right)\right) \right) \right\} \quad (87)$$

Notice that in the case of a single particle, $\mathbf{E}_1 = \mathbf{E}_0 e^{ik\mathbf{r}_1 \cdot \mathbf{u}_k}$, and hence the phase cancels. In fact the solution is invariant under a translation of the whole system because the exciting fields $\mathbf{E}_n$ and $\mathbf{H}_n$ are proportional to the phase of the field, this phase if canceled by the conjugate of the incoming external field appearing in the above equation . Explicitly, for a single particle we have.

$$P_{ext} = \frac{2\pi}{Zk^2}\mathrm{Im}\left\{ \alpha_E^{(n)} \left|\mathbf{E}_0\right|^2 + \alpha_M^{(n)} \left|\mathbf{H}_0\right|^2 \right\} \quad (88)$$

Notice also that the terms proportional to $\exp\left(\pm 2ikr\right)$ do not enter in the final result because the total contribution has the form $\mathrm{Re}\left(z - z^*\right) = 0$. On the contrary, the terms without the phase $\exp\left(\pm 2ikr\right)$ contribute in the form $\mathrm{Re}\left(z + z^*\right) \neq 0$ in general.

4.3 Absorption cross section and absorbed power in each particle.

if we consider a source free region, then, $\int d\Omega\, \mathbf{S}_i \cdot \mathbf{u}_n = 0$, hence the absorbed power in a region bounded by the surface Ω can be calculated as the difference between the integral of the scattering Poynting vector and the extinction pointing vector by virtue of the Poynting theorem:

$$P_{abs} = \int d\Omega\, \mathbf{n} \cdot \left(\mathbf{S}_{ext.} - \mathbf{S}_{scat.}\right) \quad (89)$$

Let us assume that inside this volume, there is only one particle (with induced electric and magnetic dipole). We then have

$$P_{scatt}^{(i)} = \frac{4\pi}{3Zk^2}\left[\left|\alpha_E^{(i)}\right|^2 \left|\mathbf{E}_i\right|^2 + \left|\alpha_M^{(i)}\right|^2 \left|\mathbf{H}_i\right|^2 \right] \quad (90)$$

where $\mathbf{E}_i$ and $\mathbf{H}_i$ ar the total exciting fields for the $i-th$ particle.

On the other hand, the extinction power for each particle is

$$P_{ext}^{(i)} = \frac{2\pi}{Zk^2}\mathrm{Im}\left\{ \alpha_E^{(i)} \left|\mathbf{E}_i\right|^2 + \alpha_M^{(i)} \left|\mathbf{H}_i\right|^2 \right\} \quad (91)$$

Then, the absorbed power is

$$P_{abs}^{(i)} = \frac{2\pi}{Zk^2}\left[\left(\mathrm{Im}\left\{\alpha_E^{(i)}\right\} - \frac{2}{3}\left|\alpha_E^{(i)}\right|^2 \right) \left|\mathbf{E}_i\right|^2 + \left(\mathrm{Im}\left\{\alpha_M^{(i)}\right\} - \frac{2}{3}\left|\alpha_M^{(i)}\right|^2 \right) \left|\mathbf{H}_i\right|^2 \right] \quad (92)$$

5 Summary of expressions

$$
\begin{aligned}
P_{scat} = \int d\Omega\, \mathbf{S}_s \cdot \mathbf{u}_r = \frac{4\pi}{3Zk^2} \left[\sum_i |\mathbf{p}_i|^2 + \sum_i |\mathbf{m}_i|^2 \right] \\
+ \frac{4\pi}{Zk^2} \mathrm{Re} \left\{ \sum_{i>j} \mathbf{p}_i^t \mathrm{Im} \left\{ \mathbb{G}_E \left(\mathbf{r}_i, \mathbf{r}_j \right) \right\} \mathbf{p}_j^* + \mathbf{m}_i^t \mathrm{Im} \left\{ \mathbb{G}_E \left(\mathbf{r}_i, \mathbf{r}_j \right) \right\} \mathbf{m}_j^* \right\} \\
+ \frac{4\pi}{Zk^2} \sum_{i>j} \mathrm{Im} \left\{ -\mathbf{p}_j^* \cdot \mathrm{Im} \left\{ \mathbb{G}_m \left(\mathbf{r}_j, \mathbf{r}_i \right) \right\} \mathbf{m}_i + \mathbf{p} \cdot \mathrm{Im} \left\{ \mathbb{G}_m \left(\mathbf{r}_j, \mathbf{r}_i \right) \right\} \mathbf{m}_j \right\} \\
P_{ext} = \frac{2\pi}{Zk^2} \sum_i \mathrm{Im} \left\{ \left(\alpha_E^{(i)} \left(\mathbf{E}_i \cdot \mathbf{E}_0^* \left(\mathbf{r}_i \right) \right) + \alpha_M^{(i)} \left(\mathbf{H}_i \cdot \mathbf{H}_0^* \left(\mathbf{r}_i \right) \right) \right) \right\} \\
P_{abs} = \frac{2\pi}{Zk^2} \sum_i \left[\left(\mathrm{Im} \left\{ \alpha_E^{(i)} \right\} - \frac{2}{3} \left| \alpha_E^{(i)} \right|^2 \right) |\mathbf{E}_i|^2 + \left(\mathrm{Im} \left\{ \alpha_M^{(i)} \right\} - \frac{2}{3} \left| \alpha_M^{(i)} \right|^2 \right) |\mathbf{H}_i|^2 \right]
\end{aligned}
$$

Part III
The Julia Package

6 DDA core functionalities: DDA.jl

6.1 Choosing the solver

7 Utilities

7.1 Input Fields

7.2 Mie Theory

7.3 Polarizabilities

7.4 Cross sections computation

8 Examples

8.1 Scattering, extinction and absorbtion corss sections for