

# Supplementary Informations for ”CoupledElectricMagneticDipoles.jl, an Electric and Magnetic Coupled Dipoles Julia Library for Multiple Scattering Calculations”

Augustin Muster, Diego Romero Abujetas, Luis S. Froufe-Pérez

June 2023

## 1 Induced Electric and Magnetic Dipoles

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

$$\mathbf{p} = \epsilon_0 \tilde{\alpha}_E \mathbf{E}_i(\mathbf{r}_0), \quad (1a)$$

$$\mathbf{m} = \tilde{\alpha}_M \tilde{\mathbf{H}}_i(\mathbf{r}_0). \quad (1b)$$

Where  $\mathbf{E}_i(\mathbf{r}_0)$  and  $\tilde{\mathbf{H}}_i(\mathbf{r}_0)$  are respectively the exciting incident electric and magnetic fields at the particle’s position and  $\tilde{\alpha}_E, \tilde{\alpha}_M$  are the electric, respectively magnetic, polarizabilities of the dipoles (complex scalars or tensors with units of volume). On the other hand, the electromagnetic field generated by electric and magnetic dipoles is

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

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

Where  $k$  is the wavenumber in the medium,  $Z = \sqrt{\mu_0 \mu_h / \epsilon_0 \epsilon_h}$  the impedance in the medium and the electric and magnetic Green’s tensors  $\mathbb{G}_E$  and  $\mathbb{G}_M$  are defined as

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

$$\tilde{\mathbb{G}}_M(\mathbf{r}, \mathbf{r}_0) = \frac{e^{ikr}}{4\pi r} k \left( \frac{ikr - 1}{kr} \right) \mathbf{u}_r \times. \quad (3b)$$

Where  $r \equiv |\mathbf{r} - \mathbf{r}_0|$ , and  $\mathbf{u}_r \equiv (\mathbf{r} - \mathbf{r}_0)/r$ . Then, the electromagnetic that is scattered by a particle located at  $\mathbf{r}_0$  in an incident field  $\mathbf{E}_i$  is given by

$$\mathbf{E}_s(\mathbf{r}) = k^2 \tilde{\mathbb{G}}_E(\mathbf{r}, \mathbf{r}_0) \tilde{\alpha}_E \mathbf{E}_i(\mathbf{r}_0) + iZk \tilde{\mathbb{G}}_M(\mathbf{r}, \mathbf{r}_0) \tilde{\alpha}_M \tilde{\mathbf{H}}_i(\mathbf{r}_0), \quad (4a)$$

$$\tilde{\mathbf{H}}_s(\mathbf{r}) = \frac{-i}{Z} k \tilde{\mathbb{G}}_M(\mathbf{r}, \mathbf{r}_0) \tilde{\alpha}_E \mathbf{E}_i(\mathbf{r}_0) + k^2 \tilde{\mathbb{G}}_E(\mathbf{r}, \mathbf{r}_0) \tilde{\alpha}_M \tilde{\mathbf{H}}_i(\mathbf{r}_0). \quad (4b)$$

## 2 Units and Renormalization of Variables

To simplify the expressions, we redefine Green's tensors to be dimensionless as follows,

$$\mathbb{G}_E(\mathbf{r}, \mathbf{r}_0) = \frac{e^{ikr}}{kr} \left\{ \frac{(kr)^2 + ikr - 1}{(kr)^2} \mathbb{I} + \frac{-(kr)^2 - 3ikr + 3}{(kr)^2} \mathbf{u}_r \mathbf{u}_r \right\} = \frac{4\pi}{k} \tilde{\mathbb{G}}_E(\mathbf{r}, \mathbf{r}_0), \quad (5a)$$

$$\mathbb{G}_M(\mathbf{r}, \mathbf{r}_0) = \frac{e^{ikr}}{kr} \left( \frac{ikr - 1}{kr} \right) \mathbf{u}_r \times = \frac{4\pi}{k^2} \tilde{\mathbb{G}}_M(\mathbf{r}, \mathbf{r}_0). \quad (5b)$$

The advantage of this redefinition is that we can now compute the green tensors using the dimensionless positions  $kr$  and  $kr_0$ . We also redefine the polarizabilities to be dimensionless by multiplying it by  $k^3/4\pi$ , we have

$$\alpha_E = \frac{k^3 \tilde{\alpha}_E}{4\pi}, \quad (6)$$

$$\alpha_M = \frac{k^3 \tilde{\alpha}_M}{4\pi}. \quad (7)$$

Finally, we renormalize the magnetic field as

$$\mathbf{H} = Z \tilde{\mathbf{H}}. \quad (8)$$

With this renormalization, the magnetic field has the same units as the electric field. The scattered field by a electric and magnetic dipolar particle is then

$$\mathbf{E}_s(\mathbf{r}) = \mathbb{G}_E(\mathbf{r}, \mathbf{r}_0) \alpha_E \mathbf{E}_i(\mathbf{r}_0) + i \mathbb{G}_M(\mathbf{r}, \mathbf{r}_0) \alpha_M \mathbf{H}_i(\mathbf{r}_0), \quad (9)$$

$$\mathbf{H}_s(\mathbf{r}) = -i \mathbb{G}_M(\mathbf{r}, \mathbf{r}_0) \alpha_E \mathbf{E}_i(\mathbf{r}_0) + \mathbb{G}_E(\mathbf{r}, \mathbf{r}_0) \alpha_M \mathbf{H}_i(\mathbf{r}_0). \quad (10)$$

Note that the electric and magnetic dipoles are also renormalized, now

$$\mathbf{p} = \frac{k^3 \tilde{\mathbf{p}}}{4\pi\epsilon_0}, \quad (11)$$

$$\mathbf{m} = \frac{k^3 \tilde{\mathbf{m}}}{4\pi\epsilon_0}. \quad (12)$$

## 3 Electric and Magnetic Coupled Dipoles Method

Let's now consider a collection of  $N$  electric and magnetic dipoles at positions  $\mathbf{r}_i$ ,  $i = 1, \dots, N$  and with polarizabilities  $\alpha_E^{(i)}$ ,  $\alpha_M^{(i)}$  (scalars or 3x3 tensors). Considering that all these dipoles are placed in an input electric and magnetic field  $\mathbf{E}_0(\mathbf{r})$  and  $\mathbf{H}_0(\mathbf{r})$ , the incident fields (i.e. input field plus scattered field by all the other dipoles)  $\mathbf{E}_i = \mathbf{E}(\mathbf{r}_i)$  and  $\mathbf{H}_i = \mathbf{H}(\mathbf{r}_i)$  on each dipole  $i$  are given by

$$\mathbf{E}_i = \mathbf{E}_0(\mathbf{r}_i) + \sum_{j \neq i} \mathbb{G}_E(\mathbf{r}_i, \mathbf{r}_j) \alpha_E^{(j)} \mathbf{E}_j + i \mathbb{G}_M(\mathbf{r}_i, \mathbf{r}_j) \alpha_M^{(j)} \mathbf{H}_j, \quad (13)$$

$$\mathbf{H}_i = \mathbf{H}_0(\mathbf{r}_i) + \sum_{j \neq i} -i \mathbb{G}_M(\mathbf{r}_i, \mathbf{r}_j) \alpha_E^{(j)} \mathbf{E}_j + \mathbb{G}_E(\mathbf{r}_i, \mathbf{r}_j) \alpha_M^{(j)} \mathbf{H}_j. \quad (14)$$

This is a set of linear equations that can be solved numerically. To simplify the notation, let's define

$$\Phi(\mathbf{r}) := (\mathbf{E}(\mathbf{r}), \mathbf{H}(\mathbf{r}))^T \quad (15)$$

the electromagnetic field (6 components complex vector) and

$$\mathbb{G}(\mathbf{r}, \mathbf{r}_0) := \begin{pmatrix} \mathbb{G}_{\mathbb{E}}(\mathbf{r}, \mathbf{r}_0) & i\mathbb{G}_{\mathbb{M}}(\mathbf{r}, \mathbf{r}_0) \\ -i\mathbb{G}_{\mathbb{M}}(\mathbf{r}, \mathbf{r}_0) & \mathbb{G}_{\mathbb{E}}(\mathbf{r}, \mathbf{r}_0) \end{pmatrix} \quad (16)$$

the electromagnetic green tensor (6x6 complex matrix). Then, if we write the polarizability to be

$$\alpha := \begin{pmatrix} \alpha_E & 0 \\ 0 & \alpha_M \end{pmatrix} \quad \text{or} \quad \alpha := \begin{pmatrix} \alpha_E \mathbb{I}_3 & 0 \\ 0 & \alpha_M \mathbb{I}_3 \end{pmatrix}, \quad (17)$$

depending if it's a scalar or a 3x3 tensor. With these changes in the notation, we can rewrite equations (13) and (14) as

$$\Phi_i = \Phi_0(\mathbf{r}_i) + \sum_{j \neq i}^N \mathbb{G}(\mathbf{r}_i, \mathbf{r}_j) \alpha \Phi_j. \quad (18)$$

This system of equations can be even more reduced by vectorizing it. For this, we define  $\overleftrightarrow{\Phi} = (\Phi_1, \dots, \Phi_N)^T$  and  $\overleftrightarrow{\Phi}_0 = (\Phi_0(\mathbf{r}_1), \dots, \Phi_0(\mathbf{r}_N))^T$  that are 6N dimensional complex vectors as well as  $\overleftrightarrow{\mathbb{G}} = (\mathbb{G}(\mathbf{r}_i, \mathbf{r}_j)_{ij})$  and  $\overleftrightarrow{\alpha} = (\delta_{ij} \alpha^{(i)})_{ij}$   $i, j = 1, \dots, N$ , two 6Nx6N complex matrix. With this, we obtain:

$$\overleftrightarrow{\Phi}_0 = [\mathbb{I}_{6N} - \overleftrightarrow{\mathbb{G}} \overleftrightarrow{\alpha}] \overleftrightarrow{\Phi} = \mathbb{A} \overleftrightarrow{\Phi}. \quad (19)$$

Solving the CEMDS (DDA) problem remains then to invert the  $\mathbb{A}$  matrix so

$$\overleftrightarrow{\Phi} = \mathbb{A}^{-1} \overleftrightarrow{\Phi}_0. \quad (20)$$

### 3.1 Reduction to Only Electric Coupled Dipoles

When the magnetic polarizability is zero, this remains in solving only the CEMD (DDA) problem for electric dipoles. Equations (13) and (14) reduce to

$$\mathbf{E}_i = \mathbf{E}_0(\mathbf{r}_i) + \sum_{j \neq i} \mathbb{G}_E(\mathbf{r}_i, \mathbf{r}_j) \alpha_E^{(j)} \mathbf{E}_j. \quad (21)$$

## 4 Polarizabilities

### 4.1 Clausius-Mossotti Polarizabilities

It is possible to compute quasistatic electric polarizabilities  $\tilde{\alpha}_{0E}$  using the Clausius-Mossotti relations. For an arbitrary particle the scalar electric polarizability (in units of volume) reads

$$\tilde{\alpha}_{0E} = 3V (\epsilon - \epsilon_h) (\epsilon + 2\epsilon_h)^{-1}. \quad (22)$$

Where  $V$  is the volume of the sphere,  $\epsilon$  is the dielectric constant of the medium, and  $\epsilon_h$  is the dielectric constant of the embedding medium (complex scalars or 3x3 tensors). If the particle is a sphere of radius  $a$ , the polarizability can obviously be written as

$$\tilde{\alpha}_{0E} = 4\pi a^3 (\epsilon - \epsilon_h) (\epsilon + 2\epsilon_h)^{-1}. \quad (23)$$

In the case of a parallelepiped of edges  $l_x, l_y$  and  $l_z$ , the electric polarizability tensor reads

$$\tilde{\alpha}_{0E} = l_x l_y l_z (\epsilon - \epsilon_h) ((\epsilon - \epsilon_h) + L^{-1} \epsilon_h)^{-1} L^{-1}, \quad (24)$$

where  $L = (L)_{ij}$ ,  $i, j = x, y, z$  is the depolarization tensor defined by

$$L_{ij} = \delta_{ij} \frac{2}{\pi} \arctan \left( \frac{l_x l_y l_z}{l_i^2 \sqrt{l_x^2 + l_y^2 + l_z^2}} \right). \quad (25)$$

Note that  $L_{xx} + L_{yy} + L_{zz} = 1$  and that for a cube  $L_{ii} = 1/3$ .

## 4.2 Radiative Correction

In general, the expressions for the polarizabilities are fulfilling the optical theorem (energy balance). To solve this, the radiative correction can be applied using

$$\alpha = \frac{k^3}{4\pi} \left( \tilde{\alpha}_0 - i \frac{k^3}{6\pi} \right)^{-1} \quad (26)$$

in the case of a scalar polarizability. If the polarizability is a tensor. We just multiply the second term of the parenthesis by the identity matrix. Note also that we are multiplying by  $k^3/4\pi$  in order to renormalize the polarizability and then get a dimensionless quantity.

## 4.3 Polarizability from Mie Coefficients

For a sphere, it is also possible to get the polarizability from its first Mie coefficients  $a_1$  and  $b_1$  (dipoles). We use

$$\alpha_E = i \frac{3}{2} a_1 \quad \alpha_M = i \frac{3}{2} b_1 \quad (27)$$

Note that it satisfy the optical theorem and that it is already dimensionless.

# 5 Input Fields

## 5.1 Plane Wave

A plane wave electromagnetic source with wavevector  $\mathbf{k}$  and electric field amplitude  $\mathbf{E}_0$  is given by

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_0 e^{i\mathbf{k} \cdot \mathbf{r}}, \quad \mathbf{H}(\mathbf{r}) = \mathbf{u}_k \times \mathbf{E}(\mathbf{r}). \quad (28)$$

## 5.2 Dipole Source

The field emitted at  $\mathbf{r}$  by an dipole source placed at  $\mathbf{r}_0$  is defined as

$$\Phi(\mathbf{r}) = \mathbb{G}(\mathbf{r}, \mathbf{r}_0) \begin{pmatrix} \mathbf{p} \\ \mathbf{m} \end{pmatrix}, \quad (29)$$

where  $(\mathbf{p}, \mathbf{m})^T$  is the dipole moment that characterized the dipole source.

### 5.3 Gaussian Beam

By using the angular spectrum representation of an electromagnetic (EM) field [Lukas Novotny, Bert Hecht, Principles of Nano-Optics], the field distributions of a Gaussian beam polarized electric (PE) and polarized along the  $x$ -axis that propagates along the  $z$ -axis can be written as

$$\mathbf{E}^{PE}(x, y, z) = \int \int_{k_x^2 + k_y^2 \leq k^2} \hat{E}_x^G(k_x, k_y; 0) \frac{1}{k_z} [k_z \hat{x} - k_x \hat{z}] e^{i(k_x x + k_y y + k_z z)} dk_x dk_y, \quad (30)$$

$$\mathbf{H}^{PE}(x, y, z) = \int \int_{k_x^2 + k_y^2 \leq k^2} \hat{E}_x^G(k_x, k_y; 0) \frac{1}{k k_z} [-k_x k_y \hat{x} + (k_x^2 + k_z^2) \hat{y} - k_y k_z \hat{z}] e^{i(k_x x + k_y y + k_z z)} dk_x dk_y, \quad (31)$$

being  $k_z = \sqrt{k^2 - k_x^2 - k_y^2}$  and  $\hat{E}_x^G(k_x, k_y; 0)$  is the Fourier transform of the  $x$ -component of the electric field at the object plane,  $E_x^G(x, y, 0)$ ,

$$\begin{aligned} \hat{E}_x^G(k_x, k_y; 0) &= \frac{1}{4\pi^2} \iint E_x^G(x, y, 0) e^{-i(k_x x + k_y y)} dx dy \\ &= E_0 \frac{\omega_0^2}{4\pi} e^{-(k_x^2 + k_y^2) \frac{w_0^2}{4}}, \end{aligned} \quad (32)$$

where  $\omega_0$  is the beam waist radius and

$$E_x^G(x, y, 0) = E_0 e^{-\frac{x^2 + y^2}{w_0^2}}. \quad (33)$$

Note that the integral in Eqs. 30 - 31 runs up to  $k$ , meaning that only the propagating waves are considered. Nonetheless, in practical situations the integral runs up to a  $k_{max} \leq k$  that will depend on the optical system.

Equations 30 - 31 are proportional to  $1/k_z$ . Therefore, the evaluation of the integral at  $k_x^2 + k_y^2 = k^2$  (the boundary between propagating and evanescent waves) diverges. In order to avoid this issue, we can do the next change of variable,

$$k_x = \sqrt{k^2 - Q^2} \cos \theta, \quad k_y = \sqrt{k^2 - Q^2} \sin \theta, \quad \rightarrow \quad k_z = Q. \quad (34)$$

By applying the change of variable to the propagating component of the field we get

$$\mathbf{E}^{PE}(x, y, z) = \int_0^k \int_0^{2\pi} E_0 \frac{\omega_0^2}{4\pi} e^{-(k^2 - Q^2) \frac{w_0^2}{4}} [Q \hat{x} - k_x \hat{z}] e^{i(k_x x + k_y y + Qz)} d\theta dQ, \quad (35)$$

where for simplicity  $k_x$  and  $k_y$  are written, but they should be expressed as a function of  $Q$  and  $\theta$ . Now, Eq. 37 can be numerically integrated. The magnetic field will follow a similar expression.

Also notice that the integral on  $\theta$  can be done analytically with the aid of the relationships

$$\begin{aligned} \int_0^{2\pi} \cos n\theta e^{iz \cos(\theta - \varphi)} d\theta &= 2\pi(i^n) J_n(z) \cos n\varphi, \\ \int_0^{2\pi} \sin n\theta e^{iz \cos(\theta - \varphi)} d\theta &= 2\pi(i^n) J_n(z) \sin n\varphi, \end{aligned} \quad (36)$$

and hence

$$\mathbf{E}^{PE}(x, y, z) = E_0 \frac{\omega_0^2}{2} \int_0^k e^{-k_{\parallel}^2 \frac{w_0^2}{4}} \left[ Q J_0(k_{\parallel} R) \hat{x} - i k_{\parallel}^2 J_1(k_{\parallel} R) \cos \varphi \hat{z} \right] e^{iQz} dQ, \quad (37)$$

with  $k_{\parallel} = \sqrt{k^2 - Q^2}$ ,  $R = \sqrt{x^2 + y^2}$ , and  $\varphi = \arctan y/x$ . Similarly, the magnetic field can be written as

$$\begin{aligned} \mathbf{H}^{PE}(x, y, z) = E_0 \frac{\omega_0^2}{2} \int_0^k e^{-k_{\parallel}^2 \frac{w_0^2}{4}} \frac{1}{k} \left\{ \frac{1}{2} k_{\parallel}^2 J_2(k_{\parallel} R) \sin 2\varphi \hat{x} \right. \\ \left. \left[ \left( \frac{1}{2} k_{\parallel}^2 + Q^2 \right) J_0(k_{\parallel} R) - \frac{1}{2} k_{\parallel}^2 J_2(k_{\parallel} R) \cos 2\varphi \right] \hat{y} \right. \\ \left. - i k_{\parallel} Q J_1(k_{\parallel} R) \sin \varphi \hat{z} \right\} e^{iQz} dQ. \end{aligned} \quad (38)$$

Finally, for polarized magnetic (PM) beams, the expressions are similar, where the exchange  $\mathbf{E} \rightarrow \mathbf{H}$  and  $\mathbf{H} \rightarrow -\mathbf{E}$  can be done. Also, for another polarization in the  $xy$ -plane, a rotation in this plane can be applied.

#### 5.4 Hermite-Gaussian Beam

The x-component of the field distribution at the focus of a PE Hermite-Gaussian beam of order  $n$  and  $m$  is given by

$$E_{nm,x}^H(x, y, 0) = E_0 e^{-\frac{x^2 + y^2}{w_0^2}} H_n \left( \sqrt{2} \frac{x}{w_0} \right) H_m \left( \sqrt{2} \frac{y}{w_0} \right), \quad (39)$$

where  $H_n(x)$  is the physicist's Hermite polynomials of order  $n$ .

The Fourier transform of this profile is

$$\hat{E}_{nm,x}^H(k_x, k_y; 0) = \hat{E}_x^G(x, y, 0) \left( -\sqrt{2}i \right)^{n+m} He_n(k_x \omega_0) He_m(k_y \omega_0), \quad (40)$$

being  $He_n(x)$  the probability's Hermite polynomials of order  $n$ . Thus, the field profile at any  $z$  can be calculated by means of the inverse Fourier transform using its angular spectrum representation

$$\hat{\mathbf{E}}_{nm}^H(k_x, k_y; 0) = \hat{\mathbf{E}}^G(k_x, k_y; 0) \hat{E}_{nm,x}^H(k_x, k_y; 0), \quad (41)$$

with

$$\hat{\mathbf{E}}^G(k_x, k_y; 0) = \hat{E}_x^G(k_x, k_y; 0) \frac{1}{k_z} [k_z \hat{x} - k_x \hat{z}]. \quad (42)$$

#### 5.5 Laguerre-Gaussian Beam

In a similar way, the x-component of the field distribution at the focus of a PE Laguerre-Gaussian beam of order  $n$  and  $m$  is given by

$$E_{nm,x}^L(x, y, 0) = E_0 e^{-\frac{\rho^2}{w_0^2}} \left( \sqrt{2} \frac{\rho}{w_0} \right)^m L_n^{(m)} \left( 2 \frac{\rho^2}{w_0^2} \right) e^{im\phi}, \quad (43)$$

where  $L_n^{(m)}(x)$  is the generalized Laguerre polynomials of order  $n$  and  $m$ , while  $\rho^2 = x^2 + y^2$  and  $\tan \phi = y/x$ .

The Fourier transform of the Laguerre-Gaussian beam profile is

$$\hat{E}_{nm,x}^L(k_{\parallel}, \theta; 0) = \hat{E}_x^G(k_{\parallel}, \theta; 0) i^m \frac{(-1)^{m+n}}{\sqrt{2}^m} k_{\parallel}^m w_0^m L_n^{(m)}\left(k_{\parallel}^2 \frac{w_0^2}{2}\right) e^{im\theta}, \quad (44)$$

with  $k_{\parallel}^2 = k_x^2 + k_y^2$  and  $\tan \theta = k_y/k_x$ . Thus, its angular spectrum representation is given by

$$\hat{\mathbf{E}}_{nm}^L(k_x, k_y; 0) = \hat{\mathbf{E}}^G(k_x, k_y; 0) \hat{E}_{nm,x}^L(k_x, k_y; 0). \quad (45)$$

## 5.6 Derivative of the fields

The spatial derivatives of the fields, as for the Green function, are defined adimensional. For example, the derivative of the electric field respect to the  $x$ -axis would be

$$\mathbf{E}'(\mathbf{r}) = \frac{\partial}{\partial(kx)} \mathbf{E}(\mathbf{r}). \quad (46)$$

Thus, the unit of the field and its derivatives are the same.

## 6 Extinction, Absorption and Scattering Cross Sections in a Plane Wave Field

Total cross sections are defined by a power normalized by the intensity of the input plane wave

$$\sigma = \frac{P}{I}. \quad (47)$$

The scattered, extinction and absorbed powers are given by

$$\begin{aligned} P_{scat} &= \int d\Omega \mathbf{S}_s \cdot \mathbf{u}_r = \frac{4\pi}{3Zk^2} \left[ \sum_i |\mathbf{p}_i|^2 + \sum_i |\mathbf{m}_i|^2 \right] \\ &+ \frac{4\pi}{Zk^2} \text{Re} \left\{ \sum_{i>j} \mathbf{p}_i^t \text{Im} \{ \mathbb{G}_E(\mathbf{r}_i, \mathbf{r}_j) \} \mathbf{p}_j^* + \mathbf{m}_i^t \text{Im} \{ \mathbb{G}_E(\mathbf{r}_i, \mathbf{r}_j) \} \mathbf{m}_j^* \right\} \\ &+ \frac{4\pi}{Zk^2} \sum_{i>j} \text{Im} \{ -\mathbf{p}_j^* \cdot \text{Im} \{ \mathbb{G}_m(\mathbf{r}_j, \mathbf{r}_i) \} \mathbf{m}_i + \mathbf{p}_i \cdot \text{Im} \{ \mathbb{G}_m(\mathbf{r}_j, \mathbf{r}_i) \} \mathbf{m}_j \} \\ P_{ext} &= \frac{2\pi}{Zk^2} \sum_i \text{Im} \{ \mathbf{p}_i \cdot \mathbf{E}_0^*(\mathbf{r}_i) + (\mathbf{m}_i \cdot \mathbf{H}_0^*(\mathbf{r}_i)) \} \\ P_{abs} &= \frac{2\pi}{Zk^2} \text{Im} \left\{ \mathbf{p}_i \cdot \left( \alpha_0^{(i)} \mathbf{p}_i \right)^* + \mathbf{m}_i \cdot \left( \alpha_0^{(i)} \mathbf{m}_i \right)^* \right\}. \end{aligned}$$

Then, the cross section is just obtained by normalizing the scattered power by the intensity of an input plane wave. For the emitted power, we just need to add the input field to the scattered

field. Here,  $\alpha_0$  is the polarizability at which the radiative correction have been removed. The, these powers can be renomalized by the plane wave intensity

$$I_0 = \frac{1}{2Z} |\mathbf{E}_0|^2 \quad (48)$$

in order to get the cross sections. For the only electric dipoles systems, we just need to set the magnetic polarizability equal to 0.

## 7 Differential Scattering Cross Section and Differential emitted Power

We compute the differential scattered power in the direction of  $\mathbf{R}$  (way bigger as the size of the system) as

$$\frac{dP}{d\Omega} = R^2 \mathbf{S}_s \cdot \mathbf{u}_R, \quad (49)$$

where the scattering pointing vector is

$$\mathbf{S}_s = \frac{1}{2Z} \text{Re} \{ \mathbf{E}_s \times \mathbf{H}_s^2 \} \quad (50)$$

and the scattered field is defined by equations (9) and (10), but taking the far field approximation of the green tensors:

$$\mathbb{G}_E(\mathbf{r}, \mathbf{r}_0) \simeq \frac{e^{ikr}}{kr} e^{-ik\mathbf{r}_0 \cdot \mathbf{u}_r} (\mathbb{I} - \mathbf{u}_r \mathbf{u}_r) \quad (51a)$$

$$\mathbb{G}_M(\mathbf{r}, \mathbf{r}_0) \simeq i \frac{e^{ikr}}{kr} e^{-ik\mathbf{r}_0 \cdot \mathbf{u}_r} \mathbf{u}_r \times . \quad (51b)$$

## 8 Local Density of States

The projected local density of states (LDOS) of a collection of dipoles at  $\mathbf{r}_0$ ,  $\text{LDOS}(\mathbf{r}_0)$ , can be calculated as the power emitted by a point dipole placed at  $\mathbf{r}_0$  normalized by the power emitted by the isolated dipole source (i.e., in absence of the collection of dipoles).

The power emitted by a point dipole of dipole moment,  $(\mathbf{p}, \mathbf{m})^T$ , is

$$\frac{dW}{dt} = \frac{\omega}{2} \Im [(\mathbf{p}, \mathbf{m})^\dagger \cdot \Phi(\mathbf{r}_0)], \quad (52)$$

where  $\Phi(\mathbf{r}_0)$  is the field at the position of the dipole. If the dipole source is placed in an electromagnetic environment defined by the collection of dipoles, the total field,  $\Phi(\mathbf{r})$ , emitted by the system would be equal to

$$\Phi(\mathbf{r}) = \mathbb{G}(\mathbf{r}, \mathbf{r}_0) \begin{pmatrix} \mathbf{p} \\ \mathbf{m} \end{pmatrix} + \overleftrightarrow{\mathbb{G}}_l(\mathbf{r}) \overleftrightarrow{\alpha} \overleftrightarrow{\Phi}_i, \quad (53)$$



where  $\overleftrightarrow{\mathbb{G}}_l(\mathbf{r}) = (\mathbb{G}(\mathbf{r}, \mathbf{r}_j)_{ij})$  is a  $6 \times 6N$  complex matrix that contains the field propagators from the collection of dipoles (placed at  $\mathbf{r}_j$ ) to the observational point  $(\mathbf{r})$ , and  $\overleftrightarrow{\Phi}_i$  is the total incident field on the collection of dipoles, defined by self-scattering problem (Eq. 20)

$$\overleftrightarrow{\Phi}_i = \mathbb{A}^{-1} \overleftrightarrow{\Phi}_0, \quad (54)$$

being  $\overleftrightarrow{\Phi}_0$  the external incident field. Since  $\overleftrightarrow{\Phi}_0$  is given by the own dipole source,

$$\begin{aligned} \Phi_0(\mathbf{r}_j) &= \mathbb{G}(\mathbf{r}_j, \mathbf{r}_0) \begin{pmatrix} \mathbf{p} \\ \mathbf{m} \end{pmatrix}, \\ \rightarrow \overleftrightarrow{\Phi}_0 &= \overleftrightarrow{\mathbb{G}}_r(\mathbf{r}_0) \begin{pmatrix} \mathbf{p} \\ \mathbf{m} \end{pmatrix}, \end{aligned} \quad (55)$$

with  $\overleftrightarrow{\mathbb{G}}_r(\mathbf{r}_0) = (\mathbb{G}(\mathbf{r}_j, \mathbf{r}_0)_{ij})$  a  $6N \times 6$  complex matrix that contains the field propagators from the dipole source to the collection of dipoles, the total field can be written as

$$\Phi(\mathbf{r}) = \mathbb{G}(\mathbf{r}, \mathbf{r}_0) \begin{pmatrix} \mathbf{p} \\ \mathbf{m} \end{pmatrix} + \overleftrightarrow{\mathbb{G}}_l(\mathbf{r}_0) \overleftrightarrow{\alpha} \mathbb{A}^{-1} \overleftrightarrow{\mathbb{G}}_r(\mathbf{r}_0) \begin{pmatrix} \mathbf{p} \\ \mathbf{m} \end{pmatrix}, \quad (56)$$

and the projected LDOS can be finally expressed as

$$\text{pLDOS}(\mathbf{r}_0) = 1 + \frac{1}{|(\mathbf{p}, \mathbf{m})|^2} \frac{3}{2} \Im \left[ \begin{pmatrix} \mathbf{p} \\ \mathbf{m} \end{pmatrix}^\dagger \cdot \overleftrightarrow{\mathbb{G}}_l(\mathbf{r}_0) \overleftrightarrow{\alpha} \mathbb{A}^{-1} \overleftrightarrow{\mathbb{G}}_r(\mathbf{r}_0) \begin{pmatrix} \mathbf{p} \\ \mathbf{m} \end{pmatrix} \right]. \quad (57)$$

Note that

$$\frac{1}{|(\mathbf{p}, \mathbf{m})|^2} \Im \left[ \begin{pmatrix} \mathbf{p} \\ \mathbf{m} \end{pmatrix}^\dagger \cdot \overleftrightarrow{\mathbb{G}}_l(\mathbf{r}_0) \overleftrightarrow{\alpha} \mathbb{A}^{-1} \overleftrightarrow{\mathbb{G}}_r(\mathbf{r}_0) \begin{pmatrix} \mathbf{p} \\ \mathbf{m} \end{pmatrix} \right] = \frac{2}{3}, \quad (58)$$

for any  $(\mathbf{p}, \mathbf{m})$ .

Finally, the LDOS would be

$$\text{LDOS}(\mathbf{r}_0) = 1 + \frac{1}{2} \text{Tr} \Im \left[ \overleftrightarrow{\mathbb{G}}_l(\mathbf{r}_0) \overleftrightarrow{\alpha} \mathbb{A}^{-1} \overleftrightarrow{\mathbb{G}}_r(\mathbf{r}_0) \right], \quad (59)$$

where the trace must be done in the electric (or magnetic part). The software also provides functions to compute the normalized radiative and non-radiative local density of states. These are computed using

$$\text{LDOS}_R = \frac{3Zk^2}{4\pi} \frac{P_{sca}}{|p_0|^2 + |m_0|^2} \quad (60)$$

and

$$\text{LDOS}_{NR} = \frac{3Zk^2}{4\pi} \frac{P_{abs}}{|p_0|^2 + |m_0|^2}. \quad (61)$$

With this the energy balance is fulfilled, i.e.

$$\text{LDOS} = \text{LDOS}_R + \text{LDOS}_{NR}. \quad (62)$$

## 9 Optical Forces

The optical force (as implemented in the library) on the particle  $i$  along the  $\beta$ -axis (defined by the unit vector  $\hat{\mathbf{u}}_\beta$ ),  $F_\beta^{(i)} = \mathbf{F}^{(i)} \cdot \hat{\mathbf{u}}_\beta$ , can be written as

$$F_\beta^{(i)} = \frac{1}{2} \Re \left[ \left\langle \alpha_E^{(i)} \mathbf{E}_i(\mathbf{r}_i) \cdot \mathbf{E}_i'^*(\mathbf{r}_i) + \alpha_M^{(i)} \mathbf{H}_i(\mathbf{r}_i) \cdot \mathbf{H}_i'^*(\mathbf{r}_i) - \frac{2}{3} \left( \alpha_E^{(i)} \mathbf{E}_i(\mathbf{r}_i) \right) \times \left( \alpha_M^{(i)} \mathbf{H}_i(\mathbf{r}_i) \right)^* \cdot \hat{\mathbf{u}}_\beta \right\rangle \right] \quad (63)$$

where  $'$  denotes the derivative with respect to  $\beta$ .

Since the unit of this force is  $[F_\beta^{(i)}] = [E]^2$  (remember that the derivative of the field is adimensional), in order to get the forces in Newton, Eq. 63 must be multiplied by  $1/k$  (for the adimensional derivative), by  $4\pi/k^3$  (for the renormalization of the polarizability) and by  $\epsilon_0\epsilon_h$  (for the definition of the force), where all values must be expressed in SI base units. Hence, it is necessary a total factor  $\epsilon_0\epsilon_h 4\pi/k^2$  and then, if  $\tilde{F}_\beta^{(i)}$  is the force in unit of force (forgive the redundancy), we have

$$\tilde{F}_\beta^{(i)} = \epsilon_0\epsilon_h \frac{4\pi}{k^2} F_\beta^{(i)}. \quad (64)$$

Coming back to our issue, expressing the total incident field as in Eq. 15 and vectorizing the notation, the force can be expressed as the trace of a tensor

$$F_\beta = \frac{1}{2} \Re \text{Tr} \left[ \left\langle \overleftrightarrow{\alpha} \overleftrightarrow{\Phi} \overleftrightarrow{\Phi}^\dagger + \frac{2}{3} \left( \overleftrightarrow{\alpha} \overleftrightarrow{\Phi} \right) \left( \overleftrightarrow{\alpha} \overleftrightarrow{\Phi} \right)^\dagger \overleftrightarrow{\varepsilon}_\beta \right\rangle \right], \quad (65)$$

and the force at an individual particle would be equal to a partial trace of the matrix. In the previous expression,  $\overleftrightarrow{\varepsilon}_\beta$  is a 6Nx6N tensor representing the projection of the cross product along the  $\beta$ -axis (its matrix elements are related to the Levy-Civita tensor).

Finally, using Eq. 20 the force can be written as a function of the external incident field

$$F_\beta = \frac{1}{2} \Re \text{Tr} \left[ \left\langle \overleftrightarrow{\alpha} \mathbb{A}^{-1} \left( \overleftrightarrow{\Phi}_0 \overleftrightarrow{\Phi}_0^\dagger + \overleftrightarrow{\Phi}_0 \overleftrightarrow{\Phi}_0^{\dagger'} \left( \overleftrightarrow{\alpha} \mathbb{A}^{-1} \right)^\dagger + \frac{2}{3} \overleftrightarrow{\Phi}_0 \overleftrightarrow{\Phi}_0^\dagger \left( \overleftrightarrow{\alpha} \mathbb{A}^{-1} \right)^\dagger \overleftrightarrow{\varepsilon}_\beta \right) \right\rangle \right]. \quad (66)$$