Supplementary Informations for "CoupledElectricMagneticDipoles.jl - Julia modules for coupled electric and magnetic dipoles method for light scattering, and optical forces in three dimensions"

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

1 Induced Electric and Magnetic Dipoles

A similar derivation of the method can be found in [1]. We consider dipole electric and magnetic particles. For a particle placed at $\mathbf{r}_0$ the induced electric and magnetic dipoles are

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

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

Where $\mathbf{E}_i \left(\mathbf{r}_0\right)$ and $\tilde{\mathbf{H}}_i \left(\mathbf{r}_0\right)$ 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

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

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

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

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

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

Where $r \equiv |\mathbf{r} - \mathbf{r}_0|$, $\mathbf{u}_r \equiv \left(\mathbf{r} - \mathbf{r}_0\right)/r$ and

$$\mathbf{u}_r \times \equiv \begin{pmatrix} 0 & -u_{rz} & u_{ry} \\ u_{rz} & 0 & -u_{rx} \\ -u_{ry} & u_{rx} & 0 \end{pmatrix}. \tag{4}$$

Then, the electromagnetic that is scattered by a particle located at $\mathbf{r}_0$ in an incident field $\mathbf{E_i}$ is given by

$$\mathbf{E}_s(\mathbf{r}) = k^2 \tilde{G}_E(\mathbf{r}, \mathbf{r}_0) \tilde{\alpha}_E \mathbf{E}_i(\mathbf{r}_0) + iZk\tilde{G}_M(\mathbf{r}, \mathbf{r}_0) \tilde{\alpha}_M \tilde{\mathbf{H}}_i(\mathbf{r}_0), \tag{5a}$$

$$\tilde{\mathbf{H}}_s(\mathbf{r}) = \frac{-i}{Z} k\tilde{G}_M(\mathbf{r}, \mathbf{r}_0) \tilde{\alpha}_E \mathbf{E}_i(\mathbf{r}_0) + k^2 \tilde{G}_E(\mathbf{r}, \mathbf{r}_0) \tilde{\alpha}_M \tilde{\mathbf{H}}_i(\mathbf{r}_0). \tag{5b}$$

2 Units and Renormalization of Variables

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

$$G_E(\mathbf{r}, \mathbf{r}_0) = \frac{e^{ikr}}{kr} \left\{ \frac{(kr)^2 + ikr - 1}{(kr)^2} \mathbb{I} + \frac{-(kr)^2 - 3ikr + 3}{(kr)^2} \mathbf{u}_r \otimes \mathbf{u}_r \right\} = \frac{4\pi}{k} \tilde{G}_E(\mathbf{r}, \mathbf{r}_0), \tag{6a}$$

$$G_M(\mathbf{r}, \mathbf{r}_0) = \frac{e^{ikr}}{kr} \left(\frac{ikr - 1}{kr} \right) \mathbf{u}_r \times = \frac{4\pi}{k^2} \tilde{G}_M(\mathbf{r}, \mathbf{r}_0). \tag{6b}$$

The advantage of this redefinition is that we can now compute the Green tensors using the dimensionless positions $k\mathbf{r}$ and $k\mathbf{r}_0$. We also redefine the polarizabilities to be dimensionless by multiplying it by $k^3/4\pi$, we have

$$\alpha_E = \frac{k^3 \tilde{\alpha}_E}{4\pi}, \tag{7a}$$

$$\alpha_M = \frac{k^3 \tilde{\alpha}_M}{4\pi}. \tag{7b}$$

Finally, we renormalize the magnetic field as

$$\mathbf{H} = Z\tilde{\mathbf{H}}. \tag{8}$$

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

$$\mathbf{E}_s(\mathbf{r}) = G_E(\mathbf{r}, \mathbf{r}_0) \alpha_E \mathbf{E}_i(\mathbf{r}_0) + iG_M(\mathbf{r}, \mathbf{r}_0) \alpha_M \mathbf{H}_i(\mathbf{r}_0), \tag{9a}$$

$$\mathbf{H}_s(\mathbf{r}) = -iG_M(\mathbf{r}, \mathbf{r}_0) \alpha_E \mathbf{E}_i(\mathbf{r}_0) + G_E(\mathbf{r}, \mathbf{r}_0) \alpha_M \mathbf{H}_i(\mathbf{r}_0). \tag{9b}$$

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

$$\mathbf{p} = \frac{k^3 \tilde{\mathbf{p}}}{4\pi\epsilon_0}, \tag{10a}$$

$$\mathbf{m} = \frac{k^3 \tilde{\mathbf{m}}}{4\pi\epsilon_0}. \tag{10b}$$

3 Coupled Electric and Magnetic Dipoles (CEMD) Method

Let us now consider a collection of N electric and magnetic dipoles at positions $\mathbf{r}_i$, $i = 1, ..., N$ 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

$$\mathbf{E}_i = \mathbf{E}_0\left(\mathbf{r}_i\right) + \sum_{j\neq i} G_E\left(\mathbf{r}_i, \mathbf{r}_j\right)\alpha_E^{(j)}\mathbf{E}_j + iG_M\left(\mathbf{r}_i, \mathbf{r}_j\right)\alpha_M^{(j)}\mathbf{H}_j, \tag{11a}$$

$$\mathbf{H}_i = \mathbf{H}_0\left(\mathbf{r}_i\right) + \sum_{j\neq i} -iG_M\left(\mathbf{r}_i, \mathbf{r}_j\right)\alpha_E^{(j)}\mathbf{E}_j + G_E\left(\mathbf{r}_i, \mathbf{r}_j\right)\alpha_M^{(j)}\mathbf{H}_j. \tag{11b}$$

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

$$\mathbf{\Phi}\left(\mathbf{r}\right) \equiv \left(\mathbf{E}\left(\mathbf{r}\right), \mathbf{H}\left(\mathbf{r}\right)\right)^T \tag{12}$$

the electromagnetic field (6 components complex vector) and

$$G\left(\mathbf{r}, \mathbf{r}_0\right) \equiv \begin{pmatrix} G_E\left(\mathbf{r}, \mathbf{r}_0\right) & iG_M\left(\mathbf{r}, \mathbf{r}_0\right) \\ -iG_M\left(\mathbf{r}, \mathbf{r}_0\right) & G_E\left(\mathbf{r}, \mathbf{r}_0\right) \end{pmatrix} \tag{13}$$

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

$$\alpha \equiv \begin{pmatrix} \alpha_E & 0 \\ 0 & \alpha_M \end{pmatrix} \quad \text{or} \quad \alpha \equiv \begin{pmatrix} \alpha_E \mathbb{I}_3 & 0 \\ 0 & \alpha_M \mathbb{I}_3 \end{pmatrix}, \tag{14}$$

depending if it's a scalar or a 3x3 tensor. With these changes in the notation, we can rewrite equation (11) as

$$\mathbf{\Phi}_i = \mathbf{\Phi}_0\left(\mathbf{r}_i\right) + \sum_{i\neq j}^{N} G\left(\mathbf{r_i}, \mathbf{r}_j\right)\alpha\mathbf{\Phi}_j. \tag{15}$$

This system of equations can be even more reduced by vectorizing it. For this, we define

$$\mathbf{\Phi}\left(\boldsymbol{r}\right) \equiv \begin{pmatrix} \boldsymbol{E}\left(\boldsymbol{r}\right) \\ \boldsymbol{H}\left(\boldsymbol{r}\right) \end{pmatrix} \tag{16}$$

and

$$\vec{\mathbf{\Phi}} \equiv \begin{pmatrix} \mathbf{\Phi}_1 \\ \vdots \\ \mathbf{\Phi}_N \end{pmatrix} = \begin{pmatrix} \mathbf{\Phi}_{ind}\left(\boldsymbol{r}_1\right) \\ \vdots \\ \mathbf{\Phi}_{ind}\left(\boldsymbol{r}_N\right) \end{pmatrix} \tag{17}$$

that are 6N dimensional complex vectors as well as $\mathbb{G} = (G(\mathbf{r}_i, \mathbf{r}_j))$ and $\overleftrightarrow{\alpha} = \left(\delta_{ij}\alpha^{(i)}\right)\ i, j = 1, ..., N$, two 6Nx6N complex matrix. With this, we obtain:

$$\vec{\mathbf{\Phi}}_0 = \left[\mathbb{I}_{6N} - \mathbb{G}\overleftrightarrow{\alpha}\right]\vec{\mathbf{\Phi}} \equiv \mathbb{A}\vec{\mathbf{\Phi}}. \tag{18}$$

Solving the CEMD (DDA) problem ammounts to invert the $\mathbb{A}$ matrix, so

$$\vec{\mathbf{\Phi}} = \mathbb{A}^{-1}\vec{\mathbf{\Phi}}_0. \tag{19}$$

3.1 Reduction to Only Electric Coupled Dipoles

When the magnetic polarizability is zero, the magnetic dipoles are zero and only the DDA problem remains to be solved. Equations (11a) and (11b) reduce to

$$\mathbf{E}_i = \mathbf{E}_0\left(\mathbf{r}_i\right) + \sum_{j\neq i} G_E\left(\mathbf{r}_i, \mathbf{r}_j\right)\alpha_E^{(j)}\mathbf{E}_j. \tag{20}$$

4 Polarizabilities

4.1 Clausisus-Mossotti Polarizabilities

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

$$\tilde{\alpha}_{0E} = 3V\left(\epsilon - \epsilon_h\right)\left(\epsilon + 2\epsilon_h\right)^{-1}. \tag{21}$$

Where V is the volume of the sphere, ϵ is the dielectric constant of the medium, and ϵ_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

$$\tilde{\alpha}_{0E} = 4\pi a^3\left(\epsilon - \epsilon_h\right)\left(\epsilon + 2\epsilon_h\right)^{-1}. \tag{22}$$

In a similar way, the expression of the quasistatic polarizability of a cube of side L reads

$$\tilde{\alpha}_{0E} = 3L^3\left(\epsilon - \epsilon_h\right)\left(\epsilon + 2\epsilon_h\right)^{-1}. \tag{23}$$

4.2 Radiative Correction

In general, the expressions for the polarizabilities are not fulfilling the optical theorem (energy balance). To solve this, the radiative correction can be applied using [2]

$$\alpha = \frac{k^3}{4\pi}\left(\tilde{\alpha}_0^{-1} - i\frac{k^3}{6\pi}\right)^{-1} \tag{24}$$

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, as done in [2]. 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

$$\alpha_E = i\frac{3}{2}a_1 \quad \alpha_M = i\frac{3}{2}b_1 \tag{25}$$

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

5 Input Fields

5.1 Plane Wave

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

$$\mathbf{E}\left(\mathbf{r}\right) = \mathbf{E}_0 e^{i\mathbf{k}\cdot\mathbf{r}}, \quad \mathbf{H}\left(\mathbf{r}\right) = \mathbf{u}_k \times \mathbf{E}\left(\mathbf{r}\right). \tag{26}$$

5.2 Dipole Source

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

$$\mathbf{\Phi}(\mathbf{r}) = G(\mathbf{r}, \mathbf{r}_0) \begin{pmatrix} \mathbf{p} \\ \mathbf{m} \end{pmatrix}, \tag{27}$$

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

5.3 Gaussian Beams

The Gaussian beams are defined as polarized electric along the x-axis, that propagate along the z-axis. They are implemented using its angular spectrum representation [3], calculated assuming that at the focal plane, the x-component of the fields follow the well-known expressions, i.e.,

$$\mathbf{E}^G(x, y, z=0) \cdot \hat{\mathbf{x}} = E_0 e^{-\frac{x^2+y^2}{w_0^2}}, \tag{28a}$$

$$\mathbf{E}^H_{n,m}(x, y, z=0) \cdot \hat{\mathbf{x}} = H_n\left(\sqrt{2}\frac{x}{w_0}\right) H_m\left(\sqrt{2}\frac{y}{w_0}\right) \mathbf{E}^G(x, y, z=0) \cdot \hat{\mathbf{x}}, \tag{28b}$$

$$\mathbf{E}^L_{n,m}(x, y, z=0) \cdot \hat{\mathbf{x}} = \left(\sqrt{2}\frac{\sqrt{x^2+y^2}}{w_0}\right)^m L_n^m\left(2\frac{x^2+y^2}{w_0^2}\right) \mathbf{E}^G(x, y, z=0) \cdot \hat{\mathbf{x}}. \tag{28c}$$

$\mathbf{E}^G$ is the field distribution of a Gaussian beam, and $\mathbf{E}^H_{n,m}$, $\mathbf{E}^L_{n,m}$ are the field distributions of the Hermite-Gaussian and Laguerre-Gaussian beam of order n, m, respectively. Also, E_0 is the constant field, w_0 the beam waist, $H_n(x)$ the Hermite polynomial of order n, and L_n^m the associated Laguerre polynomial of order n, m.

Explicitly, the angular spectrum representation of the Gaussian beams, $\widetilde{\mathbf{E}}^B(k_x, k_y; z=0)$ (with $B = G, H, L$), is analytically calculated from

$$\widetilde{\mathbf{E}}^B(k_x, k_y; z=0) = \frac{1}{4\pi^2} \int\int_{-\infty}^{\infty} \mathbf{E}^B(x', y', z'=0) e^{-i\left(k_x x' + k_y y'\right)} \mathrm{d}x' \mathrm{d}y', \tag{29}$$

and the field at any position is then numerically calculated from the angular spectrum representation as

$$\mathbf{E}^B(x, y, z) = \int\int_{k_x^2+k_y^2<k^2} \widetilde{\mathbf{E}}^B(k_x, k_y; z=0) e^{i(k_x x + k_y y + k_z z)} \mathrm{d}k_x \mathrm{d}k_y, \tag{30}$$

with $k_z = \sqrt{k^2 - k_x^2 - k_y^2}$. Note that, for physical reasons, the integral runs for propagating waves ($k_x^2 + k_y^2 < k^2$). Thus, the field distribution at the focal plane does not have to be exactly the same as Eq. 28a- 28c.

The x-component of the field is calculated from Eq. 28a- 28c, while the other field components are obtained by requiring that the the angular spectrum representation is divergence-free, i. e.,

$$\widetilde{\mathbf{E}}^B(k_x, k_y; z=0) \cdot \hat{\mathbf{z}} = -\frac{k_x}{k_z} \widetilde{\mathbf{E}}^B(k_x, k_y; z=0) \cdot \hat{\mathbf{x}}. \tag{31}$$

Similarly, the magnetic field is calculated as

$$\widetilde{\mathbf{H}}^B(k_x, k_y; z=0) \cdot \hat{\mathbf{x}} = -\frac{k_x k_y}{k k_z} \widetilde{\mathbf{E}}^B(k_x, k_y; z=0) \cdot \hat{\mathbf{x}}. \tag{32a}$$

$$\widetilde{\mathbf{H}}^B(k_x, k_y; z=0)\cdot\hat{\mathbf{y}} = \frac{kx^2 + kz^2}{kk_z}\widetilde{\mathbf{E}}^B(k_x, k_y; z=0)\cdot\hat{\mathbf{x}}. \tag{32b}$$

$$\widetilde{\mathbf{H}}^B(k_x, k_y; z=0)\cdot\hat{\mathbf{z}} = -\frac{ky}{k}\widetilde{\mathbf{E}}^B(k_x, k_y; z=0)\cdot\hat{\mathbf{x}}. \tag{32c}$$

For another kind of polarization, a rotation of the field in the xy plane can be done. For polarized magnetic Gaussian beams, it is possible to swap the electric and magnetic field as $\mathbf{E}\to\mathbf{H}$, $\mathbf{H}\to-\mathbf{E}$.

As details for the implementation, the evaluation of the integral for $k_x^2+k_y^2<k^2$ (for propagating waves) is done by using the next change of variable,

$$k_x = \sqrt{k^2-Q^2}\cos\theta, \qquad k_y = \sqrt{k^2-Q^2}\sin\theta, \qquad \to \qquad k_z = Q. \tag{33}$$

where the integral runs for $\theta = [0, 2\pi]$, $Q = [0, k]$.

Additionally, for the Gaussian beam of order $n = m = 0$ the integral on θ is done analytically with the aid of the relationships

$$\begin{aligned}\int_0^{2\pi} \cos n\theta e^{iz\cos(\theta-\varphi)}\mathrm{d}\theta &= 2\pi(i^n)J_n(z)\cos n\varphi,\\ \int_0^{2\pi} \sin n\theta e^{iz\cos(\theta-\varphi)}\mathrm{d}\theta &= 2\pi(i^n)J_n(z)\sin n\varphi.\end{aligned} \tag{34}$$

For the shake of completeness, the angular spectrum representation of the Gaussian Beams are given:

$$\widetilde{\mathbf{E}}^G(k_x, k_y; z=0)\cdot\hat{\mathbf{x}} = E_0\frac{w_0^2}{4\pi}e^{-\left(k_x^2+k_y^2\right)\frac{w_0^2}{4}}, \tag{35a}$$

$$\widetilde{\mathbf{E}}^H_{n,m}(k_x, k_y; z=0)\cdot\hat{\mathbf{x}} = \left(-\sqrt{2}i\right)^{n+m} He_n\left(k_x w_0\right) He_m\left(k_y w_0\right)\widetilde{\mathbf{E}}^G(k_x, k_y; z=0)\cdot\hat{\mathbf{x}}, \tag{35b}$$

$$\widetilde{\mathbf{E}}^L_{n,m}(k_\parallel, \theta; z=0)\cdot\hat{\mathbf{x}} = i^m\frac{(-1)^{m+n}}{\sqrt{2}^m}k_\parallel^m w_0^m L_n^{(m)}\left(k_\parallel^2\frac{w_0^2}{2}\right)e^{im\theta}\widetilde{\mathbf{E}}^G(k_x, k_y; z=0)\cdot\hat{\mathbf{x}}, \tag{35c}$$

where $He_n\left(x\right)$ is the probability's Hermite polynomial of order n, and we have defined $k_\parallel^2 = k_x^2 + k_y^2$ and $\theta = \arctan\left(k_y/k_x\right)$.

Finally, assuming the paraxial approximation, we can describe the electric field of the Gaussian beams simply by its x-component. Thus, the intensity of the beam at the focal plane will be given by

$$I^B = \frac{1}{2Z}|E_x^B|^2, \tag{36}$$

where $E_x^B = \widetilde{\mathbf{E}}^B(k_x, k_y; z=0)\cdot\hat{\mathbf{x}}$ is the x-component of the field at the focal plane.

The power of the beam, P^B, can be calculated as the integral of the intensity in the focal plane, leading to

$$P^G = \int I^G\mathrm{dA} = \frac{1}{2Z}E_0^2\pi\frac{w_0^2}{2}, \tag{37}$$

$$P^H = \int I^H\mathrm{dA} = \frac{1}{2Z}E_0^2\pi\frac{w_0^2}{2}2^{n+m}n!m!, \tag{38}$$

$$P^L = \int I^L\mathrm{dA} = \frac{1}{2Z}E_0^2\pi\frac{w_0^2}{2}\frac{(n+m)!}{n!}, \tag{39}$$

relating the power of the beam with the field constant E_0. If the paraxial approximation cannot be assumed, the vectorial character of the field must be considered.

5.4 Derivative of the fields

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

$$\mathbf{E}'(\mathbf{r}) = \frac{\partial}{\partial\,(kx)}\mathbf{E}(\mathbf{r}). \tag{40}$$

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

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

The scattered, extincted and absorbed powers by a set of electric and magnetic dipoles under any arbitrary input field are given by [1]

$$\begin{aligned} P_{scat} = \int d\Omega\, \mathbf{S}_s \cdot \mathbf{u}_r = \frac{4\pi}{3Zk^2}\left[\sum_i |\mathbf{p}_i|^2 + \sum_i |\mathbf{m}_i|^2\right] \\ + \frac{4\pi}{Zk^2}\mathrm{Re}\left\{\sum_{i>j} \mathbf{p}_i^* \cdot \mathrm{Im}\left\{G_E\left(\mathbf{r}_i, \mathbf{r}_j\right)\right\}\mathbf{p}_j + \mathbf{m}_i^* \cdot \mathrm{Im}\left\{G_E\left(\mathbf{r}_i, \mathbf{r}_j\right)\right\}\mathbf{m}_j\right\} \\ + \frac{4\pi}{Zk^2}\mathrm{Im}\left\{\sum_{i>j} -\mathbf{p}_j^* \cdot \mathrm{Im}\left\{G_M\left(\mathbf{r}_j, \mathbf{r}_i\right)\right\}\mathbf{m}_i + \mathbf{p}^* \cdot \mathrm{Im}\left\{G_M\left(\mathbf{r}_j, \mathbf{r}_i\right)\right\}\mathbf{m}_j\right\} \end{aligned} \tag{41a}$$

$$P_{ext} = \frac{2\pi}{Zk^2}\sum_i \mathrm{Im}\left\{\mathbf{p}_i \cdot \mathbf{E}_0^*\left(\mathbf{r}_i\right) + \left(\mathbf{m}_i \cdot \mathbf{H}_0^*\left(\mathbf{r}_i\right)\right)\right\} \tag{41b}$$

$$P_{abs} = \frac{2\pi}{Zk^2}\sum_i \left(\mathrm{Im}\left\{\mathbf{E}_i \cdot \mathbf{p}_i\right\} - \frac{2}{3}\left|\mathbf{p}_i\right|^2 + \mathrm{Im}\left\{\mathbf{H}_i \cdot \mathbf{m}_i\right\} - \frac{2}{3}\left|\mathbf{m}_i\right|^2\right). \tag{41c}$$

On the other hand, total cross sections are defined by a power normalized by the intensity of the input plane wave

$$\sigma = \frac{P}{I}. \tag{42}$$

Then, the cross section is just obtained by normalizing the scattered power by the intensity of an input plane wave. Then, these powers can be renomalized by the plane wave intensity

$$I_0 = \frac{1}{2Z}|\mathbf{E}_0|^2 \tag{43}$$

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 Emission Pattern

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

$$\frac{\mathrm{d}P}{\mathrm{d}\Omega} = R^2 \mathbf{S}_s \cdot \mathbf{u}_R, \tag{44}$$

where the scattering pointing vector is

$$\mathbf{S}_s = \frac{1}{2Z} \operatorname{Re}\{\mathbf{E}_s \times \mathbf{H}_s\} \tag{45}$$

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

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

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

For the emission pattern, the functions in the software are outputting the emitted power normalized by the total radiated power of the dipole emitter ($\mathbf{p}_0$, $\mathbf{m}_0$ or both) defined as

$$P_0 \equiv \frac{k^4 c}{12\pi\epsilon_0} \left(|\tilde{\mathbf{p}_0}|^2 + |\tilde{\mathbf{m}_0}|^2 \right) = \frac{4\pi Z}{3k^2} \left(|\mathbf{p}_0|^2 + |\mathbf{m}_0|^2 \right) \tag{47}$$

8 Local Density of States

The normalized projected local density of states (LDOS) of a collection of dipoles at $\mathbf{r}_0$, 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

$$\frac{\mathrm{d}W}{\mathrm{d}t} = \frac{\omega}{2} \operatorname{Im}\left[(\mathbf{p}, \mathbf{m})^\dagger \cdot \mathbf{\Phi}(\mathbf{r}_0) \right], \tag{48}$$

where $\mathbf{\Phi}(\mathbf{r}_0)$ 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, $\mathbf{\Phi}(\mathbf{r})$, emitted by the system would be equal to

$$\mathbf{\Phi}(\mathbf{r}) = G(\mathbf{r}, \mathbf{r}_0) \begin{pmatrix} \mathbf{p} \\ \mathbf{m} \end{pmatrix} + \mathbb{G}_l(\mathbf{r}) \overleftrightarrow{\alpha} \vec{\mathbf{\Phi}}, \tag{49}$$

where $\mathbb{G}_l(\mathbf{r}) = (G(\mathbf{r}, \mathbf{r}_j))$ is a 6x6N complex matrix that contains the field propagators from the collection of dipoles (placed at $\mathbf{r}_j$) to the observational point ($\mathbf{r}$), and $\vec{\mathbf{\Phi}}$ is the total incident field on the collection of dipoles, defined by self-scattering problem (Eq. 20)

$$\vec{\mathbf{\Phi}} = \mathbb{A}^{-1} \vec{\mathbf{\Phi}}_0, \tag{50}$$

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

$$\mathbf{\Phi}_0(\mathbf{r_j}) = G(\mathbf{r}_j, \mathbf{r}_0) \begin{pmatrix} \mathbf{p} \\ \mathbf{m} \end{pmatrix}, \text{hence,}$$

$$\vec{\mathbf{\Phi}}_0 = \mathbb{G}_r(\mathbf{r}_0) \begin{pmatrix} \mathbf{p} \\ \mathbf{m} \end{pmatrix}, \tag{51}$$

with $\mathbb{G}_r(\mathbf{r}_0) = (G(\mathbf{r}_j, \mathbf{r}_0)_{ij})$ a 6Nx6 complex matrix that contains the field propagators from the dipole source to the collection of dipoles, the total field can be written as

$$\mathbf{\Phi}(\mathbf{r}) = G(\mathbf{r}, \mathbf{r}_0) \begin{pmatrix} \mathbf{p} \\ \mathbf{m} \end{pmatrix} + \mathbb{G}_l(\mathbf{r}) \overleftrightarrow{\alpha} \mathbb{A}^{-1} \mathbb{G}_r(\mathbf{r}_0) \begin{pmatrix} \mathbf{p} \\ \mathbf{m} \end{pmatrix}, \tag{52}$$

and the projected LDOS can be finally expressed as

$$\mathrm{pLDOS}(\mathbf{r}_0) = 1 + \frac{1}{|(\mathbf{p}, \mathbf{m})|^2} \frac{3}{2} \mathrm{Im} \left[\begin{pmatrix} \mathbf{p} \\ \mathbf{m} \end{pmatrix}^\dagger \cdot \mathbb{G}_l(\mathbf{r}_0) \overleftrightarrow{\alpha} \mathbb{A}^{-1} \mathbb{G}_r(\mathbf{r}_0) \begin{pmatrix} \mathbf{p} \\ \mathbf{m} \end{pmatrix} \right]. \tag{53}$$

Note that

$$\frac{1}{|(\mathbf{p}, \mathbf{m})|^2} \mathrm{Im} \left[\begin{pmatrix} \mathbf{p} \\ \mathbf{m} \end{pmatrix}^\dagger \cdot G(\mathbf{r}_0, \mathbf{r}_0) \begin{pmatrix} \mathbf{p} \\ \mathbf{m} \end{pmatrix} \right] = \frac{2}{3}, \tag{54}$$

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

Finally, the LDOS would be

$$\mathrm{LDOS}(\mathbf{r}_0) = 1 + \frac{1}{2} \mathrm{Tr} \left(\mathrm{Im} \left[\mathbb{G}_l(\mathbf{r}_0) \overleftrightarrow{\alpha} \mathbb{A}^{-1} \mathbb{G}_r(\mathbf{r}_0) \right] \right), \tag{55}$$

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 [4]

$$\mathrm{LDOS}_R = \frac{3Zk^2}{4\pi} \frac{P_{sca}}{|\mathbf{p}_0|^2 + |\mathbf{m}_0|^2} \tag{56}$$

and

$$\mathrm{LDOS}_{NR} = \frac{3Zk^2}{4\pi} \frac{P_{abs}}{|\mathbf{p}_0|^2 + |\mathbf{m}_0|^2}. \tag{57}$$

The scattered and the absorbed powers P_{sca} and P_{abs} can be computed using expressions from section 6. With this, the energy balance is fulfilled, i.e.

$$\mathrm{LDOS} = \mathrm{LDOS_R} + \mathrm{LDOS_{NR}}. \tag{58}$$

9 Optical Forces

The optical force (as implemented in the library) on the particle i along the β-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 [5]

$$F_\beta^{(i)} = \frac{1}{2} \mathrm{Re} \left\langle \alpha_E^{(i)} \mathbf{E}_i(\mathbf{r}_i) \cdot \mathbf{E}_i^{'*}(\mathbf{r}_i) + \alpha_M^{(i)} \mathbf{H}_i(\mathbf{r}_i) \cdot \mathbf{H}_i^{'*}(\mathbf{r}_i) - \frac{2}{3} \left(\alpha_E^{(i)} \mathbf{E}_i(\mathbf{r}_i) \right) \times \left(\alpha_M^{(i)} \mathbf{H}_i(\mathbf{r}_i) \right)^* \cdot \hat{\mathbf{u}}_\beta \right\rangle \tag{59}$$

where $'$ denotes the derivative with respect to β.

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. 59 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 $\widetilde{F}_\beta^{(i)}$ is the force in unit of force (forgive the redundancy), we have

$$\widetilde{F}_\beta^{(i)} = \epsilon_0\epsilon_h \frac{4\pi}{k^2} F_\beta^{(i)}. \tag{60}$$

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

$$F_\beta = \frac{1}{2}\mathrm{Re}\left(\mathrm{Tr}\left\langle \overleftrightarrow{\alpha}\vec{\mathbf{\Phi}}\vec{\mathbf{\Phi}}^{\dagger\prime} + \frac{2}{3}\left(\overleftrightarrow{\alpha}\vec{\mathbf{\Phi}}\right)\left(\overleftrightarrow{\alpha}\vec{\mathbf{\Phi}}\right)^{\dagger}\overleftrightarrow{\varepsilon}_\beta\right\rangle\right), \tag{61}$$

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 β-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

$$F_\beta = \frac{1}{2}\mathrm{Re}\left(\mathrm{Tr}\left\langle \overleftrightarrow{\alpha}\mathbb{A}^{-1}\left[\vec{\mathbf{\Phi}}_0\vec{\mathbf{\Phi}}_0^{\dagger} + \vec{\mathbf{\Phi}}_0\vec{\mathbf{\Phi}}_0^{\dagger\prime}\left[\overleftrightarrow{\alpha}\mathbb{A}^{-1}\right)^{\dagger} + \frac{2}{3}\vec{\mathbf{\Phi}}_0\vec{\mathbf{\Phi}}_0^{\dagger}\left(\overleftrightarrow{\alpha}\mathbb{A}^{-1}\right)^{\dagger}\overleftrightarrow{\varepsilon}_\beta\right]\right\rangle\right). \tag{62}$$

10 Comparison with other DDA codes

The performance of CoupledElectricMagneticDipoles.jl with only electric dipoles can be compared with other DDA codes. To do it, we use DDSCAT 7.3 [6] and PyGDM 1.1.6 [7]. Figure 1 shows the comparison of the runtime between CoupledElectricMagneticDipoles.jl and these two other software packages for the computation of extinction, scattering and absorption cross sections of a polystyrene sphere of radius $a = 250nm$ discretized in a different number of dipoles. We show that, for a number of dipoles until $\approx 10^3$, the performance of CoupledElectricMagneticDipoles.jl is better than the one of PyGDM, which is an advantage because our software is mostly dedicated to do computations for a number of dipoles in this range. On the other hand DDSCAT, which is using FFT acceleration for solving the system of equations, looks to be substantially more performant. We notice that DDSCAT does not allow outputting $\mathbb{A}^{-1}$, which is another advantage of CoupledElectricMagneticDipoles.jl for some applications, as discussed in the main text.

11 Use of tensor permittivity

In order to check that the results obtained with our code when a tensor (anisotropic) dielectric constant is used, we compare the results obtained with CoupledElectriMagneticDipoles.jl for the extinction, absorption and scattering efficiencies of a rectangular block of dimensions $0.1\mu m \times 0.2\mu m \times 0.2\mu m$ (discretized in 4000 cubes with the Clausius-Mossotti polarizability with radiative correction) with the results obtained with the DDSCAT software [6]. The dielectric constant of the block is taken to be

$$\epsilon = \begin{pmatrix} 1.33+0.01i & 0 & 0 \\ 0 & 1.33+0.01i & 0 \\ 0 & 0 & 1.50+0.01i \end{pmatrix}. \tag{63}$$

Figure 2 shows the results of such a comparison, we observe a good nice agreement between our code and DDSCAT.

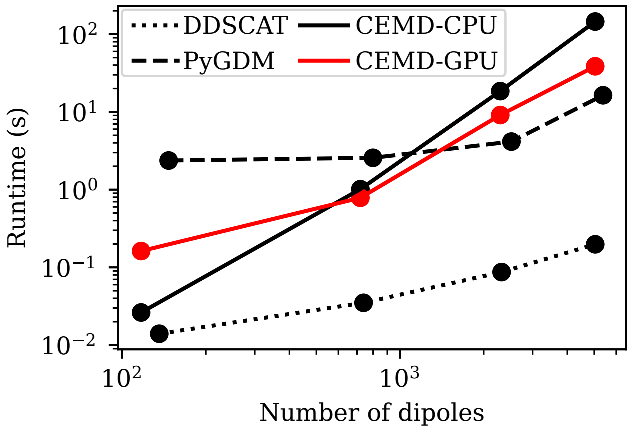

Figure 1: Comparison of the performance of a selection of codes implementing the DDA. The runtime is the time to compute extinction, scattering and absorption cross section for a polystyrene sphere discretized in various number of dipoles. Calculations have been done in single core 11th Gen Intel Core i9-11900K @ 3.50GHz and offloaded to GPU (Nvidia RTX3090). Note that compilation time is not included in the runtimes when the DDSCAT or CEMD code is used.

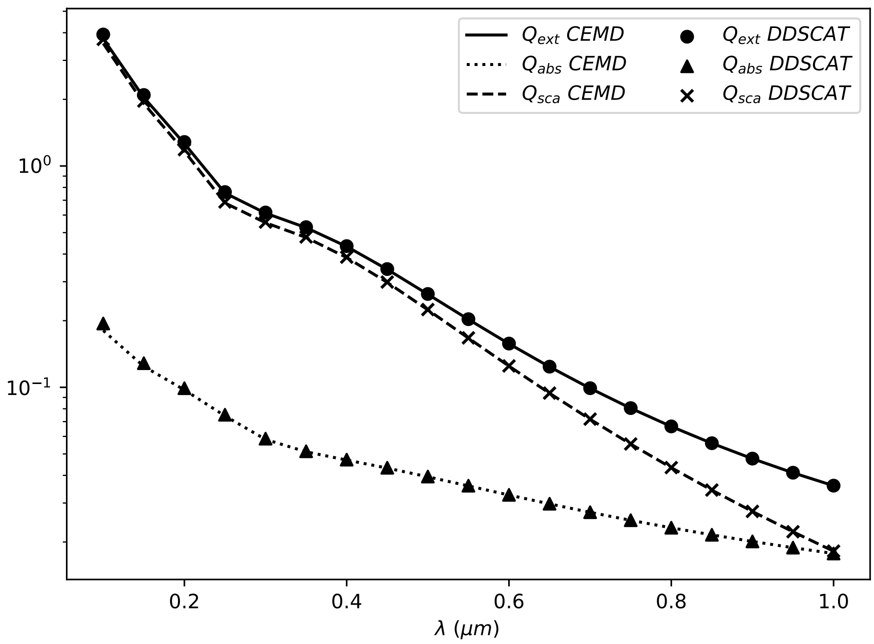

Figure 2: Comparison of the extinction, absorption and scattering efficiencies Q_{ext}, Q_{abs} and Q_{sca} of a block of size $0.1\mu m \times 0.2\mu m \times 0.2\mu m$ with tensor permittivity given by equation (63). Lines are results obtained with CoupledElectricMagneticDipoles.jl and markers are results obtained with DDSCAT.

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