An analytical approach to light scattering from small cubic and rectangular cuboidal nanoantennas - Supplementary data

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0.1 Definitions

In the following it is shown how to calculate the scattering, extinction and absorption cross sections of a rectangular cuboid embedded into a medium using the Green’s function formalism, showing also expressions for the scattered field. Consider a cuboid of volume $V$ placed with its centre at the origin with length equal to $L_a = 2a$, width equal to $L_b = 2b$ and height equal to $L_c = 2c$. The cuboid is composed of a material with a complex, wavelength dependent, dielectric constant $\epsilon$ and is surrounded by a background with a dielectric constant $\epsilon_B$. The incident electromagnetic field is a plane wave $E(r) = E_0 e^{ik_B z}$, where, in all the following, it will be assumed the time varying dependence of the field is given by $e^{-i\omega t}$. The electric field $E_0$ is along the $x$ direction and the wave-vector in the background is $k_B = \sqrt{\epsilon_B k_0} = \sqrt{\epsilon_B \omega / c}$.

0.2. Scattered field

The starting point is to consider the Green’s function formula in the far field, which can be written as:

$$G_{FF} = \frac{e^{ik_B R}}{4\pi R} \left[ \frac{I - RR}{R^2} \right],$$

(1)
where $R = r - r'$ and $R = |r - r'|$. The scattered field in the far field is therefore:

$$E_{sca}^{FF} = \int_V \frac{1}{4\pi R} \frac{e^{ik_B R}}{R^2} k_0^2 \Delta \epsilon \mathbf{E}(r') \cdot \mathbf{r}' \, dr' = \int_V \frac{1}{4\pi R} \frac{e^{ik_B R}}{R^2} k_0^2 \Delta \epsilon \mathbf{E}(r').$$

(2)

The geometrical symmetry of the scatterer gives rise to the following relationships for the electric field:

$$E_x(x) = E_x(-x); \quad E_y(y) = E_y(-y); \quad E_z(z) = E_z(-z),$$

(3)
which are valid for each $z = \text{constant}$ plane. If we consider the case of a constant electric field $E_{int}$ inside the scatterer, than the symmetry relationships give the following expressions for $E_{int}$ in the volume of the scatterer:

$$\begin{cases} \text{For } x > 0, y > 0 \\
E_{int} = (E_{x,int}, E_{y,int}, E_{z,int}) \end{cases}; \quad \begin{cases} \text{For } x < 0, y > 0 \\
E_{int} = (E_{x,int}, -E_{y,int}, -E_{z,int}) \end{cases},$$

$$\begin{cases} \text{For } x > 0, y < 0 \\
E_{int} = (E_{x,int}, -E_{y,int}, E_{z,int}) \end{cases}; \quad \begin{cases} \text{For } x < 0, y < 0 \\
E_{int} = (E_{x,int}, E_{y,int}, -E_{z,int}) \end{cases}.$$
By doing the approximation in formula (2) of $1/R \approx 1/r$ and $R \approx r - r' \cos \gamma$, where $\gamma$ is the angle between $\mathbf{r}$ and $\mathbf{r}'$, and by taking out from the integral the term $[1 - \frac{RR}{R^2}] \approx [1 - \frac{rr}{r^2}]$ since the higher order terms generate contributions that go to zero faster than $1/r^2$ which are negligible in the far field, one obtains:

$$E_{FF}^{sc} = \frac{e^{ikBr^2}k_0^2\Delta\epsilon}{4\pi r} \left( I - \frac{rr}{r^2} \right) \int_V \, dr' e^{-ikBr'\cos\gamma} \mathbf{E}_{int}.$$  \hspace{1cm} (5)

By writing Eq. 5 using the symmetry relationship given by Eq. 4 one obtains for the $x$ component of the electric field:

$$E_{FF}^{sc} = \frac{e^{ikBr^2}k_0^2\Delta\epsilon}{4\pi r} \left\{ \int_{V,x',0,y',0} \, dr' e^{-ikBr'\cos\gamma} \left\{ \left[ 1 - \frac{x'^2}{r'^2} \right] E_{x,\text{int}} - \frac{xy}{r'^2} E_{y,\text{int}} - \frac{xz}{r'^2} E_{z,\text{int}} \right\} + \frac{xz}{r'^2} E_{z,\text{int}} \right\}.$$  \hspace{1cm} (6)

By doing the change of variable $x' \to -x'$ and $y' \to -y'$ in order to express all the integrals in terms of $\int_{V,x',0,y',0} = \int_{V,+}$, by putting together the common terms and by using also the identity $\cos \gamma = (xx' + yy' + zz')/(rr')$, one obtains:

$$E_{FF}^{sc} = \frac{e^{ikBr^2}k_0^2\Delta\epsilon}{4\pi r} \left\{ \left[ 1 - \frac{x'^2}{r'^2} \right] E_{x,\text{int}} \left( \int_{V,+} \, dr' e^{-ikB(xx' + yy' + zz')/r} + \int_{V,+} \, dr' e^{-ikB(-xx' + yy' + zz')/r} \right) + \int_{V,+} \, dr' e^{-ikB(-xx' + yy' + zz')/r} \right\} + \int_{V,+} \, dr' e^{-ikB(-xx' + yy' + zz')/r} \right\}$$  \hspace{1cm} (7)

Since we are considering small particles the term $e^{-ikBr'\cos\gamma}$ can be approximated further by using the definition of the exponential, which gives:

$$e^{-ikBr'\cos\gamma} = 1 - ikBr'\cos\gamma - \frac{1}{2}k^2Br'^2\cos^2\gamma + O((kBr')^3).$$  \hspace{1cm} (8)

We are left with the evaluation of integrals of the type $\int_V \, dr' r'^d \cos^l \gamma$, which can be evaluated using the definition of the scalar product as:

$$\int_V \, dr' r'^d \cos^l \gamma = \frac{1}{r^l} \int_V \, dr'(xx' + yy' + zz')^l.$$  \hspace{1cm} (9)
Therefore Eq. 7 can be expressed as:

\[
E^{FF}_{x,sea} = \frac{e^{ik_B r} k_B^2 \Delta \epsilon}{4 \pi r} \left\{ \left[ 1 - \frac{x^2}{r^2} \right] E_{x,\text{int}} \left( 8abc - \frac{4k_B^2}{3r^2} \left[ a^3 bc x^2 + ab^3 cy^2 + abc^3 z^2 \right] \right) + \frac{4k_B^2 a^2 bc \frac{x^2 y^2}{r^3} E_{y,\text{int}} + 4ik_B a^2 bc \frac{x^2 z}{r^3} E_{z,\text{int}} + O(k_B)}{r^3} \right\}.
\]
By using Eq. 5 and the symmetry relationship given by Eq. 4 one obtains for the y component of the electric field:

\[
E_{y, sca}^{FF} = \frac{e^{ik_BT_0^2} \Delta \epsilon}{4\pi r} \left\{ \int_{V, x' > 0, y' > 0} dV \frac{e^{-ik_BT_0^2 \cos \gamma} \left\{ -\frac{yx}{r^2} E_{x, int} + \left[ 1 - \frac{y^2}{r^2} \right] E_{y, int} \right\}}{4\pi r} - \frac{yz}{r^2} E_{z, int} \right\} + \\
\int_{V, x' > 0, y' < 0} dV \frac{e^{-ik_BT_0^2 \cos \gamma} \left\{ -\frac{yx}{r^2} E_{x, int} - \left[ 1 - \frac{y^2}{r^2} \right] E_{y, int} + \frac{yz}{r^2} E_{z, int} \right\}}{4\pi r} + \\
\int_{V, x' < 0, y' > 0} dV \frac{e^{-ik_BT_0^2 \cos \gamma} \left\{ -\frac{yx}{r^2} E_{x, int} + \left[ 1 - \frac{y^2}{r^2} \right] E_{y, int} + \frac{yz}{r^2} E_{z, int} \right\}}{4\pi r} \right\}.
\]

By doing the change of variable \( x' \to -x' \) and \( y' \to -y' \) in order to express all the integrals in terms of \( \int_{V, x' > 0, y' > 0} = \int_{V_+} \), by putting together the common terms and by using also the identity \( \cos \gamma = (xx' + yy' + zz')/(rr') \), one obtains:

\[
E_{y, sca}^{FF} = \frac{e^{ik_BT_0^2} \Delta \epsilon}{4\pi r} \left\{ \int_{V_+} dV \frac{e^{-ik_BT_0^2 (xx' + yy' + zz')/r} + \\
\int_{V_+} dV \frac{e^{-ik_BT_0^2 (xx' - yy' + zz')/r} + \\
\int_{V_+} dV \frac{e^{-ik_BT_0^2 (-xx' - yy' + zz')/r} + \\
\int_{V_+} dV \frac{e^{-ik_BT_0^2 (-xx' + yy' + zz')/r} - \\
\int_{V_+} dV \frac{e^{-ik_BT_0^2 (-xx' - yy' + zz')/r} - \\
\int_{V_+} dV \frac{e^{-ik_BT_0^2 (-xx' + yy' + zz')/r} - \\
\int_{V_+} dV \frac{e^{-ik_BT_0^2 (-xx' - yy' + zz')/r} - \\
\int_{V_+} dV \frac{e^{-ik_BT_0^2 (-xx' + yy' + zz')/r})} {4\pi r} + \\
\int_{V_+} dV \frac{e^{-ik_BT_0^2 (-xx' + yy' + zz')/r})} \right\} \right\}.
\]

The integrals in parenthesis have already been evaluated, therefore the scattered field in the y direction is:

\[
E_{y, sca}^{FF} = \frac{e^{ik_BT_0^2} \Delta \epsilon}{4\pi r} \left\{ \int_{V_+} dV \frac{e^{-ik_BT_0^2 (xx' + yy' + zz')/r} + \\
\int_{V_+} dV \frac{e^{-ik_BT_0^2 (xx' - yy' + zz')/r} + \\
\int_{V_+} dV \frac{e^{-ik_BT_0^2 (-xx' - yy' + zz')/r} + \\
\int_{V_+} dV \frac{e^{-ik_BT_0^2 (-xx' + yy' + zz')/r} - \\
\int_{V_+} dV \frac{e^{-ik_BT_0^2 (-xx' - yy' + zz')/r} - \\
\int_{V_+} dV \frac{e^{-ik_BT_0^2 (-xx' + yy' + zz')/r} - \\
\int_{V_+} dV \frac{e^{-ik_BT_0^2 (-xx' - yy' + zz')/r})} {4\pi r} + \\
\int_{V_+} dV \frac{e^{-ik_BT_0^2 (-xx' + yy' + zz')/r})} \right\} \right\}.
\]

Finally, by using Eq. 5 and the symmetry relationship given by Eq. 4 one obtains for the z component of the electric field:

\[
E_{z, sca}^{FF} = \frac{e^{ik_BT_0^2} \Delta \epsilon}{4\pi r} \left\{ \int_{V_+} dV \frac{e^{-ik_BT_0^2 (xx' + yy' + zz')/r} + \\
\int_{V_+} dV \frac{e^{-ik_BT_0^2 (xx' - yy' + zz')/r} + \\
\int_{V_+} dV \frac{e^{-ik_BT_0^2 (-xx' - yy' + zz')/r} + \\
\int_{V_+} dV \frac{e^{-ik_BT_0^2 (-xx' + yy' + zz')/r} - \\
\int_{V_+} dV \frac{e^{-ik_BT_0^2 (-xx' - yy' + zz')/r} - \\
\int_{V_+} dV \frac{e^{-ik_BT_0^2 (-xx' + yy' + zz')/r})} {4\pi r} + \\
\int_{V_+} dV \frac{e^{-ik_BT_0^2 (-xx' + yy' + zz')/r})} \right\} \right\}.
\]
\[ E_{z,\text{sca}}^{\text{FF}} = \frac{e^{ik_B r_0^2} \Delta \epsilon}{4\pi r} \left\{ \int_{V,x'>0,y'>0} dr' e^{-ik_B r' \cos \gamma} \left\{ \frac{-zx}{r^2} E_{x,\text{int}} + \frac{-zy}{r^2} E_{y,\text{int}} + \left[ 1 - \frac{z^2}{r^2} \right] E_{z,\text{int}} \right\} + \left[ 1 - \frac{z^2}{r^2} \right] E_{z,\text{int}} \right\} + \int_{V,x'>0,y'<0} dr' e^{-ik_B r' \cos \gamma} \left\{ \frac{-zx}{r^2} E_{x,\text{int}} + \frac{zy}{r^2} E_{y,\text{int}} + \left[ 1 - \frac{z^2}{r^2} \right] E_{z,\text{int}} \right\} + \int_{V,x'<0,y'>0} dr' e^{-ik_B r' \cos \gamma} \left\{ \frac{-zx}{r^2} E_{x,\text{int}} - \frac{zy}{r^2} E_{y,\text{int}} - \left[ 1 - \frac{z^2}{r^2} \right] E_{z,\text{int}} \right\} \right\} \]

By doing the change of variable \( x' \rightarrow -x' \) and \( y' \rightarrow -y' \) in order to express all the integrals in terms of \( \int_{V,x'>0,y'>0} = \int_{V_+} \), by putting together the common terms and by using also the identity \( \cos \gamma = (xx' + yy' + zz')/(rr') \), one obtains:

\[ E_{z,\text{sca}}^{\text{FF}} = \frac{e^{ik_B r_0^2} \Delta \epsilon}{4\pi r} \left\{ \int_{V_+} dr' e^{-ik_B (xx' + yy' + zz')/r} + \int_{V_+} dr' e^{-ik_B (-xx' - yy' + zz')/r} + \int_{V_+} dr' e^{-ik_B (-xx' - yy' + zz')/r} + \frac{zy}{r^2} E_{y,\text{int}} - \int_{V_+} dr' e^{-ik_B (xx' + yy' + zz')/r} + \int_{V_+} dr' e^{-ik_B (-xx' - yy' + zz')/r} + \left[ 1 - \frac{z^2}{r^2} \right] E_{z,\text{int}} \left( \int_{V_+} dr' e^{-ik_B (xx' + yy' + zz')/r} - \int_{V_+} dr' e^{-ik_B (-xx' - yy' + zz')/r} \right) + \int_{V_+} dr' e^{-ik_B (xx' - yy' + zz')/r} - \int_{V_+} dr' e^{-ik_B (-xx' - yy' + zz')/r} \right\} \]  

The integrals in parenthesis have already been evaluated and are given by Eq. 10, 11, 12, therefore the scattered field in the \( z \) direction is:

\[ E_{z,\text{sca}}^{\text{FF}} = \frac{e^{ik_B r_0^2} \Delta \epsilon}{4\pi r} \left\{ \int_{V_+} dr' e^{-ik_B r' \cos \gamma} \left\{ \frac{-zx}{r^2} E_{x,\text{int}} + \frac{4k_B^2}{3r^2} \left[ a^2bcx^2 + ab^3cy^2 + abc^3z^2 \right] + 4k_B^2 a^2b^2c \frac{xy^2 z^2}{r^4} E_{y,\text{int}} - 4ik_B a^2bc \left[ 1 - \frac{z^2}{r^2} \right] E_{z,\text{int}} + O(k_B^3) \right\} \right\} \]

0.3. Scattering cross section

The scattering cross section can be calculated using the formula:

\[ \sigma = \frac{1}{E_0^2} \int_S dS \frac{1}{r^2} |E_{z,\text{sca}}^{\text{FF}}|^2 = \frac{1}{E_0^2} \int_S dS \frac{1}{r^2} \left( |E_{x,\text{sca}}^{\text{FF}}|^2 + |E_{y,\text{sca}}^{\text{FF}}|^2 + |E_{z,\text{sca}}^{\text{FF}}|^2 \right) \]
where S is a spherical surface in the limit with \( r \to +\infty \). Therefore by using Eq. 13, 16 and 19 one obtains:

\[
\sigma_{sca} = \frac{k_0^2 |\Delta \epsilon|^2}{16\pi^2 E_0^2} \int_S \left[ 1 - \frac{x^2}{r^2} \right] E_{x,\text{int}} \left( 8abc - \frac{4k_B^2}{3r^2} \left[ a^3bcr^2 + ab^3cy^2 + abc^3z^2 \right] \right) +
\]

\[
+4k_B^2 a^2b^2c \frac{x^2y^2}{r^4} E_{y,\text{int}} + 4ik_Ba^2bc \frac{x^2z}{r^3} E_{z,\text{int}} + O(k_B^3)
\]

\[
+ \left| \frac{-y}{r} E_{x,\text{int}} \right| \left( 8abc - \frac{4k_B^2}{3r^2} \left[ a^3bcr^2 + ab^3cy^2 + abc^3z^2 \right] \right) -
\]

\[
-4k_B^2 a^2b^2c \left[ 1 - \frac{y^2}{r^2} \right] \frac{xy}{r^2} E_{y,\text{int}} + 4ik_Ba^2bc \frac{xz}{r^3} E_{z,\text{int}} + O(k_B^3)
\]

\[
+ \left| \frac{-z}{r} E_{x,\text{int}} \right| \left( 8abc - \frac{4k_B^2}{3r^2} \left[ a^3bcr^2 + ab^3cy^2 + abc^3z^2 \right] \right) +
\]

\[
+4k_B^2 a^2b^2c \frac{x^2y^2}{r^4} E_{y,\text{int}} - 4ik_Ba^2bc \left[ 1 - \frac{z^2}{r^2} \right] \frac{x}{r} E_{z,\text{int}} + O(k_B^3)
\]

\[
(21)
\]

The squared moduli inside the integral term can be expanded using the identity:

\[
|z_1 + z_2 + z_3|^2 = |z_1|^2 + |z_2|^2 + |z_3|^2 + z_1z_2 + z_1z_3 + z_2z_3 + z_1z_2 + z_1z_3 + z_2z_3.
\]

\[
(22)
\]

For the first term \( |E_{x,\text{sca}}|^2 \) \( z_1, z_2, z_3 \) are expressed by:

\[
z_1 = \left[ 1 - \frac{x^2}{r^2} \right] E_{x,\text{int}} \left( 8abc - \frac{4k_B^2}{3r^2} \left[ a^3bcr^2 + ab^3cy^2 + abc^3z^2 \right] \right)
\]

\[
z_2 = 4k_B^2 a^2b^2c \frac{x^2y^2}{r^4} E_{y,\text{int}}
\]

\[
z_3 = 4ik_Ba^2bc \frac{x^2z}{r^3} E_{z,\text{int}}.
\]

The integrals for each term can be expressed in spherical coordinates. The first term gives:

\[
\int_S dS|z_1|^2 = \int_S dS \left[ 1 - \frac{x^2}{r^2} \right]^2 \left( 8abc - \frac{4k_B^2}{3r^2} \left[ a^3bcr^2 + ab^3cy^2 + abc^3z^2 \right] \right)^2
\]

\[
\int_S \left[ 1 - \sin^2 \theta \cos^2 \phi \right]^2 \left\{ 8abc - \frac{4k_B^2}{3} \left[ a^3bc \sin^2 \theta \cos^2 \phi + ab^3 \sin^2 \phi \sin^2 \phi + abc^3 \cos^2 \theta \right] \right\}^2 \sin \theta d\theta d\phi,
\]

which can be carried out analytically to give the following expression:

\[
\int_S dS|z_1|^2 = \frac{512}{2835} \pi [a^2b^2c^2 (756 - k_B^2 (36a^2 + 108b^2 + 108c^2)) +
\]

\[
+ k_B^2 (a^4 + 6b^4 + 6c^4 + 2a^2b^2 + 2a^2c^2 + 4b^2c^2))]|E_{x,\text{int}}|^2.
\]

\[
(25)
\]

The second term can be calculated as:

\[
\int_S dS|z_2|^2 = \int_S dS \left| 4k_B^2 a^2b^2c \frac{x^2y^2}{r^4} E_{y,\text{int}} \right|^2
\]

\[
= 16k_B^4 a^4b^2c^2 |E_{y,\text{int}}|^2 \int_S d\theta d\phi \sin^6 \theta \sin^4 \phi \cos^4 \phi = \frac{64}{105} \pi k_B^4 a^4b^4c^2 |E_{y,\text{int}}|^2.
\]

\[
(27)
\]
The third term can be calculated as:

\[ \int dS |z_3|^2 = \int dS \left| 4i k_B a^2 b c \frac{x^2 z}{r^3} E_{z,int} \right|^2 = 16 k_B^2 a^4 b^2 c^2 |E_{z,int}|^2 \int d\theta d\phi \sin^3 \theta \sin^4 \phi \cos^2 \theta = \frac{64}{35} \pi k_B^2 a^4 b^2 c^2 |E_{z,int}|^2. \]

(28)

The terms \(z_1 \bar{z}_3, z_2 \bar{z}_3, \bar{z}_1 z_3, \bar{z}_2 \bar{z}_3\) give identically 0. The term \(z_1 \bar{z}_2\) gives:

\[ \int dS z_1 \bar{z}_2 = \frac{128}{945} \pi k_B^2 a^3 b^3 c^2 \left[ 36 - k_B^2 (2a^2 + 3b^2 + c^2) \right] E_{x,int} E_{y,int}, \]

(29)

whereas the term \(\bar{z}_1 z_2\) gives:

\[ \int dS z_1 \bar{z}_2 = \frac{128}{945} \pi k_B^2 a^3 b^3 c^2 \left[ 36 - k_B^2 (2a^2 + 3b^2 + c^2) \right] E_{x,int} E_{y,int}. \]

(30)

For the second term \(|E_{y,scal}|^2\), \(z_1, z_2, z_3\) are expressed by:

\[ z_1 = -\frac{y x}{r^2} E_{x,int} \left( 8abc - \frac{4 k_B^2}{3r^2} \left[ a^3 b c x^2 + a^3 b c y^2 + a b^3 c z^2 \right] \right) \]

\[ z_2 = -4 k_B^2 a b c \left[ 1 - \frac{y^2}{r^2} \right] \frac{x y}{r^2} E_{y,int} \]

\[ z_3 = 4 i k_B a^2 b c \frac{x y z}{r^3} E_{z,int}. \]

(31)

The integrals, expressed in spherical coordinates, give for the first term:

\[ \int dS |z_1|^2 = \int dS \left\{ -\frac{y x}{r^2} \left( 8abc - \frac{4 k_B^2}{3r^2} \left[ a^3 b c x^2 + a^3 b c y^2 + a b^3 c z^2 \right] \right) \right\}^2 |E_{x,int}|^2 = \frac{64}{2835} \pi |a^2 b^2 c^2 (756 - k_B^2 (108a^2 + 108b^2 + 36c^2) + k_B^2 (5a^4 + 5b^4 + c^4 + 6a^2 b^2 + 2a^2 c^2 + 2b^2 c^2))||E_{x,int}||^2. \]

(32)

The second term can be calculated as:

\[ \int dS |z_2|^2 = \int dS \left| -4 k_B^2 a^2 b^2 c \left[ 1 - \frac{y^2}{r^2} \right] \frac{x y}{r^2} E_{y,int} \right|^2 = \frac{512}{315} \pi k_B^4 a^4 b^4 c^2 |E_{y,int}|^2. \]

(33)

The third term can be calculated as:

\[ \int dS |z_3|^2 = \int dS \left| 4 i k_B a^2 b c \frac{x y z}{r^3} E_{z,int} \right|^2 = \frac{64}{105} \pi k_B^2 a^4 b^2 c^2 |E_{z,int}|^2. \]

(34)

The terms \(z_1 \bar{z}_3, z_2 \bar{z}_3, \bar{z}_1 z_3, \bar{z}_2 \bar{z}_3\) give identically 0. The term \(z_1 \bar{z}_2\) gives:

\[ \int dS z_1 \bar{z}_2 = \frac{128}{945} \pi k_B^2 a^3 b^3 c^2 \left[ 36 - k_B^2 (3a^2 + 2b^2 + c^2) \right] E_{x,int} E_{y,int}, \]

(35)

whereas the term \(\bar{z}_1 z_2\) gives:

\[ \int dS \bar{z}_1 z_2 = -\frac{128}{945} \pi k_B^2 a^3 b^3 c^2 \left[ 36 - k_B^2 (3a^2 + 2b^2 + c^2) \right] E_{x,int} E_{y,int}. \]

(36)
For the third term \( |E_{z,\text{sca}}| \), \( z_1, z_2, z_3 \) are expressed by:

\[
z_1 = -\frac{zx}{r^2} E_{x,\text{int}} \left( 8abc - \frac{4k_B^2}{3r^2} \left[ a^3bcx^2 + ab^3cy^2 + abc^3z^2 \right] \right)
\]

\[
z_2 = 4k_B^2a^2b^2c \frac{x^2y^2z}{r^4} E_{y,\text{int}}
\]

\[
z_3 = -4i k_B a^2 bc \left[ 1 - \frac{z^2}{r^2} \right] x E_{z,\text{int}}.
\]

The integrals, expressed in spherical coordinates, give for the first term:

\[
\int_S dS |z_1|^2 = \int_S dS \left\{ -\frac{zx}{r^2} E_{x,\text{int}} \left( 8abc - \frac{4k_B^2}{3r^2} \left[ a^3bcx^2 + ab^3cy^2 + abc^3z^2 \right] \right) \right\}^2 |E_{x,\text{int}}|^2 = \frac{64}{2835} \pi [a^2b^2c^2(756 - k_B^2(108a^2 + 36b^2 + 108c^2) + k_B^4(5a^4 + b^4 + 5c^4 + 2a^2b^2 + 6a^2c^2 + 2b^2c^2))]|E_{x,\text{int}}|^2.
\]  

(37)

The second term can be calculated as:

\[
\int_S dS |z_2|^2 = \int_S dS \left\{ 4k_B^2a^2b^2c \frac{x^2y^2z}{r^4} E_{y,\text{int}} \right\}^2 = \frac{64}{315} \pi k_B^4a^4b^2c^2 |E_{y,\text{int}}|^2.
\]  

(39)

The third term can be calculated as:

\[
\int_S dS |z_3|^2 = \int_S dS \left\{ 4i k_B a^2 bc \frac{x^2y^2z}{r^4} E_{z,\text{int}} \right\}^2 = \frac{512}{35} \pi k_B^2a^4b^2c^2 |E_{z,\text{int}}|^2.
\]  

(40)

The terms \( \overline{z}_1z_3, \overline{z}_2z_3, \overline{z}_1z_2, \overline{z}_2z_2 \) give identically 0. The term \( \overline{z}_1z_2 \) gives:

\[
\int_S dS \overline{z}_1z_2 = -\frac{128}{945} \pi k_B^2a^3b^2c^2 \left[ 36 - k_B^2(2a^2 + 2b^2 + 2c^2) \right] E_{x,\text{int}} \overline{E_{y,\text{int}}},
\]

(41)

whereas the term \( \overline{z}_1z_2 \) gives:

\[
\int_S dS \overline{z}_1z_2 = -\frac{128}{945} \pi k_B^2a^3b^2c^2 \left[ 36 - k_B^2(2a^2 + 2b^2 + 2c^2) \right] \overline{E_{x,\text{int}}} E_{y,\text{int}}.
\]

(42)

Finally the scattering cross section can be written as:

\[
\sigma_{\text{sca}} = \frac{k_0^4 |\Delta c|^2}{15\pi E_0^2} \left\{ \frac{8}{63} [a^2b^2c^2(1260 - k_B^2(84a^2 + 168b^2 + 168c^2) + k_B^4(3a^4 + 9b^4 + 9c^4 + 4a^2b^2 + 4a^2c^2 + 6b^2c^2))]|E_{x,\text{int}}|^2 + 16k_B^2a^4b^2c^2 (k_B^2b^2|E_{y,\text{int}}|^2 + |E_{z,\text{int}}|^2) + \frac{4}{63} \pi k_B^2a^3b^3c^2 [18 + k_B^2(3a^2 - b^2 + c^2)] (E_{x,\text{int}} E_{y,\text{int}} + E_{x,\text{int}} \overline{E_{y,\text{int}}}) + O(k_B^3) \right\}.
\]

(43)

0.4. Extinction cross section

The extinction cross section can be calculated using the optical theorem:

\[
\sigma_{\text{ext}} = \frac{4\pi}{k_B^2} \Re[\mathbf{X} \cdot \mathbf{n}_{E_0}]_{z \to +\infty; x, y = 0},
\]

(44)

where \( \mathbf{n}_{E_0} \) is a unit vector in the direction of the polarization of the incoming wave (x direction) and the scattering amplitude \( \mathbf{X} \) is defined as:

\[
\mathbf{E}_{\text{sca}} = -\frac{e^{ik_B r}}{ik_B r} \mathbf{X} E_0.
\]

(45)
Therefore by using Eq. (13) the extinction cross section can be expressed as:

\[
\sigma_{ext} = -\frac{k_0^2}{k_B E_0} \Re[i \Delta \epsilon E_{x,int} \left( 8abc - \frac{4k_B^2}{3} abc^3 \right)].
\] (46)

0.5. Absorption cross section

The absorption cross section can be expressed as:

\[
\sigma_{abs} = \frac{k_B}{E_0^2} \int_V \Im(\epsilon)|E(r)|^2 dV.
\] (47)

Given the constant field inside the cuboid the absorption cross section readily calculate as:

\[
\sigma_{abs} = \frac{8k_B}{E_0^2} \Im(\epsilon)(|E_{x,int}|^2 + |E_{y,int}|^2 + |E_{z,int}|^2)abc,
\] (48)

otherwise can be expressed simply as \(\sigma_{abs} = \sigma_{ext} - \sigma_{sca}\).

0.6. Internal electric field

If we assume that the polarization of the cuboid is homogeneous in its volume the following equation applies:

\[
P = \epsilon_0 (\epsilon - \epsilon_B)(E_0 + E_{dep}),
\] (49)

where \(E_{dep}\) is the depolarization field generated by the matter surrounding a point in the volume.

The field \(E_{dep}\) can be determined by assigning a dipole moment \(dp(r) = P dV\) to each volume element, calculating the retarder dipolar field \(dE_{dep}\) generated at the specific point and integrating over the entire volume. The electric field produced by a retarded dipole \(dp(r)\) oriented along \(x\) in spherical coordinates can be expressed as:

\[
E_r = \frac{2 \cos \theta}{4\pi \epsilon_0 \epsilon_B} \frac{e^{ik_B r}}{r} \left[ \frac{1}{k_B^2 r^2} - \frac{i}{k_B r} \right] |dp|,
E_\theta = \frac{\sin \theta}{4\pi \epsilon_0 \epsilon_B} \frac{e^{ik_B r}}{r} \left[ \frac{1}{k_B^2 r^2} - \frac{i}{k_B r} - 1 \right] |dp|,
\] (50)

with \(E_\phi = 0\).

The projection of the electric field along the \(x\) direction is:

\[
E_\parallel = E_r \cos \theta - E_\theta \sin \theta.
\] (51)

In particular if we consider the point in the centre of the cuboid and the \(dE_{dep}\) parallel to the \(x\) axis, the expression is:

\[
dE_{dep,x} = \frac{1}{4\pi \epsilon_0 \epsilon_B} \left[ \frac{1}{r^3} (3 \cos^2 \theta - 1) + \frac{k_B^2}{2r} (\cos^2 \theta + 1) + \frac{2}{3} i k_B^3 \right] P_x dV.
\] (52)

By integrating this expression over the cube we are left with three terms. The first term diverges as \(1/r^3\), and it is precisely the divergent part of the Green’s function. Its expression is tabulated and it is given by \(-2\Omega\) where \(\Omega\) is the solid angle subtended by a side of the cuboid orthogonal to the \(x\) axis.
The expression of the solid angle of a cuboid subtended by the side perpendicular to the x axis can be written as:

$$\Omega = 4 \arcsin \left( \frac{bc}{\sqrt{(a^2 + b^2)(a^2 + c^2)}} \right).$$  \hfill (53)

The second term is integrable but with a rather long expression, and can be written as:

$$\frac{k_B^2 \beta}{2} = \int_{-c}^{c} \int_{-b}^{b} \int_{-a}^{a} \frac{k_B^2}{2 \sqrt{x^2 + y^2 + z^2}} \left( 1 + \frac{x^2}{x^2 + y^2 + z^2} \right) dx dy dz =$$

$$= k_B^2 \left\{ 4c \left[ a \arctanh \left( \frac{\sqrt{a^2 + b^2 + c^2}}{b} \right) - c \arctan \left( \frac{ab}{c\sqrt{a^2 + b^2 + c^2}} \right) \right] +$$

$$+ b \arctanh \left( \frac{\sqrt{a^2 + b^2 + c^2}}{a} \right) \right] - 4b^2 \arctan \left( \frac{ac}{b\sqrt{a^2 + b^2 + c^2}} \right) +$$

$$+ 2ab \log \left( c + \sqrt{a^2 + b^2 + c^2} \right) + 2ac \log \left( b + \sqrt{a^2 + b^2 + c^2} \right) + 4bc \log \left( a + \sqrt{a^2 + b^2 + c^2} \right) -$$

$$- 4ac \arctanh \left( \frac{\sqrt{a^2 + b^2 + c^2}}{b} \right) - 4bc \arctan \left( \frac{\sqrt{a^2 + b^2 + c^2}}{a} \right) - 2ab \log \left( \sqrt{a^2 + b^2 + c^2 - c} \right) -$$

$$- 2ac \log \left( \sqrt{a^2 + b^2 + c^2 - b} \right) - 4bc \log \left( \sqrt{a^2 + b^2 + c^2 - a} \right) \right\},$$

which in case of a cube gives:

$$\beta_{cube} = a^2 \int_{-1}^{1} \int_{-1}^{1} \int_{-1}^{1} \frac{1}{\sqrt{x^2 + y^2 + z^2}} \left( 1 + \frac{x^2}{x^2 + y^2 + z^2} \right) dx dy dz \approx 12.6937a^2. \hfill (55)$$

The integral is therefore just a function of the aspect ratio of the cuboid.

The third term can be integrated in a simple way to give $\frac{16}{3}ik_B^3abc$, therefore the expression of the depolarizing field is:

$$E_{dep,x} = \frac{1}{4\pi \varepsilon_0 \varepsilon_B} \left[ -2\Omega + \frac{k_B^2}{2} \beta + \frac{16}{3}ik_B^3abc \right] P_x. \hfill (56)$$

By inserting Eq. 56 into 49 we obtain an expression for the field inside the particles $E_{int} = E_0 + E_{dep}$ along the x direction:

$$E_{int,x} = \frac{E_0}{1 - \frac{c - \varepsilon_B}{4\pi \varepsilon_B} \left[ -2\Omega + \frac{k_B^2}{2} \beta + \frac{16}{3}ik_B^3abc \right]}.$$

By considering also the effect of polarization charges at the planar ends of the cuboid orthogonal to the x direction, another term in the expression of $E_{dep,x}$ appears. Using equation $\mathbf{P} \cdot \mathbf{n} = \sigma$ where $\sigma$ is the surface charge at the planar ends and $\mathbf{n}$ is the external normal vector, we obtain that the charge at the surfaces, which we consider concentrated at each of the eight vertices, is given by $q = P_x bc$, where $q$ is positive in the $x = a$ and negative in the $x = -a$ planar surfaces. The contribution to the field along x at the centre of the cuboid given by the charges at the vertices is:

$$E_{vert,x} = -\frac{8}{4\pi \varepsilon_0 \varepsilon (a^2 + b^2 + c^2)^{3/2}} abc P_x.$$  \hfill (58)
where we have taken into account the projection of the electric field along $x$ generated by the charges. Therefore the expression of the depolarizing field becomes:

$$E_{dep,x}^\prime = E_{dep,x} + E_{vert,x} = \frac{1}{4\pi\epsilon_0\epsilon_B} \left[ -2\Omega + \frac{k_B^2}{2}\beta + \frac{16}{3}ik_B^3abc - \frac{8abc}{(a^2 + b^2 + c^2)^{3/2}} \right] \frac{\epsilon_B}{\epsilon} P_x,$$

where we have assumed a polarization charge at each vertex polarization charges at the planar ends of the cuboid orthogonal to the $x$ direction. Using the previous expression and defining $\delta$ as:

$$\delta = \frac{8abc}{(a^2 + b^2 + c^2)^{3/2}} \frac{\epsilon_B}{\epsilon},$$

Eq. 59 gives as a final expression:

$$E_{int,x} = \frac{E_0}{1 - \frac{\epsilon - \epsilon_B}{4\pi\epsilon_B} \left[ -2\Omega - \delta + \frac{k_B^2}{2}\beta + \frac{16}{3}ik_B^3abc \right]}.$$