Irreducible Cartesian multipole decomposition of scattered light with explicit contribution of high order toroidal moments

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Abstract. Multipole decomposition is a powerful tool for analysis of electromagnetic systems. This work considers high order irreducible Cartesian multipole moments in approximation of electric 32-pole and magnetic 16-pole. The explicit contributions to scattering of high order toroidal moments up to toroidal electric octupole and toroidal magnetic quadrupole are demonstrated for a dielectric high refractive index scatterer.

1. Introduction:
Multipoles are simplest configurations of charges and currents excited in a medium suitable for an electromagnetic analysis. Many years multipole concept remained unchanged before the work of Ya. Zeldovich, who first specified the features of a toroidal moment (he called it anapole moment) in connection with the problem of violation of parity symmetry in an atomic system with broken space-time mirror symmetry [1].

Recently, toroidal moments attract much interest in metamaterials science. Unlike naturally occurring media those artificial ones were for first time shown to produce electrical toroidal response [2,3]. It was demonstrated in microwave frequencies that metamaterials with the toroidal response produce strong circular dichroism [2] and possess extremely high Q-factor, due to destructive interference of dipolar and toroidal parts (this nonradiative state was called anapole state), etc.

In the optical frequency range, the investigation of high order multipoles and high order toroidal moments has been started since the magnetic responses have been found in high refractive index materials [4,5], such as Si, Ge. High order multipoles were applied for optical forces analysis [6], scattering light directivity control [7,8], studying of nonradiative states (e.g lasing and nonradiative mode transfer [9–12]), photovoltaics [13–15], cloaking [16,17], etc.
There are frequently used approaches for multipole decomposition, e.g., Cartesian [18–21], spherical [22], fractional [23], Fano-Feshbach modes [24], and others. The most popular one is Cartesian multipole decomposition. It allows to get explicit contribution of toroidal type multipole moments to scattering, and reveals their interference with basic ones. In this work we demonstrate multipole decomposition of a scattered electric field in far-field zone in limitation of 5th order Cartesian multipoles (electric 32 pole and magnetic 16 pole) with explicit contribution of high order toroidal multipoles up to the toroidal electric octupole and toroidal magnetic quadrupole.

2. Results
To obtain multipole decomposition of the scattered electric field in Lorentz gauge \( \mathbf{E} = -\dot{\mathbf{A}} - \nabla \Phi \) the scalar \( \Phi \) and vector \( \mathbf{A} \) retarded potentials are expanded to Taylor series:

\[
\Phi(\mathbf{R}, t) = \frac{1}{4\pi \varepsilon_0} \int_V \frac{\rho(\mathbf{r}, t' + \Delta t)}{|\mathbf{R} - \mathbf{r}|} \, d\mathbf{r},
\]

\[
\mathbf{A}(\mathbf{R}, t) = \frac{\mu_0}{4\pi} \int_V \frac{\mathbf{J}(\mathbf{r}, t' + \Delta t)}{|\mathbf{R} - \mathbf{r}|} \, d\mathbf{r},
\]

where \( \rho \) and \( \mathbf{J} \) are charge and current densities in an infinitesimal volume \( d\mathbf{r} \), \( \varepsilon_0 \) and \( \mu_0 \) are vacuum permittivity and permeability, \( \mathbf{R} \) is a radius vector from the origin to a distant point and \( \mathbf{r} \) is a radius vector from origin to a point with considered distribution of charges and currents; retarded time at \( d\mathbf{r} \) is \( t' + \Delta t = t - |\mathbf{R} - \mathbf{r}| / c \), where \( c \) is speed of light in vacuum and \( t' = t - |\mathbf{R}| / c \) is the time retardation at the coordinates origin [19]. Symmetrisation and detracing [25] of primitive high order multipoles [21] allow to obtain tensors, which produce an independent contribution to the electric field in far-field. The symmetrized and traceless tensors match requirement for a Cartesian tensor to stay invariant under its translation and rotation in respect to SO3 group.

Using Einstein index notation the final equation for the scattered power in far-field zone is introduced in the irreducible representation of high order multipoles and explicit contributions of high order toroidal moments:

\[
P_{\text{scat}} = \frac{k^4 \varepsilon_d}{12\pi \varepsilon_0^2 c \mu_0} |p_i + \frac{ik}{c} \bar{r}^{(e)}(c) + \frac{ik^3}{c} T_i^{(2e)}|^2 + \frac{k^4 \varepsilon_d \varepsilon_e}{12\pi \varepsilon_0 c} |m_i + \frac{ik}{c} T_i^{(m)}|^2 + \]

\[
+ \frac{k^6 \varepsilon_d \varepsilon_e}{160\pi \varepsilon_0^2 c \mu_0} |\bar{Q}_{ij}^{(e)} + \frac{ik}{c} \bar{P}_{ij}^{(e)}|^2 + \frac{k^6 \varepsilon_d \varepsilon_e}{160\pi \varepsilon_0 c} |\bar{Q}_{ij}^{(m)} + \frac{ik}{c} \bar{P}_{ij}^{(m)}|^2 + \]

\[
+ \frac{k^8 \varepsilon_d \varepsilon_e^2}{3780\pi \varepsilon_0^2 c \mu_0} |\bar{Q}_{ijk}^{(e)} + \frac{ik}{c} \bar{P}_{ijk}^{(e)}|^2 + \frac{k^8 \varepsilon_d \varepsilon_e^2}{3780\pi \varepsilon_0 c} |\bar{Q}_{ijk}^{(m)} + \frac{ik}{c} \bar{P}_{ijk}^{(m)}|^2 + \]

\[
+ \frac{k^{10} \varepsilon_d \varepsilon_e^3}{145152\pi \varepsilon_0^2 c \mu_0} |\bar{S}_{ijk}^{(e)} + \frac{ik}{c} \bar{V}_{ijk}^{(e)}|^2 + \frac{k^{10} \varepsilon_d \varepsilon_e^3}{145152\pi \varepsilon_0 c} |\bar{S}_{ijk}^{(m)} + \frac{ik}{c} \bar{V}_{ijk}^{(m)}|^2 + \]

\[
+ \frac{k^{12} \varepsilon_d^2}{831600\pi \varepsilon_0^2 c \mu_0} |\bar{X}_{ijk}^{(e)}|^2.
\]

Here \( k \) is a vacuum wave number, \( \varepsilon_0 \) and \( \mu_0 \) are vacuum permittivity and permeability, \( \varepsilon_d \) is relative permittivity, \( \mathbf{n} \) is a unit vector codirected with \( \mathbf{R} \), \( R \) is length of \( \mathbf{R} \), \( \mathbf{p} \) and \( \mathbf{m} \) are basic electric and magnetic dipoles, \( \bar{Q}_{jk}^{(e)} \) and \( \bar{Q}_{jp}^{(e)} \) are electric and magnetic quadrupoles (the double overline denotes symmetrized and detraced tensor), \( \bar{Q}_{jkp}^{(e)} \) and \( \bar{Q}_{jpm}^{(m)} \) are electric and magnetic octupoles, \( \bar{S}_{jkpl}^{(e)} \) and \( \bar{V}_{jpl}^{(e)} \)
are electric and magnetic 16 poles, and $\tilde{X}_{jkp\ell\ell}$ is electric 32 pole. Toroidal moments in Equation 3 contain superscript, which refers to the corresponding multipole and shown in Table 1.

**Table 1.** The high order toroidal moments

| Order | Toroidal electric multipoles | Toroidal magnetic multipoles |
|-------|-----------------------------|-----------------------------|
| 1     | $T^{(e)}_j = \frac{1}{10} \int (\mathbf{J} \cdot \mathbf{r}) r_j - 2 r^2 J_j d\nu$ | $-$ |
|       | $T^{(2e)}_j = \frac{1}{280} \int 3 r^4 J_j - 2 r^2 (\mathbf{r} \cdot \mathbf{J}) r_j d\nu$ | |
| 2     | $T^{(0e)}_{jk} = \frac{1}{42} \int 4 (\mathbf{r} \cdot \mathbf{J}) r_j r_k + 2 (\mathbf{J} \cdot \mathbf{r}) r^2 \delta_{jk} - 5 r^2 (\mathbf{r} \mathbf{J}_k + r_k \mathbf{J}_j) d\nu$ | $T^{(m)}_j = \frac{i \omega}{20} \int r^2 (\mathbf{r} \times \mathbf{J})_j d\nu$ |
| 3     | $T^{(0e)}_{jk\ell\ell} = \frac{1}{300} \int 35 (\mathbf{r} \cdot \mathbf{J}) r_j r_k r_\ell - 20 r^2 (J_l r_k r_\ell + J_k r_l r_\ell + J_\ell r_k r_l) + (\delta_{lj} \delta_{k\ell} + \delta_{jk} \delta_{l\ell} + \delta_{j\ell} \delta_{k\ell}) \cdot [ (\mathbf{r} \cdot \mathbf{J}) r^2 r_p + 4 J_p r^4 ] d\nu$ | $T^{(qm)}_{\ell p} = \frac{i \omega}{42} \int r^2 (\mathbf{r} \times \mathbf{J})_p + (\mathbf{r} \times \mathbf{J})_p r_\ell d\nu$ |

Taking into account a normalization of the scattered power on incident wave energy flux $I_0 = \frac{1}{2} \sqrt{\varepsilon_0} \varepsilon_d$ and geometrical cross-section of the scatterer we have obtained the multipole decomposition of the scattering efficiency for a spherical scatterer with refractive index $n=4$

![Figure1](image.png)

**Figure 1.** Scattering efficiency with explicit contributions of toroidal moments of 1st order: TED and TED2 – toroidal electric dipoles (a), the 2nd order toroidal moments TMD - toroidal magnetic dipole and TEQ - toroidal electric quadrupole (b), and the 3rd order: TMQ toroidal magnetic quadrupole and TEO toroidal electric octupole (c).
Figure 1 shows that irreducible representation provides an additional information about configurations of charges and currents inside a scatterer and the integral contribution of basic and toroidal moments in the far field. Panels (a,b,c) demonstrate shifts of scattering efficiency minima, so-called anapole states, for basic moments having toroidal contributions. The scattering efficiency minima are explained by the destructive interference of basic and toroidal moments in far-field. At the same time the introduced toroidal moments reveal spectral points, where they have predominant contribution in the scattered field. Those spectral points are observed at the minima of basic multipole moments.

Conclusion:
Irreducible representation match the requirement for the tensors to be invariant regarding transformations on SO3 group. The primitive Cartesian multipoles were simplified to irreducible form using symmetrization and detracing processes. The combination of residual terms allows to reveal explicit contribution of toroidal moments to the scattered power. Toroidal moments have identical propagators as corresponding basic counterpart. Proposed multipole decomposition method allows to separate scattering contribution of the basic and toroidal multipoles in far-field zone.

Acknowledgement
The authors acknowledge the financial support provided by Russian Fund for Basic Research (Projects No. 18-02-00414, 18-52-00005); Government of Russian Federation, Grant 08-08.

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