Multipole matrix elements of Green function of Laplace equation

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Multipole matrix elements of Green function of Laplace equation are calculated. The multipole matrix elements of Green function in electrostatics describe potential on a sphere which is produced by a charge distributed on the surface of a different (possibly overlapping) sphere of the same radius. The matrix elements are defined by double convolution of two spherical harmonics with the Green function of Laplace equation. The method we use relies on the fact that in the Fourier space the double convolution has simple form. Therefore we calculate the multipole matrix from its Fourier transform. An important part of our considerations is simplification of the three dimensional Fourier transformation of general multipole matrix by its rotational symmetry to the one-dimensional Hankel transformation.

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I. INTRODUCTION

Metallic spheres in a vacuum, minute spherical particles in a fluid, and spherical inclusions in a solid body are often considered in statistical physics of dispersive media [1]. Equations which describe those systems are linear and have spherical symmetry. It is the case of Laplace equation in dielectrics [2], Stokes equations in suspensions [3] and Lamé equations [4] describing solid body. The first step in considerations of dispersive media is often to solve a single particle problem. In dielectrics it means to find distribution of charge on the surface of a single metallic sphere in an external electrostatic potential. To find the solution of single particle problem it is convenient to take spherical symmetry into account [5]. To this end one introduces a set of scalar functions on the sphere which is invariant under rotations. That is how spherical harmonics \( Y_{lm}(\hat{r}) \) enter calculations.

To pass from considerations of a single particle to the analysis of many particles it demands to answer the following question. What is the electrostatic potential produced by a charge distributed in one spherical surface in the area occupied by a different sphere. The answer to the above question can be inferred from the following multipole matrix element

\[
[G(R, R')]_{lm, l'm'} = \int d^3r \int d^3r' \frac{1}{a} \delta (|r - R| - a) \phi^*_{lm} (r - R) G (r - r') \frac{1}{a} \delta (|r' - R'| - a) \phi_{l'm'} (r' - R').
\]  

In the above definition \( G(r) \) is the Green function of Laplace equation [2],

\[
G(r) = \frac{1}{4\pi r},
\]

\( a \) is radius of particles, and one-dimensional Dirac delta distribution \( \delta (x) \) is used. Moreover \( \phi_{lm} (r) \) are solid harmonics defined by

\[
\phi_{lm} (r) = r^l Y_{lm}(\hat{r}),
\]

with spherical harmonics \( Y_{lm}(\hat{r}) \) numbered by order \( l \) and azimuthal number \( m = -l, \ldots, l \) [6]. In our notation an argument of spherical harmonics is a versor \( \hat{r}(\theta, \phi) \) in direction described by angles \( \theta, \phi \) in spherical coordinates. Dirac delta distributions in equation (1) reduce three-dimensional integrations to integrals over the surface of the spheres with radius \( a \) centered at positions \( R \) and \( R' \).

We can differentiate between two situations. The first situation corresponds to nonoverlapping spheres, i.e. when \( |R - R'| > 2a \). In this case the matrix elements defined by equation (1) can be inferred from the results in the literature [1]. They have application e.g. in numerical simulations. The second situation is the case of overlapping configurations, \( |R - R'| < 2a \). Even if the particles in the system cannot overlap there may appear a need of calculation of overlapping configurations of the multipole matrix elements \( G(R, R') \) defined by equation (1). For example, it has been recognized that overlapping configurations appear in microscopic explanation of the famous Clausius-Mossotti formula for dielectric constant [5]. In this context integral \( \int_{|R-R'|<2a} d^3r' (G(R, R')) \exp (-ikR')_{lm, l'm'} \) for low multipole numbers \( l, l' \) has been considered. Therefore the multipole matrix elements \( G(R, R') \) for overlapping configurations play an important role in statistical physics considerations of dispersive media.

In this article we give general expression for the multipole matrix elements \( G(R, R') \) defined by equation (1). The new contribution of the current article is the calculation of \( G(R, R') \) for overlapping configurations \( |R - R'| < 2a \). We are going to use the result for overlapping configurations in our statistical physics considerations of transport properties of dispersive media in further work.

The method of calculation of the multipole matrix elements defined by equation (1) is the following. We observe that \( G(R, R') \) has the form of a double convolution of three functions - two solid harmonics and the Green function. Therefore we calculate the Fourier transform of the three functions, take their product, and then perform the inverse Fourier transform to obtain \( G(R, R') \). An important element of our calculations is to use spherical symmetry which allows to reduce the three-dimensional Fourier transform of the multipole matrix to the one-dimensional Hankel transform.

II. MULTIPOLe MATRIX IN THE FOURIER SPACE

The aim of this article is calculation of integral (1). We can simplify it using homogeneity of the Laplace equation which implies that the multipole matrix \( G(R, R') \) depends on the relative positions \( R - R' \). Therefore from now on we consider multipole matrix \( G(R) \) defined by
\[ G(R - R')_{lm,l'm'} = [G(R,R')]_{lm,l'm'} \]
depending on the relative positions.

Next, we observe that the multipole matrix given by the formula (1) has a form of a double convolution of three functions. The three functions are \( \omega_{l+m'}(r) \equiv \delta((r-a) \phi_{l+m'}(r))/a \), conjugated function \( \omega^*_{lm}(r) \), and the Green function \( G(r) \). The Fourier transform of a double convolution of the three functions is given by the product of their Fourier transforms, therefore

\[ \hat{G}(k)_{lm,l'm'} = \hat{\omega}^*_{lm}(k) \hat{G}(k) \hat{\omega}_{l'm'}(k). \]

In our calculations we use the following definition of the three-dimensional Fourier transform

\[ \hat{G}_{lm,l'm'}(k) = \int d^3R \exp(-ikR) G_{lm,l'm'}(R), \] 

with the inverse transformation given by the formula

\[ G_{lm,l'm'}(R) = \frac{1}{(2\pi)^3} \int d^3k \exp(ikR) \hat{G}_{lm,l'm'}(k). \]

In this situation the Fourier transforms of \( \omega_{lm}(r) \) and \( G(r) \) are given respectively by

\[ \hat{G}(k) = \frac{1}{k^2}, \]

and

\[ \hat{\omega}_{lm}(k) = 4\pi a^{l+1} (-i)^l j_l (ka) Y_{lm}(\hat{k}). \]

The last expression can be calculated with the use of equation (5.8.3) from Ref. [6] and with the use of orthonormality of spherical harmonics. The expression contains spherical Bessel functions \( j_l(x) \) of the order \( l \). Finally, the Fourier transform of multipole matrix (1) is given by the following formula

\[ \hat{G}(k)_{lm,l'm'} = (4\pi)^2 (-i)^{-l+l'} a^{l+l'+2} \frac{\hat{j}_l(ka) j_{l'}(ka)}{k^2} Y_{lm}(\hat{k}) Y_{l'm'}(\hat{k}). \]

(3)

According to the above expression, the Fourier transform of \[ G(R)_{lm,l'm'} \] is given by the spherical harmonics and the spherical Bessel functions. At this point we face the main difficulty in our calculations of \[ G(R)_{lm,l'm'}. \] The inverse Fourier transform of the above formula has to be calculated. To this end we consider rotational symmetry of the multipole matrix.

### III. ROTATIONAL SYMMETRY OF A MULTIPOLe MATRIX

In the definition of the multipole matrix (1) there appear solid harmonics \( \phi_{lm}(r) \) and Green function \( G(r) \). Transformation of solid harmonics under rotation is given by the formula

\[ \phi_{lm}(D(\alpha,\gamma,\beta) r) = \sum_{m_1=-l}^{l} [D^{(l)}(\alpha,\gamma,\beta)]^*_{m_1m} \phi_{lm_1}(r). \]

(4)

The above expression can be inferred from Ref. [6] from which we adopt notation in this article. There, formula (4.1.1) defines three-dimensional rotation matrix \( D(\alpha,\beta,\gamma) \) characterized by the Euler angles \( \alpha,\beta,\gamma \). Moreover, \( D^{(l)}_{m_1m}(\alpha,\beta,\gamma) \) denotes the Wigner matrix. Isotropy of the Laplace equation implies that its Green function \( G(r) \) is invariant under rotation, i.e. \( G(D(\alpha,\beta,\gamma) r) = G(r) \).
Changing the variables in the integrals in Eq. (1) and the above properties of the solid harmonics and the Green function lead us to the following transformation of the multipole matrix elements under rotation

$$G_{l,m',m'}(D(\alpha, \beta, \gamma) R) = \sum_{m_1, m_1'} D_{m,m_1}^{(l)}(\alpha, \beta, \gamma) \left[ D_{m',m_1'}^{(l)}(\alpha, \beta, \gamma) \right]^{*} G_{lm',m'_m}(R).$$

(5)

It is worth mentioning here that the above transformation applied for $R$ in $z$ direction, $R = R\hat{e}_z$, and for any rotations around axis $z$, thus for $\beta = 0$ and any other Euler angles, implies that the multipole matrix is diagonal in indexes $m$, i.e.

$$G_{l,m',m'}(R\hat{e}_z) = \delta_{m,m'}G_{lm',m'}(R\hat{e}_z),$$

where Kronecker delta $\delta_{m,m'}$ appears. It is easy to prove similar diagonality in case of the Fourier transform,

$$\hat{G}_{l,m',m'}(k\hat{e}_z) = \delta_{m,m'}\hat{G}_{lm',m'}(k\hat{e}_z),$$

(6)

which appears as a result of Fourier transformation of equation (5) and considerations for proper rotations and wave vector $k = k\hat{e}_z$.

**IV. FOURIER TRANSFORM OF MULTIPole MATRIX - SIMPLIFICATION BY ROTATIONAL SYMMETRY**

The key point of our calculations is simplification of the Fourier transform of a matrix satisfying symmetry property given by equation (6). We simplify the Fourier transform for a wave vector along $z$ direction because then the multipole matrix is diagonal in indexes $m$, as is shown by equation (7). For the case $k = k\hat{e}_z$ expression (2) written in spherical coordinates reads

$$\hat{G}_{l,m',m'}(k\hat{e}_z) = \int_{0}^{\infty} dR \int_{0}^{\pi} d\theta \int_{0}^{2\pi} d\phi R^2 \sin \theta \exp(-ikR \cos \theta) G_{lm',m'}(R, \theta, \phi).$$

(7)

We express vector $R(\theta, \phi)$ by a product of the vector $R\hat{e}_z$ and the rotation matrix $D(\alpha, \beta, \gamma)$ characterized with proper Euler angles. The angles can be deduced from formula (4.1.1) in Ref. [6]. These angles are $\beta = -\theta, \gamma = -\phi$, and any $\alpha$, e.g. $\alpha = 0$. Therefore $R(\theta, \phi) = D(0, -\theta, -\phi) R\hat{e}_z$. For this rotation and $R = R\hat{e}_z$ we use symmetry property (5) which leads to the following expression for multipole matrix $G$

$$G_{lm',m'}(R(\theta, \phi)) = \sum_{m_1, m_1'} D_{m,m_1}^{(l)}(0, -\theta, -\phi) \left[ D_{m',m_1'}^{(l)}(0, -\theta, -\phi) \right]^{*} G_{lm',m'_m}(R\hat{e}_z).$$

(8)

In the next step we represent $\exp(-ikR \cos \theta)$ from expression (7) in the form of an infinite series of spherical Bessel functions

$$\exp(-ikR \cos \theta) = \sum_{l_1 = 0}^{\infty} (-i)^{l_1}(2l_1 + 1) j_{l_1}(kR) D_{00}^{(l_1)}(0, -\theta, -\phi), number$$

which is deduced from formula (5.8.1) and (4.1.26) in the reference [6]. Taking into consideration the last two formulae in expression (7) yields

$$\hat{G}_{l,m',m'}(k\hat{e}_z) = \int_{0}^{\infty} dRR^2 \sum_{l_1 = 0}^{\infty} (-i)^{l_1}(2l_1 + 1) j_{l_1}(kR) G_{lm',m'_m}(R\hat{e}_z) \times$$

$$\sum_{m_1, m_1'} \int_{0}^{\pi} d\theta \int_{0}^{2\pi} d\phi \sin \theta D_{00}^{(l_1)}(0, \theta, \phi) D_{m,m_1}^{(l)}(0, \theta, \phi) \left[ D_{m',m_1'}^{(l)}(0, \theta, \phi) \right]^{*}.$$  

(9)

Integration over variables $\theta, \phi$ in the above formula is performed with the use of formulae (4.6.2), (4.1.12) and (4.2.7) from the reference [6]. They lead to expression

$$\int_{0}^{\pi} d\theta \int_{0}^{2\pi} d\phi \sin \theta D_{00}^{(l_1)}(0, \theta, \phi) D_{m,m_1}^{(l)}(0, \theta, \phi) \left[ D_{m',m_1'}^{(l)}(0, \theta, \phi) \right]^{*}$$

$$= 4\pi (-1)^{m'-m_1} \begin{pmatrix} l & l' & l_1 \\ m & -m' & 0 \end{pmatrix} \begin{pmatrix} l & l' & l_1 \\ m_1 & -m_1' & 0 \end{pmatrix},$$
which contains Wigner 3-$j$ symbols. Taking into account the above integral in expression (9) yields

$$
\hat{G}_{l,m',m} (k\hat{e}_z) = 4\pi \sum_{l_1=|l-l'|}^{l+l'} \sum_{m_1=-l_1}^{l_1} \sum_{m'_{1}=-l_1}^{l_1} (-1)^{m'-m_1'} (2l_1 + 1) \left( \begin{array}{ccc} l & l' & l_1 \\ m & -m' & 0 \end{array} \right) \left( \begin{array}{ccc} l & l' & l_1 \\ m_1 & -m'_1 & 0 \end{array} \right) \times (-i)^{l_1} \int_0^\infty dR R^2 j_{l_1} (kR) G_{l,m',m_1} (R\hat{e}_z) .
$$

In this way the three-dimensional Fourier transform is reduced to the one dimensional Hankel transform.

It is convenient to introduce different representation of matrix $G$. Namely, instead of $G_{l,m',m} (R\hat{e}_z)$ we can consider $g_{l',m'}^j (R)$ defined in the following way

$$
g_{l',m'}^j (R) = (2j + 1) \sum_{m,m'} (-1)^m \left( \begin{array}{ccc} l & l' & j \\ m & -m' & 0 \end{array} \right) G_{l,m',m} (R\hat{e}_z) .
$$

with the inverse transformation

$$
G_{l,m',m} (R\hat{e}_z) = \delta_{m,m'} (-1)^m \sum_{j=|l-l'|}^{l+l'} \left( \begin{array}{ccc} l & l' & j \\ m & -m' & 0 \end{array} \right) g_{l',m'}^j (R) .
$$

Let us notice that only integer $j$ which satisfy condition $|l-l'| \leq j \leq l+l'$ needs to be considered in the above equations. It follows from properties of Wigner 3-$j$ symbols. The multipole matrix elements $G_{l,m',m} (R)$ for any $R$ are then related to $g_{l',m'}^j (R)$ by equation

$$
G_{l,m',m} (R, \theta, \phi) = \sum_{m_1} (-1)^{m'+m_1} \sum_{j=|l-l'|}^{l+l'} \left( \begin{array}{ccc} l & l' & j \\ m & -m' & m_1 \end{array} \right) D_{m_1\phi}^{(j)} (0, \theta, -\phi) g_{l',m'}^j (R) ,
$$

which follows from equation (5) and relation (12).

Different representations of the multipole matrix $G_{l,m',m} (R\hat{e}_z)$ in positional space given by equations (11) and (12) can be similarly introduced also in Fourier space, i.e.

$$
\hat{g}_{l',m'}^j (k) = (2j + 1) \sum_{m,m'} (-1)^m \left( \begin{array}{ccc} l & l' & j \\ m & -m' & 0 \end{array} \right) \hat{G}_{l,m',m} (k\hat{e}_z) .
$$

$$
\hat{G}_{l,m',m} (k\hat{e}_z) = \delta_{m,m'} (-1)^m \sum_{j=|l-l'|}^{l+l'} \left( \begin{array}{ccc} l & l' & j \\ m & -m' & 0 \end{array} \right) \hat{g}_{l',m'}^j (k) .
$$

By equations (10), (14), and (12) and orthogonality of Wigner 3-$j$ symbols, we get that in the new basis the Fourier transform of the multipole matrix is expressed in the following form

$$
g_{l',m'}^j (k) = 4\pi (-i)^j \int_0^\infty dR R^2 j_j (kR) g_{l',m'}^j (R) .
$$

In this way the three-dimensional Fourier transform given by expression (2) of a multipole matrix satisfying rotational symmetry is reduced to relevant Hankel transform given by expression (10).

Calculations performed in this section can be repeated with very minor modification in order to reduce the inverse three-dimensional Fourier transform of a multipole matrix to the one-dimensional Hankel transform. We omit the derivation giving only the result for the inverse Fourier transform of a multipole matrix satisfying rotational symmetry,

$$
g_{l',m'}^j (R) = \frac{1}{2\pi^2 i^d} \int_0^\infty dk k^2 j_j (kR) \hat{g}_{l',m'}^j (k) .
$$
V. MULTIPOLe MATRIX IN POSITIONAL SPACE

To calculate the inverse Fourier transform of \( \hat{G}(k) \) with the use of equation (17), \( g_{l',l}^j(k) \) is needed. We calculate it by means of transformation (13) and expression (3) for \( \hat{G}_{lm,l'm'}(k\hat{e}_z) \). The calculations yields

\[
g_{l',l}^j(k) = 4\pi (-i)^{-l+l'} (2j+1) [(2l+1)(2l'+1)]^{1/2} a^{l+l'+2} \left( \begin{array}{ccc} l & l' & j \\ 0 & 0 & 0 \end{array} \right) \frac{j_l(k\alpha) j_{l'}(k\alpha)}{k^2}. \tag{18}
\]

It is worth noting that the Wigner \( 3-j \) symbol is not vanishing only when the \( l, l', j \) satisfy triangular inequality, \( |l - l'| \leq j \leq |l + l'| \). In calculations of the above formula we used the following property of the spherical harmonics, \( Y_{jm}(\hat{e}_z) = \delta_{m,0} ((2j+1)/4\pi)^{1/2} \).

With the above expression for \( g_{l',l}^j(k) \), equation (17) yields

\[
g_{l',l}^j(R) = \mu_{j,l,l'} a^{l+l'+2} \int_0^\infty dk \ j_j(kR) j_l(k\alpha) j_{l'}(ka) \tag{19}
\]

with

\[
\mu_{j,l,l'} = \frac{2(-i)^{-l+l'+j} (-1)^j}{\pi} (2j+1) [(2l+1)(2l'+1)]^{1/2} \left( \begin{array}{ccc} l & l' & j \\ 0 & 0 & 0 \end{array} \right). \tag{20}
\]

It demands to calculate integral of three spherical Bessel functions. That has already been considered in the literature [10]. For \( R \geq 2a \), the integral is given as follows

\[
\int_0^\infty dk \ j_j(kR) j_l(k\alpha) j_{l'}(ka) = \frac{\pi^{3/2}}{8a} \delta_{l,l'} \frac{a}{R} \frac{l+l'+1}{(l+1) \Gamma(\frac{3}{2} + l + l')} \frac{\Gamma(\frac{1}{2} + l + l')}{\Gamma(\frac{1}{2} + l') \Gamma(\frac{1}{2} + l)}, \tag{21}
\]

with Euler Gamma function \( \Gamma(x) \). Whereas for \( R \leq 2a \) we have

\[
\int_0^\infty dk \ j_j(kR) j_l(k\alpha) j_{l'}(ka) = \frac{\pi^{3/2}}{2a} R \frac{a}{\alpha_{j,l,l'}} F_3 \left( \frac{l-l'}{2}, \frac{1+l-l'}{2}, \frac{1-l+l'}{2}, \frac{2+l+l'}{2}; \frac{1}{2}, \frac{3-j}{2}, \frac{4+j}{2}; \frac{R^2}{4a^2} \right) \\
+ \frac{\pi^{3/2}}{2a} R \frac{a}{\beta_{j,l,l'}} F_3 \left( \frac{l-l'}{2}, \frac{1+l-l'}{2}, \frac{1-j+l'}{2}, \frac{2+l+l'}{2}; \frac{1}{2}, \frac{3+j}{2}, \frac{3+j}{2}; \frac{R^2}{4a^2} \right) \\
- \frac{\pi^{3/2}}{2a} R \frac{a}{\gamma_{j,l,l'}} F_3 \left( \frac{l-l'}{2}, \frac{1+l-l'}{2}, \frac{1+j-l'}{2}, \frac{2+l+l'}{2}; \frac{1}{2}, \frac{3+j}{2}, \frac{3+j}{2}; \frac{R^2}{4a^2} \right) \tag{22}
\]

with coefficients \( \alpha_{j,l,l'}, \beta_{j,l,l'}, \) and \( \gamma_{j,l,l'} \) given by

\[
\alpha_{j,l,l'} = 2^{-5/2} \frac{\Gamma\left(\frac{l-l'}{2}\right)}{\Gamma\left(1+l+l'-\frac{j}{2}\right) \Gamma\left(\frac{1+l-l'}{2}\right) \Gamma\left(\frac{1+l'+l'}{2}\right)},
\]

\[
\beta_{j,l,l'} = 2^{-3/2} \frac{\Gamma\left(1-j\right) \Gamma\left(\frac{l+l+l'+l'}{2}\right)}{\Gamma\left(1+\frac{l+l-l'}{2}\right) \Gamma\left(1+\frac{l+l-l'}{2}\right) \Gamma\left(1+\frac{l+l-l'}{2}\right) \Gamma\left(\frac{3+j}{2}\right) \Gamma\left(\frac{3+j}{2}\right)},
\]

\[
\gamma_{j,l,l'} = -2^{-7/2} \frac{\Gamma\left(\frac{j}{2}\right)}{\Gamma\left(\frac{l-l}{2}\right) \Gamma\left(\frac{1+l-l'}{2}\right) \Gamma\left(2+\frac{l+l}{2}\right)}. \tag{23}
\]

Symbol \( 4F_3 \) stands for hypergeometric function

\[
4F_3(\alpha_1, \alpha_2, \alpha_3, \alpha_4; \beta_1, \beta_2, \beta_3; x) = \sum_{k=0}^{\infty} \frac{(\alpha_1)_k (\alpha_2)_k (\alpha_3)_k (\alpha_4)_k}{(\beta_1)_k (\beta_2)_k (\beta_3)_k} \frac{x^k}{k!}
\]
where $(\alpha)_k$ denotes Pochhammer symbol defined by

\[
(\alpha)_0 = 1 \\
(\alpha)_k = \alpha (\alpha + 1) \ldots (\alpha + k - 1) \quad \text{for} \quad k = 1, 2, \ldots
\]

For nonoverlapping configurations $R > 2a$, the multipole matrix elements are given by formulae (19), (20), and (21). Therefore in this regime $g_{1\nu}^l (R)$ is proportional to $1/R^{l+l'+1}$.

For overlapping configurations, $R < 2a$, the multipole matrix elements are given by formulae (19), (20), and (22) with equations (23). For small $l$ and $l'$, analysis of the poles in Euler gamma functions and in Pochhammer symbols (which may also be expressed by Euler gamma functions) reveals that for overlapping configurations $g_{1\nu}^l (R)$ is a polynomial with respect to $R$. We observe that the degree of the polynomial is $l+l'+1$. For example

\[
g_{1,1}^0 (R < 2a) = -\frac{(-2a + R)^2 (4a + R)}{16\sqrt{3}}, \quad (24)
\]

\[
g_{2,3}^3 (R < 2a) = -7\frac{(-4a^2 R + R^3)^2}{256\sqrt{3}}. \quad (25)
\]

VI. SUMMARY

In this article we calculate the multipole matrix elements of Green function for Laplace equation. The elements are defined by equation (1). The expression for nonoverlapping configurations, i.e. for $R > 2a$, is known in the literature and can be inferred e.g. from the reference [7]. The new contribution is the calculation of expression (1) for overlapping configurations, i.e. for $R < 2a$. In this case one can find related considerations for the lowest multipole numbers [8].

It is worth mentioning that the method which we use to calculate multipole matrix for Laplace equation can be generalized for other cases, because the considerations rely on simplification of the Fourier transform. For example, the method can be generalized to the multipole matrix elements of Green function for Stokes equations in hydrodynamics [11–13]. In this case overlapping configurations of multipole Green function for the lowest multipoles have been considered recently in the literature [14].

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