MULTIPOLE MATRIX OF GREEN FUNCTION OF LAPLACE EQUATION

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Multipole matrix of the Green function of the Laplace equation defined by double convolution of two spherical harmonics with the Green function of the Laplace equation is calculated. The multipole matrix elements 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. We calculate the multipole matrix from its Fourier transform. An essential part of our considerations is simplification of the three-dimensional Fourier transformation of a multipole matrix by its rotational symmetry to the one-dimensional Hankel transformation.

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1. 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 a 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 $Y_{lm}(\hat{\boldsymbol{r}})$ enter calculations.

To pass from considerations of a single particle to the analysis of many particles in a dispersive medium, it demands to answer the following question. What is the electrostatic potential produced by a charge distributed on 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

$$\left[G\left(\boldsymbol{R},\boldsymbol{R}'\right)\right]_{lm,l'm'} = \int\limits_{\mathcal{R}^3} d^3r \int\limits_{\mathcal{R}^3} d^3r' \frac{1}{a}\delta\left(\left|\boldsymbol{r}-\boldsymbol{R}\right|-a\right)\phi^*_{lm}\left(\boldsymbol{r}-\boldsymbol{R}\right)\boldsymbol{G}\left(\boldsymbol{r}-\boldsymbol{r}'\right) \times\frac{1}{a}\delta\left(\left|\boldsymbol{r}'-\boldsymbol{R}'\right|-a\right)\phi_{l'm'}\left(\boldsymbol{r}'-\boldsymbol{R}'\right) . \quad (1)$$

In the above definition, $\boldsymbol{G}\left(\boldsymbol{r}\right)$ is the Green function of Laplace equation [2],

$$\boldsymbol{G}\left(\boldsymbol{r}\right) = \frac{1}{4\pi r} ,$$

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

$$\phi_{lm}\left(\boldsymbol{r}\right) = r^{-l-1}Y_{lm}\left(\hat{\boldsymbol{r}}\right) ,$$

with spherical harmonics $Y_{lm}\left(\hat{\boldsymbol{r}}\right)$ numbered by order $l = 0, 1, \ldots$ and azimuthal number $m = -l, \ldots, l$ [6]. In our notation, an argument of spherical harmonics is a versor $\hat{\boldsymbol{r}}\left(\theta,\phi\right)$ in direction described by angles θ, ϕ 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 $\boldsymbol{R}$ and $\boldsymbol{R}'$.

We can differentiate between two situations. The first situation corresponds to non-overlapping spheres, *i.e.* when $|\boldsymbol{R}-\boldsymbol{R}'| > 2a$. In this case, the matrix elements defined by equation (1) can be inferred from the results in the literature [7]. They have application *e.g.* in numerical simulations. The second situation is the case of overlapping configurations, $|\boldsymbol{R}-\boldsymbol{R}'| < 2a$. Even if the particles in the system cannot overlap, there may appear a need of calculation of overlapping configurations of the multipole matrix elements $\left[G\left(\boldsymbol{R},\boldsymbol{R}'\right)\right]_{lm,l'm'}$. For example, it has been recognized that overlapping configurations appear in microscopic explanation of the famous Clauius–Mossotti formula for dielectric constant [8]. In this context, integral $\int_{\left|\boldsymbol{R}-\boldsymbol{R}'\right|<2a} d^3R' \left[G\left(\boldsymbol{R},\boldsymbol{R}'\right)\right]\exp\left(-i\boldsymbol{k}\left(\boldsymbol{R}'-\boldsymbol{R}\right)\right)_{lm,l'm'}$ for low multipole numbers l, l' has been considered. Therefore, the multipole matrix elements $\left[G\left(\boldsymbol{R},\boldsymbol{R}'\right)\right]_{lm,l'm'}$ for overlapping configurations play an important role in statistical physics considerations of dispersive media.

The multipole matrix for overlapping configurations calculated in our article potentially has another very important application. In nature and in industry, there are plenty of dispersive media composed of spherical particles. Numerical calculations in this context are simplified by spherical symmetry. But there are also plenty of dispersive media composed of non-spherical objects for which, due to lack of spherical symmetry of the particles, the numerical approach is more difficult. One of the possible extensions from spherical to non-spherical objects in numerical approach is to build a non-spherical particle from conglomerate of spherical particles. This approach is well known in the literature when particles in a conglomerate do not overlap. The result of our paper allows to generalize this approach to build a conglomerate made of overlapping particles. This can be of great interests for scientists interested in modelling of dispersive media of non-spherical objects.

In this article, we give general expression for the multipole matrix elements $[G(\boldsymbol{R},\boldsymbol{R}')]_{lm,l'm'}$ defined by equation (1). The method of calculation of the multipole matrix elements defined by equation (1) is the following. We observe that $[G(\boldsymbol{R},\boldsymbol{R}')]_{lm,l'm'}$ 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 $G(\boldsymbol{R},\boldsymbol{R}')$. 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.

The new contribution of the current article is the calculation of $[G(\boldsymbol{R},\boldsymbol{R}')]_{lm,l'm'}$ for overlapping configurations $|\boldsymbol{R}-\boldsymbol{R}'| < 2a$. It is worth mentioning that the reduction of the three-dimensional Fourier transform of the multipole matrix to the one-dimensional Hankel transform which we perform in this article is of general character. It means that the reduction can be performed with minor changes in the context of multipole matrices of the Green function for other differential equations like, *e.g.*, Stokes equations in hydrodynamics.

2. 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 $[G(\boldsymbol{R},\boldsymbol{R}')]_{lm,l'm'}$ depends on the relative positions $\boldsymbol{R}-\boldsymbol{R}'$. Therefore, from now on, we consider multipole matrix $[G(\boldsymbol{R})]_{lm,l'm'}$ defined by

$$\left[G\left(\boldsymbol{R}-\boldsymbol{R}'\right)\right]_{lm,l'm'} = \left[G\left(\boldsymbol{R},\boldsymbol{R}'\right)\right]_{lm,l'm'}$$

depending on the relative positions.

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

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

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

$$\hat{G}_{lm,l'm'}(\boldsymbol{k}) = \int d^3R\ \exp(-i\boldsymbol{k}\boldsymbol{R})\,G_{lm,l'm'}(\boldsymbol{R}) \ , \tag{2}$$

with the inverse transformation given by the formula

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

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

$$\hat{\boldsymbol{G}}(\boldsymbol{k}) = \frac{1}{k^2} \ ,$$

and

$$\hat{\omega}_{lm}(\boldsymbol{k}) = 4\pi a^{-l}(-i)^l\,j_l(ka)\,Y_{lm}\left(\hat{\boldsymbol{k}}\right) \ .$$

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 of l. Finally, the Fourier transform of multipole matrix (1) is given by the following formula

$$\left[\hat{G}(\boldsymbol{k})\right]_{lm,l'm'} = (4\pi)^2(-i)^{-l+l'}\,a^{-l-l'}\frac{j_l(ka)\,j_{l'}(ka)}{k^2}Y^*_{lm}\left(\hat{\boldsymbol{k}}\right)Y_{l'm'}\left(\hat{\boldsymbol{k}}\right) \ . \tag{3}$$

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

3. Rotational symmetry of a multipole matrix

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

$$\phi_{lm}(\boldsymbol{D}(\alpha,\gamma,\beta)\,\boldsymbol{r}) = \sum_{m_1=-l}^{l}\left[D^{(l)}(\alpha,\gamma,\beta)\right]^*_{mm_1}\phi_{lm_1}(\boldsymbol{r}) \,. \tag{4}$$

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 $\boldsymbol{D}(\alpha,\beta,\gamma)$ characterized by the Euler angles α,β,γ. Moreover, $D^{(l)}_{mm'}(\alpha,\beta,\gamma)$ denotes the Wigner matrix. Isotropy of the Laplace equation implies that its Green function $\boldsymbol{G}(\boldsymbol{r})$ is invariant under rotation, *i.e.* $\boldsymbol{G}(\boldsymbol{D}(\alpha,\beta,\gamma)\,\boldsymbol{r}) = \boldsymbol{G}(\boldsymbol{r})$.

Changing the variables in the integrals in Eq. (1) and the above properties of the solid harmonics and the Green function leads us to the following transformation of the multipole matrix elements under rotation

$$\begin{aligned} &G_{lm,l'm'}(\boldsymbol{D}(\alpha,\beta,\gamma)\,\boldsymbol{R}) \\ &= \sum_{m_1,m_1'} D^{(l)}_{m,m_1}(\alpha,\beta,\gamma)\left[D^{(l')}_{m',m_1'}(\alpha,\beta,\gamma)\right]^* G_{lm_1,l'm_1'}(\boldsymbol{R}) \,. \end{aligned} \tag{5}$$

It is worth mentioning here that the above transformation applied for $\boldsymbol{R}$ in z direction, $\boldsymbol{R} = R\hat{\boldsymbol{e}}_z$, 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.*

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

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

$$\hat{G}_{lm,l'm'}(k\hat{\boldsymbol{e}}_z) = \delta_{m,m'}\hat{G}_{lm,l'm}(k\hat{\boldsymbol{e}}_z) \,, \tag{6}$$

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

4. 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 (5). 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 (6). For the case $\boldsymbol{k} = k\hat{\boldsymbol{e}}_z$, expression (2) written in spherical coordinates reads

$$\hat{G}_{lm,l'm'}\left(k\hat{\boldsymbol{e}}_z\right) = \int\limits_0^\infty dR \int\limits_0^\pi d\theta \int\limits_0^{2\pi} d\phi R^2 \sin\theta \exp\left(-ikR\cos\theta\right) G_{lm,l'm'}\left(\boldsymbol{R}\left(R,\theta,\phi\right)\right) . \quad (7)$$

We express vector $\boldsymbol{R}\left(R,\theta,\phi\right)$ by a product of the vector $R\hat{\boldsymbol{e}}_z$ and the rotation matrix $\boldsymbol{D}\left(\alpha,\beta,\gamma\right)$ 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 α, *e.g.* $\alpha = 0$. Therefore, $\boldsymbol{R}\left(R,\theta,\phi\right) = \boldsymbol{D}\left(0,-\theta,-\phi\right) R\hat{\boldsymbol{e}}_z$. For this rotation and $\boldsymbol{R} = R\hat{\boldsymbol{e}}_z$, we use symmetry property (5) which leads to the following expression for multipole matrix G

$$G_{lm,l'm'}\left(\boldsymbol{R}\left(R,\theta,\phi\right)\right) = \sum_{m_1,m_1'} D^{(l)}_{m,m_1}\left(0,-\theta,-\phi\right) \left[D^{(l')}_{m',m_1'}\left(0,-\theta,-\phi\right)\right]^* G_{lm_1,l'm_1'}\left(R\hat{\boldsymbol{e}}_z\right) . \quad (8)$$

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

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

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

$$\hat{G}_{lm,l'm'}\left(k\hat{\boldsymbol{e}}_z\right) = \int\limits_0^\infty dR R^2 \sum_{l_1=0}^{\infty} \left(-i\right)^{l_1} \left(2l_1+1\right) j_{l_1}\left(kR\right) G_{lm_1,l'm_1'}\left(R\hat{\boldsymbol{e}}_z\right)$$
$$\times \sum_{m_1,m_1'} \int\limits_0^\pi d\theta \int\limits_0^{2\pi} d\phi \sin\theta D^{(l_1)}_{00}\left(0,\theta,\phi\right) D^{(l)}_{m,m_1}\left(0,\theta,\phi\right) \left[D^{(l')}_{m',m_1'}\left(0,\theta,\phi\right)\right]^* . \quad (9)$$

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

$$\begin{aligned} \hat{G}_{lm,l'm'}(k\hat{\boldsymbol{e}}_z) \;=\; & 4\pi \sum_{l_1=|l-l'|}^{|l+l'|} \sum_{m_1=-l}^{l} \sum_{m_1'=-l'}^{l'} (-1)^{m'-m_1'}(2l_1+1) \\ & \times \begin{pmatrix} l & l' & l_1 \\ m & -m' & 0 \end{pmatrix}\begin{pmatrix} l & l' & l_1 \\ m_1 & -m_1' & 0 \end{pmatrix} \\ & \times (-i)^{l_1}\int_0^{\infty} dR R^2 j_{l_1}(kR)\, G_{lm_1,l'm_1'}(R\hat{\boldsymbol{e}}_z)\,. \end{aligned} \tag{10}$$

In this way, the three-dimensional Fourier transform is reduced to the one-dimensional Hankel transform [9].

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

$$g_{l,l'}^{j}(R) = (2j+1)\sum_{m,m'}(-1)^m \begin{pmatrix} l & l' & j \\ m & -m' & 0 \end{pmatrix} G_{lm,l'm'}(R\hat{\boldsymbol{e}}_z) \tag{11}$$

with the inverse transformation

$$G_{lm,l'm'}(R\hat{\boldsymbol{e}}_z) = \delta_{m,m'}(-1)^m \sum_{j=|l-l'|}^{l+l'} \begin{pmatrix} l & l' & j \\ m & -m' & 0 \end{pmatrix} g_{l,l'}^{j}(R)\,. \tag{12}$$

Let us notice that only integer j which satisfies the condition $|l-l'| \le j \le l+l'$ needs to be considered in the above equations. It follows from properties of Wigner 3-j symbols. The multipole matrix elements $G_{lm,l'm'}(\boldsymbol{R})$ for any

$\boldsymbol{R}$ are then related to $g^{j}_{l,l'}(R)$ by equation

$$G_{lm,l'm'}\left(\boldsymbol{R}\left(R,\theta,\phi\right)\right) = \sum_{m_1}\left(-1\right)^{m'+m_1}\sum_{j=|l-l'|}^{l+l'}\begin{pmatrix} l & l' & j \\ m & -m' & m_1\end{pmatrix} D^{(j)}_{-m_1,0}\left(0,-\theta,-\phi\right) g^{j}_{l,l'}\left(R\right)\ , \tag{13}$$

which follows from equation (8) and relation (12).

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

$$\tilde{g}^{j}_{l,l'}\left(k\right) = \left(2j+1\right)\sum_{m,m'}\left(-1\right)^{m}\begin{pmatrix} l & l' & j \\ m & -m' & 0\end{pmatrix}\hat{G}_{lm,l'm'}\left(k\hat{\boldsymbol{e}}_z\right)\ , \tag{14}$$

$$\hat{G}_{lm,l'm'}\left(k\hat{\boldsymbol{e}}_z\right) = \delta_{m,m'}\left(-1\right)^{m}\sum_{j=|l-l'|}^{l+l'}\begin{pmatrix} l & l' & j \\ m & -m' & 0\end{pmatrix}\tilde{g}^{j}_{l,l'}\left(k\right)\ . \tag{15}$$

By equations (10), (12), and (14) and orthogonality of Wigner 3-j symbols [6], we get that in the new basis the Fourier transform of the multipole matrix is expressed in the following form

$$\tilde{g}^{j}_{l,l'}\left(k\right) = 4\pi\left(-i\right)^{j}\int_0^\infty dRR^2 j_j\left(kR\right) g^{j}_{l,l'}\left(R\right)\ . \tag{16}$$

In this way, the three-dimensional Fourier transform given by expression (2) of a multipole matrix satisfying rotational symmetry (5) is reduced to relevant Hankel transform given by expression (16).

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,

$$g^{j}_{l,l'}\left(R\right) = \frac{1}{2\pi^2} i^{j}\int_0^\infty dk\ k^2 j_j\left(kR\right)\tilde{g}^{j}_{l,l'}\left(k\right)\ . \tag{17}$$

5. Multipole matrix in positional space

To calculate the inverse Fourier transform of $\left[\hat{G}\left(\boldsymbol{k}\right)\right]_{lm,l'm'}$ with the use of equation (17), $\tilde{g}^{j}_{ll'}\left(k\right)$ is needed. We calculate it by means of transformation (14) and expression (3) for $\hat{G}_{lml'm'}\left(k\hat{\boldsymbol{e}}_z\right)$. The calculations yields

$$\begin{aligned}\tilde{g}^{j}_{l,l'}\left(k\right) &= 4\pi\left(-i\right)^{-l+l'}\left(2j+1\right)\left[\left(2l+1\right)\left(2l'+1\right)\right]^{1/2}a^{-l-l'}\\ &\quad\times\begin{pmatrix} l & l' & j\\ 0 & 0 & 0\end{pmatrix}\frac{j_l\left(ka\right)j_{l'}\left(ka\right)}{k^2}\,.\end{aligned}\tag{18}$$

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, $Y_{jm}\left(\hat{\boldsymbol{e}}_z\right)=\delta_{m,0}\left(\left(2j+1\right)/4\pi\right)^{1/2}$.

With the above expression for $\tilde{g}^{j}_{l,l'}\left(k\right)$, equation (17) yields

$$g^{j}_{l,l'}\left(R\right)=\mu_{j,l,l'}a^{-l-l'}\int\limits_0^\infty dk\; j_j\left(kR\right)j_l\left(ka\right)j_{l'}\left(ka\right)\tag{19}$$

with

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

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

$$\begin{aligned}&\int\limits_0^\infty dk\; j_{l_1}\left(kR\right)j_l\left(ka\right)j_{l'}\left(ka\right)\\ &=\frac{\pi^{3/2}}{8a}\delta_{l+l',l_1}\left(\frac{a}{R}\right)^{l+l'+1}\frac{\mathit{\Gamma}\left(\frac{1}{2}+l+l'\right)}{\mathit{\Gamma}\left(\frac{3}{2}+l\right)\mathit{\Gamma}\left(\frac{3}{2}+l'\right)}\,,\end{aligned}\tag{21}$$

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

$$\begin{aligned}
&\int_0^\infty dk\ j_j(kR)\, j_l(ka)\, j_{l'}(ka) \\
&= \frac{\pi^{3/2}}{2a}\frac{R}{a}\alpha_{j,l,l'}\ {}_4F_3 \\
&\times\left(\frac{-l-l'}{2},\frac{1+l-l'}{2},\frac{1-l+l'}{2},\frac{2+l+l'}{2};\frac{1}{2},\frac{3-j}{2},\frac{4+j}{2};\frac{R^2}{4a^2}\right) \\
&+\frac{\pi^{3/2}}{2a}\left(\frac{R}{a}\right)^j\beta_{j,l,l'}\ {}_4F_3 \\
&\times\left(\frac{j-l-l'-1}{2},\frac{j+l-l'}{2},\frac{j+l'-l}{2},\frac{l+l'+j+1}{2};\frac{1+j}{2},\frac{j}{2},\frac{3}{2}+j;\frac{R^2}{4a^2}\right) \\
&-\frac{\pi^{3/2}}{2a}\frac{R^2}{a^2}\gamma_{j,l,l'}\ {}_4F_3 \\
&\times\left(1-\frac{l'+l+1}{2},1+\frac{l-l'}{2},1+\frac{l'-l}{2},1+\frac{l+l'+1}{2};\frac{3}{2},2-\frac{j}{2},2+\frac{j+1}{2};\frac{R^2}{4a^2}\right)
\end{aligned} \tag{22}$$

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

$$\begin{aligned}
\alpha_{j,l,l'} &= 2^{-5/2}\frac{\Gamma\left(\frac{j-1}{2}\right)}{\Gamma\left(\frac{1+l'-l}{2}\right)\Gamma\left(\frac{1+l-l'}{2}\right)\Gamma\left(\frac{j+4}{2}\right)}\,, \\
\beta_{j,l,l'} &= 2^{-3/2}\frac{\Gamma(1-j)\,\Gamma\left(\frac{1+l+l'+j}{2}\right)}{\Gamma\left(1+\frac{1+l+l'-j}{2}\right)\Gamma\left(1+\frac{l'-l-j}{2}\right)\Gamma\left(1+\frac{l-l'-j}{2}\right)\Gamma\left(\frac{3}{2}+j\right)}\,, \\
\gamma_{j,l,l'} &= -2^{-7/2}\frac{\Gamma\left(\frac{j}{2}-1\right)}{\Gamma\left(\frac{l'-l}{2}\right)\Gamma\left(\frac{l-l'}{2}\right)\Gamma\left(2+\frac{j+1}{2}\right)}\,.
\end{aligned} \tag{23}$$

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

$$\begin{aligned}
(\alpha)_0 &= 1 \qquad \text{for} \qquad k=0\,, \\
(\alpha)_k &= \alpha(\alpha+1)\dots(\alpha+k-1) \qquad \text{for} \qquad k=1,2,\dots
\end{aligned}$$

For non-overlapping configurations $R > 2a$, the multipole matrix elements are given by formulae (19), (20), and (21). Therefore, in this regime, $g^{j}_{ll'}(R)$ 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 $g^{j}_{ll'}(R)$ is a polynomial with respect to R. We observe that the degree of the polynomial is $l + l' + 1$. For example,

$$g^{0}_{1,1}(R < 2a) = -\frac{1}{a^6}\frac{(-2a+R)^2(4a+R)}{16\sqrt{3}}\,, \tag{24}$$

$$g^{3}_{2,3}(R < 2a) = -\frac{7}{a^{12}}\frac{\left(-4a^2R+R^3\right)^2}{256\sqrt{3}}\,. \tag{25}$$

6. Summary

In this article, we calculate the multipole matrix elements of the Green function of the Laplace equation. The elements are defined by equation (1). The expression for non-overlapping configurations, *i.e.* for $|\boldsymbol{R} - \boldsymbol{R}'| > 2a$, is known in the literature and can be inferred *e.g.* from reference [7]. The new contribution is the calculation of expression (1) for overlapping configurations, *i.e.* for $|\boldsymbol{R} - \boldsymbol{R}'| < 2a$. 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 the 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 the Green function for Stokes equations in hydrodynamics [11–13]. In this case, overlapping configurations of the multipole Green function for the lowest multipoles have been considered recently in the literature [14]. We are going to use the result of this article for overlapping configuration in our further research on statistical physics of dispersive media. It should be emphasized that our result can also be of great interest in the context of numerical simulations of non-spherical objects which are constructed from overlapping spherical particles.

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