Fast, Exact, and Stable Computation of Multipole Translation and Rotation Coefficients for the 3-D Helmholtz Equation

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Abstract

We develop **exact expressions** for translations and rotations of local and multipole fundamental solutions of the Helmholtz equation in spherical coordinates. These expressions are based on recurrence relations that we develop, and to our knowledge are presented here for the first time. The symmetry and other properties of the coefficients are also examined, and based on these efficient procedures for calculating them are presented. Our expressions are direct, and do not use the Clebsch-Gordan coefficients or the Wigner 3-j symbols, though we compare our results with methods that use these, to prove their accuracy. We test our expressions on a number of simple calculations, and show their accuracy.

For evaluating a N_t term truncation of the translation (involving $O(N_t^2)$ multipoles), compared to previous exact expressions that rely on the Clebsch-Gordan coefficients or the Wigner 3-j symbol that require $O\left(N_t^5\right)$ operations, our expressions require $O(N_t^4)$ evaluations, with a small constant multiplying the order term.

The recent trend in evaluating such translations has been to use approximate "diagonalizations," that require $O(N_t^3)$ evaluations with a large coefficient for the order term. For the Helmholtz equation, these translations in addition have stabilty problems unless the accuracy of the truncation and approximate translation are balanced. We derive explicit exact expressions for achieving "diagonal" translations in $O(N_t^3)$ operations. Our expressions are based on recursive evaluations of multipole coefficients for rotations, and are accurate and stable, and have a much smaller coeffiicient for the order term, resulting practically in much fewer operations.

Future use of the developed methods in computational acoustic scattering, electromagnetic scattering (radar and microwave), optics and computational biology are expected.

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1 Introduction

The fast multipole method introduced in the work of Rokhlin and Greengard [11, 3], has been called one of the ten most influential algorithms of the 20th century [1]. The algorithm speeds up summations/matrix vector products arising from sums of the type

$$s(x_j) = \sum_i \alpha_i \phi(x_j - x_i), \quad s_j = \Phi_{ji}\alpha_i. \tag{1}$$

For M evaluation points x_j and N "source centers" x_i, the complexity of the matrix vector product $\Phi_{ji}\alpha_i$ is $O(MN)$ operations. For a given precision ϵ, the Rokhlin-Greengard method achieves the evaluation in $O(M+N)$ operations. The initial application of the algorithm [11, 3] was for the efficient computation of the field generated by multiple electrostatic or gravitational monopoles, at a large number of evaluation points. Crucial to the algorithm was the use of identities for the translation of multipole solutions of Laplace equation, and this lead to the given name for the algorithm. Instead of evaluating Equation (1) directly, equivalent N_t term multipole expansions are created at a few locations at a cost that is $f(N_t)N$ and the sum is evaluated at the M points using these expansions at a cost $g(N_t)M$. The cost is thus linear in M and N. Typically these multipole series are quickly convergent, and the functions $f(N_t)$ and $g(N_t)$ are linear or low order polynomial, and the algorithm is substantially faster than the $O(NM)$ algorithm even for moderate N and M.

This work was later extended to several other types of radial functions, for several problems arising from almost all branches of computational mathematics. Currently multipole methods are extensively used in solving problems in fluid mechanics, biomolecular force calculations, acoustics, electromagnetics, etc.

An area with significant promise for application of fast multipole methods is the fast solution of integral equations of potential theory, and there accordingly has been renewed interest in studying translation properties of multipole solutions of the Laplace and Helmholtz equations. Our interest in this algorithm arose from a desire to develop efficient algorithms for the solution of the Helmholtz equation (2) for finite and infinite domains with complex boundaries, for problems in the domain of creating virtual audio environments. Achieving fast solutions of the Helmholtz equation is an area of active research, with applications in the varied areas of acoustics, electromagnetics, etc., and some fast preliminary applications of the multipole method to the problem have appeared, and some fast computational techniques having been developed [9]. However, fast scattering codes of the type we desire are not yet available in the literature as there are several numerical problems that remain, and multipole solvers are not widely implemented. The source of most of these difficulties is associated with the efficient computation of the translations and rotations of multipoles.

Exact expressions for multipole translations for the Helmholtz equation have been presented by Epton and Dembart [7]. However these expressions are relatively cumbersome as they use the Wigner or Clebsch-Gordan coefficients, and are relatively expensive to compute ($O(N_t^5)$). Much recent interest has been focused at developing so-called diagonal translation operators, which can achieve the translation in $O(N_t^3)$ operations. However, these diagonal formulations rely on an approximate "plane-wave" integral proposed by Rokhlin, that must be computed numerically (leading to a large coefficient for the order symbol). This leads to inefficient translation operators. Further unless the error in the numerical evaluation of the integral is carefully balanced with the error in the truncation, numerical blow-up and stability problems result [10].

This report avoids these problems, by developing fast methods for evaluating the reexpansion coefficients. We derive, fast recursive relations for the translated and rotated series coefficients, which we believe are presented here for the first time.

Applications and numerical implementations are ongoing, and the obtained results will be reported shortly in other publications. This algorithm has the potential to influence many problems in acoustics (acoustic scattering), biomolecular modeling (modeling damped Coulomb or Yukawa potentials), electromagnetic propagation (radar, microwave devices), optics (optoelectronic systems), modeling the Schrödinger equation, and fluid mechanics (waves). Our initial motivation is the calculation of the head related transfer function in virtual acoustics [13].

2 Statement of the Problem

The Helmholtz equation for complex potential $\psi(\mathbf{r})$ is

$$\nabla^2\psi + k^2\psi = 0, \tag{2}$$

where ∇^2 is the Laplace operator and k is the wavenumber. The solutions to problems in external infinite domains satisfy the Sommerfeld radiation condition

$$\lim_{r\to\infty} r\left(\frac{\partial\psi}{\partial r} - ik\psi\right) = 0, \quad r = |\mathbf{r}|, \tag{3}$$

while ψ usually is required to be non-singular for problems in internal finite domains.

We consider solution of this equation in the domain $\Omega = \mathbb{R}^3/\{\mathbf{r}'_p\}$, where $\{\mathbf{r}'_p\}$ is a finite set of points with coordinates $\mathbf{r} = \mathbf{r}'_p$, $p = 1, ..., N$. Let us introduce N reference frames centered at each of the points $\mathbf{r}'_p$, $p = 1, ..., N$. In spherical polar coordinates $\mathbf{r} - \mathbf{r}'_p = \mathbf{r}_p = (r_p, \theta_p, \varphi_p)$.

At these points the potential is singular, which physically corresponds to the presence of a multipole source of the form

$$\sum_{n=0}^{\infty}\sum_{m=-n}^{m=n} A_n^{(p)m} S_n^m(\mathbf{r}_p) \tag{4}$$

being placed at each $\mathbf{r}'_p$. Here $A_n^{(p)m}$ are scalar multipole expansion coefficients, which we assume to be known, and $S_n^m(\mathbf{r})$ is a multipole (we also call it "Singular elementary solution", and accordingly use the letter "S" to denote the multipole) of degree n and order m:

$$S_n^m(\mathbf{r}_p) = h_n(kr_p) Y_n^m(\theta_p, \varphi_p), \qquad p = 1, ..., N. \tag{5}$$

Here $h_n(kr)$ are spherical Hankel functions of the 1st kind that satisfy the Sommerfeld condition, and $Y_n^m(\theta, \phi)$ are orthonormal spherical harmonics, which also can be represented in the form

$$Y_n^m(\theta,\varphi) = (-1)^m \sqrt{\frac{2n+1}{4\pi}\frac{(n-|m|)!}{(n+|m|)!}} P_n^{|m|}(\cos\theta) e^{im\varphi}, \tag{6}$$
$$n = 0, 1, 2, ..., \qquad m = -n, ..., n,$$

where $P_n^m(\mu)$ are the associated Legendre functions. (For a brief primer on the spherical solutions of the Helmholtz equation, see the appendix).

Note that we will use definition of the associated Legendre function $P_n^m(\mu)$ consistent with the value on the cut $(-1, 1)$ of the hypergeometric function $P_n^m(z)$ (see Abramowitz & Stegun, 1964). These functions can be produced from Legendre polynomials $P_n(\mu)$ using the Rodrigues' formulas:

$$P_n^m(\mu) = (-1)^m \left(1-\mu^2\right)^{m/2} \frac{d^m}{d\mu^m} P_n(\mu), \quad P_n(\mu) = \frac{1}{2^n n!}\frac{d^n}{d\mu^n}\left(\mu^2-1\right)^n, \tag{7}$$

In some of the literature the functions $(-1)^m P_n^m(\mu)$ are called associated Legendre functions. Depending on the choice, the recurrence relations involving associated Legendre functions of orders m and $m+1$ has alternating signs in different handbooks (leading to much headache in comparing results!). Also we should notice that in some literature the factor $(-1)^m$ is not included in the definition of spherical harmonics (6). Our definition of spherical harmonics coincides with that of Epton & Dembart [7], except for a factor $\sqrt{(2n+1)/4\pi}$, which we include to provide an orthonormal basis. More insight to the problem of definition of spherical harmonics with a view to developing an efficient multipole translation theory is an area of ongoing research.

Due to linearity, the solution of the Helmholtz equation that satisfies the radiation condition can be written as a combination of multipoles

$$\psi(\mathbf{r}) = \sum_{p=1}^{N}\sum_{n=0}^{\infty}\sum_{m=-n}^{m=n} A_n^{(p)m} S_n^m(\mathbf{r}_p). \tag{8}$$

The problem that we address is that of obtaining an alternative representation of the field (8) that can be used for evaluating of $\psi(\mathbf{r})$ using multipoles centered at any other point $\mathbf{r} \in \Omega$. Such a technique is known in literature as "multipole-to-multipole translation." When this evaluation can be done speedily to a specified precision a "fast multipole method" results.

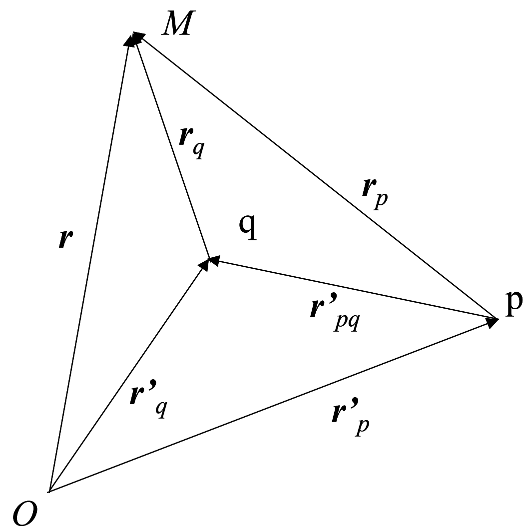


Figure 1: Coordinates of points in various reference frames.

An associated problem is the solution of equation (2) inside a regular finite domain Ω, where it can be represented as a sum of "Regular elementary solutions", $R_n^m(\mathbf{r})$:

$$\psi(\mathbf{r}) = \sum_{p=1}^{N} \sum_{n=0}^{\infty} \sum_{m=-n}^{m=n} A_n^{(p)m} R_n^m(\mathbf{r}_p), \tag{9}$$

where

$$R_n^m(\mathbf{r}_p) = j_n(kr_p) Y_n^m(\theta_p, \varphi_p), \qquad p = 1, ..., N. \tag{10}$$

Here $j_n(kr)$ are the spherical Bessel functions of the 1st kind, regular at finite r. In this case we also introduce N reference frames centered at $\mathbf{r}_p'$, $p = 1, ..., N$. In contrast to the previous case, the solution is regular at these points.

3 Multipole Reexpansions

3.1 Translations

The basic problem in reexpansion techniques is to represent $S_n^m(\mathbf{r}_p)$ and $R_n^m(\mathbf{r}_p)$ as a sum of singular or regular elementary solutions with the center of expansion specified as some *other* point $\mathbf{r} = \mathbf{r}_q'$. To obtain such representations we introduce spherical coordinates centered at $\mathbf{r} = \mathbf{r}_q'$, so $\mathbf{r} - \mathbf{r}_q' = \mathbf{r}_q = (r_q, \theta_q, \varphi_q)$. By definition we have

$$\mathbf{r} = \mathbf{r}_p + \mathbf{r}_p' = \mathbf{r}_q + \mathbf{r}_q', \quad \mathbf{r}_p = \mathbf{r}_q + \mathbf{r}_{pq}', \qquad \mathbf{r}_{pq}' = \mathbf{r}_q' - \mathbf{r}_p' = \mathbf{r}_p - \mathbf{r}_q, \tag{11}$$

where the vector $\mathbf{r}_{pq}'$ is directed from point p to point q. The value of this vector determines the radius of reexpansion $r_{pq}' = |\mathbf{r}_{pq}'|$. Inside the sphere with this radius centered at $\mathbf{r} = \mathbf{r}_q'$ the solution is regular, and can be represented as

$$S_n^m(\mathbf{r}_p) = \sum_{l=0}^{\infty} \sum_{s=-l}^{l} (S|R)_{ln}^{sm} (\mathbf{r}_{pq}') R_l^s(\mathbf{r}_q), \qquad |\mathbf{r}_q| < |\mathbf{r}_{pq}'|, \quad p \neq q. \tag{12}$$

The singular elementary solution outside this sphere satisfies the radiation conditions, and therefore we can write:

$$S_n^m(\mathbf{r}_p) = \sum_{l=0}^{\infty} \sum_{s=-l}^{l} (S|S)_{ln}^{sm} (\mathbf{r}_{pq}') S_l^s(\mathbf{r}_q), \qquad |\mathbf{r}_q| > |\mathbf{r}_{pq}'|, \tag{13}$$

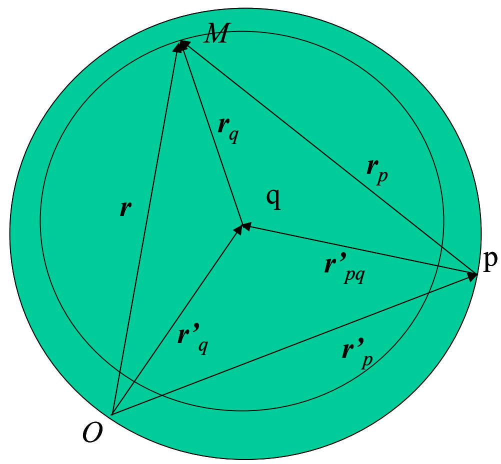


Figure 2: Illustration of the reexpansion of the singular to regular solution (12). Such reexpansion can be performed inside the dark sphere. It can be used for a field point M, since the distance to this point from point q is smaller than the radius of the dark sphere.

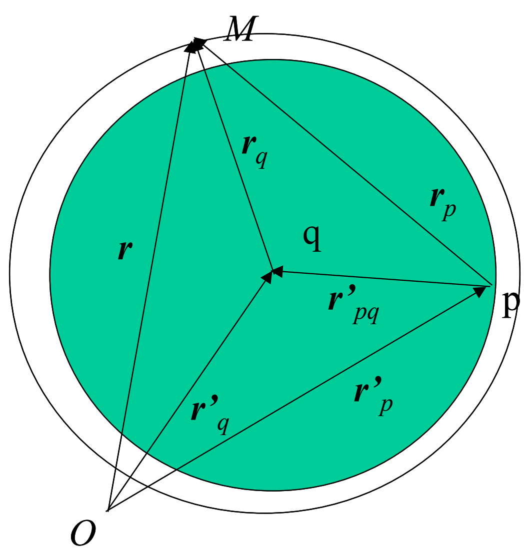


Figure 3: Illustration of the reexpansion of the singular to singular solution (13). Such reexpansion can be performed outside the dark sphere. It can be used for a field point M, since the distance to this point from point q is larger than the radius of the dark sphere.

The regular elementary solution inside a finite domain can be reexpanded near an arbitrary point, so that

$$R_n^m(\mathbf{r}_p) = \sum_{l=0}^{\infty} \sum_{s=-l}^{l} (R|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) R_l^s(\mathbf{r}_q). \tag{14}$$

In expansions (12)-(14) the symbols $(S|R), (S|S)$ and $(R|R)$ denote that singular (S) and regular (R) elementary solutions are reexpanded into series of regular or singular elementary solutions, respectively, with coefficients of reexpansion $(S|R)_{ln}^{sm}$, $(S|S)_{ln}^{sm}$ and $(R|R)_{ln}^{sm}$.

Note that we do not consider the reexpansion of regular solutions in terms multipoles, i.e. $(R|S)$. If such a reexpansion were possible, then the regular solution would be "radiating" at infinity, which cannot be true. Therefore such reexpansions cannot be used either for infinite domains, or for finite domains including the singular point of the center of the expansion. For this reason we drop consideration of the reexpansions $(R|S)$, and all cases of interest can be covered using the reexpansions $(S|R), (S|S)$ and $(R|R)$.

Using reexpansions, e.g. (12) sum (8) can be represented in the form

$$\psi(\mathbf{r}) = \sum_{l=0}^{\infty} \sum_{s=-l}^{l} B_l^s R_l^s(\mathbf{r}_q) \tag{15}$$

$$B_l^s = \sum_{p=1}^{N} \sum_{n=0}^{\infty} \sum_{m=-n}^{m=n} (S|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) A_n^{(p)m},$$

For large N these expansions can provide efficient evaluation of the field ψ, .by appropriately truncating the series in n, Usually the series can be truncated at relatively low values and coefficients B_l^s can be computed only once to evaluate of $\psi(\mathbf{r})$ at multiple field points.

3.2 Rotations

We also consider transforms of multipole expansions due to rotation of coordinate system.

3.2.1 Basic Results

We first consider the elementary case of rotation of one Cartesian system into another. Let $(\mathbf{i}_x, \mathbf{i}_y, \mathbf{i}_z)$ and $(\mathbf{i}_{\widehat{x}}, \mathbf{i}_{\widehat{y}}, \mathbf{i}_{\widehat{z}})$ be two Cartesian systems of coordinates with a common origin. Let Q be the rotation matrix that takes a vector $\mathbf{a}$ represented in the first coordinate system to the vector $\hat{\mathbf{a}}$ represented in the second coordinate systems, so that

$$\hat{\mathbf{a}} = Q\mathbf{a} \tag{16}$$

Then

$$Q = \begin{bmatrix} \mathbf{i}_{\widehat{x}} \cdot \mathbf{i}_x & \mathbf{i}_{\widehat{x}} \cdot \mathbf{i}_y & \mathbf{i}_{\widehat{x}} \cdot \mathbf{i}_z \\ \mathbf{i}_{\widehat{y}} \cdot \mathbf{i}_x & \mathbf{i}_{\widehat{y}} \cdot \mathbf{i}_y & \mathbf{i}_{\widehat{y}} \cdot \mathbf{i}_z \\ \mathbf{i}_{\widehat{z}} \cdot \mathbf{i}_x & \mathbf{i}_{\widehat{z}} \cdot \mathbf{i}_y & \mathbf{i}_{\widehat{z}} \cdot \mathbf{i}_z \end{bmatrix}. \tag{17}$$

3.2.2 Rotation Matrix to Point the z Axis to a Specified Direction

It is often convenient (and physically meaningful) to link the entries of the matrix Q to physical angles between the axes. This is usually done via one of many representations such as the Euler angles. In the present case we wish to rotate a set of axes so that the old z axis is rotated to a specified $\hat{z}$ direction (pointing to the translation location of the multipole). A simple expression for Q in terms of the direction cosines of the $\hat{z}$ direction that achieves this objective can be derived from elementary geometric considerations. We recall from Euler's theorem that any rotation of a rigid body can be uniquely specified by providing an axis of rotation and the angle of rotation through that axis.

Referring to Figure 4, the origin and the two z axes form a given plane ($Oz\hat{z}$). In this case the vector that is normal to this plane, and passes through the origin is obviously the axis of rotation. Let the direction cosines of the new $\hat{z}$ axis be $e_x, e_y.e_z$. Let the direction of the z axis in the current coordinate system be $\mathbf{i}_z$. Then the angle γ through which we must rotate the original system about the rotation axis is specified by

$$\cos\gamma = e_z. \tag{18}$$

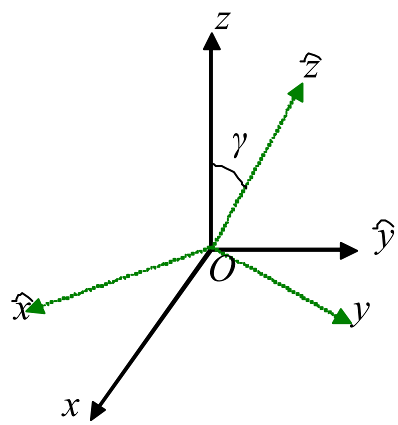


Figure 4: Rotation of axes.

The direction of the axis of rotation can be specified as

$$\mathbf{n} = \mathbf{i}_z \times \mathbf{i}_{\hat{z}} = \begin{vmatrix} \mathbf{i}_x & \mathbf{i}_y & \mathbf{i}_z \\ 0 & 0 & 1 \\ e_x & e_y & e_z \end{vmatrix} = -e_y \mathbf{i}_x + e_x \mathbf{i}_y. \tag{19}$$

Let us make a choice that the new $\mathbf{i}_{\hat{x}}$ direction is along $\mathbf{n}$. The unit vector along this direction is

$$\mathbf{i}_{\hat{x}} = \frac{-e_y \mathbf{i}_x + e_x \mathbf{i}_y}{\sqrt{(e_x^2 + e_y^2)}}. \tag{20}$$

We then have the remaining axis chosen by the cyclic order of coordinate vectors as

$$\mathbf{i}_{\hat{y}} = \mathbf{i}_{\hat{z}} \times \mathbf{i}_{\hat{x}} = \frac{1}{\sqrt{(e_x^2 + e_y^2)}} \begin{vmatrix} \mathbf{i}_x & \mathbf{i}_y & \mathbf{i}_z \\ e_x & e_y & e_z \\ -e_y & e_x & 0 \end{vmatrix} = \frac{-e_z e_x \mathbf{i}_x - e_z e_y \mathbf{i}_y}{\sqrt{(e_x^2 + e_y^2)}} + \sqrt{(e_x^2 + e_y^2)}\mathbf{i}_z \tag{21}$$

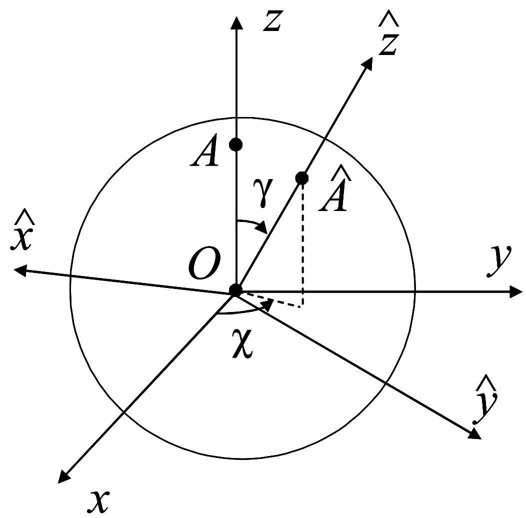
We can now evaluate the matrix Q using Equation (17) as

$$Q = \begin{bmatrix} \mathbf{i}_{\hat{x}} \cdot \mathbf{i}_x & \mathbf{i}_{\hat{x}} \cdot \mathbf{i}_y & \mathbf{i}_{\hat{x}} \cdot \mathbf{i}_z \\ \mathbf{i}_{\hat{y}} \cdot \mathbf{i}_x & \mathbf{i}_{\hat{y}} \cdot \mathbf{i}_y & \mathbf{i}_{\hat{y}} \cdot \mathbf{i}_z \\ \mathbf{i}_{\hat{z}} \cdot \mathbf{i}_x & \mathbf{i}_{\hat{z}} \cdot \mathbf{i}_y & \mathbf{i}_{\hat{z}} \cdot \mathbf{i}_z \end{bmatrix} = \begin{bmatrix} -\frac{e_y}{\sqrt{(e_x^2+e_y^2)}} & \frac{e_x}{\sqrt{(e_x^2+e_y^2)}} & 0 \\ -\frac{e_z e_x}{\sqrt{(e_x^2+e_y^2)}} & -\frac{e_z e_y}{\sqrt{(e_x^2+e_y^2)}} & \sqrt{(e_x^2 + e_y^2)} \\ e_x & e_y & e_z \end{bmatrix}. \tag{22}$$

Of course, here the choice of the $\hat{x}$ and the $\hat{y}$ axes was arbitrary. If we have a specification for the orientation of these axes (thereby fixing the 0^o meridian in the rotated coordinate system), we can compute the Q matrix as a composition of two rotations as

$$Q = \begin{bmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} -\frac{e_y}{\sqrt{(e_x^2+e_y^2)}} & \frac{e_x}{\sqrt{(e_x^2+e_y^2)}} & 0 \\ -\frac{e_z e_x}{\sqrt{(e_x^2+e_y^2)}} & -\frac{e_z e_y}{\sqrt{(e_x^2+e_y^2)}} & \sqrt{(e_x^2 + e_y^2)} \\ e_x & e_y & e_z \end{bmatrix}. \tag{23}$$

where ϕ is the rotation angle near $\mathbf{i}_{\hat{z}}$ axis.



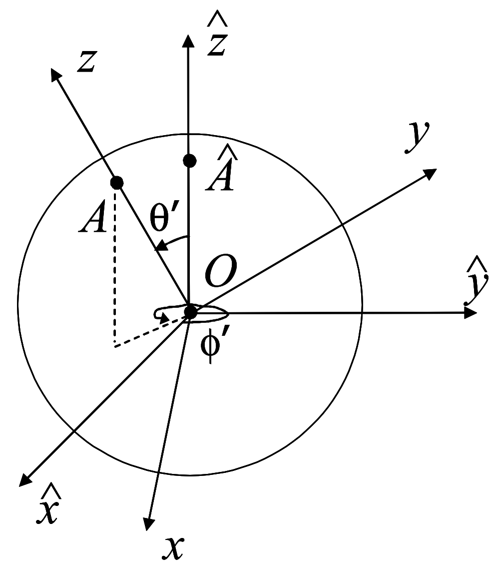


Figure 5: The figure on the left shows the transformed axes $(\hat{x}, \hat{y}, \hat{z})$ in the original reference frame (x, y, z). The spherical polar coordinates of the point $\hat{A}$ lying on the $\hat{z}$ axis on the unit sphere are (γ, χ). The figure on the right shows the original axes (x, y, z) in the transformed reference frame $(\hat{x}, \hat{y}, \hat{z})$. The coordinates of the point A lying on the z axis on the unit sphere are $(\theta' = \gamma, \varphi')$. The points O, A, and $\hat{A}$ are the same in both figures. All rotation matrices can be derived in terms of these three angles θ', φ', χ. Particularly economical expressions for multipole rotations can be obtained using these angles, as shown in the text.

For computation of rotations of spherical harmonics it is convenient to represent the rotation matrix using spherical polar angles in both coordinate systems $(\mathbf{i}_x, \mathbf{i}_y, \mathbf{i}_z)$ and $(\mathbf{i}_{\widehat{x}}, \mathbf{i}_{\widehat{y}}, \mathbf{i}_{\widehat{z}})$. Let θ' and φ' be the spherical angles of the axis $\mathbf{i}_z$ in the reference frame $(\mathbf{i}_{\widehat{x}}, \mathbf{i}_{\widehat{y}}, \mathbf{i}_{\widehat{z}})$, and let γ and χ be the spherical angles of the axis $\mathbf{i}_{\widehat{z}}$ in the reference frame $(\mathbf{i}_x, \mathbf{i}_y, \mathbf{i}_z)$. The angles θ' and γ are the same since $\cos\theta' = \mathbf{i}_z \cdot \mathbf{i}_{\widehat{z}} = \mathbf{i}_{\widehat{z}} \cdot \mathbf{i}_z = \cos\gamma = e_z$. The three independent angles θ', φ', and χ uniquely specify arbitrary rotation and can be used instead of the Euler angles.

Relation between the components of the rotation matrix (23) and angles θ' and φ' is provided by the following relations:

$$
\begin{aligned}
\cos\theta' &= \mathbf{i}_z \cdot \mathbf{i}_{\widehat{z}} = Q_{33} = e_z, \qquad \theta' = \gamma. \\
\cos\varphi' \sin\theta' &= \mathbf{i}_z \cdot \mathbf{i}_{\widehat{x}} = Q_{13} = -\sqrt{\left(e_x^2 + e_y^2\right)} \sin\phi, \\
\sin\varphi' \sin\theta' &= \mathbf{i}_z \cdot \mathbf{i}_{\widehat{y}} \ = Q_{23} = \sqrt{\left(e_x^2 + e_y^2\right)} \cos\phi.
\end{aligned}
\tag{24}
$$

Thus, the rotation angle ϕ and the polar angle φ' are related as

$$
\phi = \varphi' - \frac{\pi}{2}. \tag{25}
$$

At the same time we have

$$
\begin{aligned}
e_x &= \mathbf{i}_{\widehat{z}} \cdot \mathbf{i}_x = \sin\gamma\cos\chi = \sin\theta'\cos\chi, \\
e_y &= \mathbf{i}_{\widehat{z}} \cdot \mathbf{i}_y = \sin\gamma\sin\chi = \sin\theta'\sin\chi.
\end{aligned}
\tag{26}
$$

The matrix Q representing the rotation between the axes can be represented in terms of these angles in the form

$$Q\left(\theta',\varphi',\chi\right) = \begin{bmatrix} \sin\varphi' & \cos\varphi' & 0 \\ -\cos\varphi' & \sin\varphi' & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} -\sin\chi & \cos\chi & 0 \\ -\cos\theta'\cos\chi & -\cos\theta'\sin\chi & \sin\theta' \\ \sin\theta'\cos\chi & \sin\theta'\sin\chi & \cos\theta' \end{bmatrix} \tag{27}$$

$$= \begin{bmatrix} -\sin\varphi'\sin\chi - \cos\theta'\cos\varphi'\cos\chi & \sin\varphi'\cos\chi - \cos\theta'\cos\varphi'\sin\chi & \sin\theta'\cos\varphi' \\ \cos\varphi'\sin\chi - \cos\theta'\sin\varphi'\cos\chi & -\left(\cos\varphi'\cos\chi + \cos\theta'\sin\varphi'\sin\chi\right) & \sin\theta'\sin\varphi' \\ \sin\theta'\cos\chi & \sin\theta'\sin\chi & \cos\theta' \end{bmatrix}.$$

Since Q is an orthonormal rotation matrix, it satisfies

$$\left[Q\left(\theta',\varphi',\chi\right)\right]^{-1} = \left[Q\left(\theta',\varphi',\chi\right)\right]^{T} = Q\left(\theta',\chi,\varphi'\right). \tag{28}$$

The last equality holds because we can exchange the symbols χ and φ' if we exchange symbols $(\mathbf{i}_x,\mathbf{i}_y,\mathbf{i}_z)$ and $(\mathbf{i}_{\widehat{x}},\mathbf{i}_{\widehat{y}},\mathbf{i}_{\widehat{z}})$. Note also that Q can be represented as a composition of three rotations:

$$Q\left(\theta',\varphi',\chi\right) = \begin{bmatrix} \sin\varphi' & \cos\varphi' & 0 \\ -\cos\varphi' & \sin\varphi' & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} -1 & 0 & 0 \\ 0 & -\cos\theta' & \sin\theta' \\ 0 & \sin\theta' & \cos\theta' \end{bmatrix}\begin{bmatrix} \sin\chi & -\cos\chi & 0 \\ \cos\chi & \sin\chi & 0 \\ 0 & 0 & 1 \end{bmatrix} = A(\varphi')B\left(\theta'\right)A^{T}(\chi). \tag{29}$$

Here $B\left(\theta'\right) = \left[B\left(\theta'\right)\right]^{-1} = \left[B\left(\theta'\right)\right]^{T}$ and

$$\left[Q\left(\theta',\varphi',\chi\right)\right]^{-1} = \left[A(\varphi')B\left(\theta'\right)A^{T}(\chi)\right]^{-1} = \left[A^{T}(\chi)\right]^{-1}\left[B\left(\theta'\right)\right]^{-1}\left[A(\varphi')\right]^{-1} = A(\chi)B\left(\theta'\right)A^{T}(\varphi') = Q\left(\theta',\chi,\varphi'\right). \tag{30}$$

Such a symmetrical representation using the angles θ', φ', and χ has advantages in that leads to compact expressions for transforming the spherical coordinates of vectors in the rotated reference frames.

3.2.3 Rotation of the Spherical Harmonics for Specified Q

From group theory (Wigner [17]), we have the following transform of the spherical harmonics due to rotation of coordinates

$$Y_n^m\left(\theta,\varphi\right) = \sum_{\nu=-n}^{n} T_n^{\nu m}\left(Q\right) Y_n^j\left(\widehat{\theta},\widehat{\varphi}\right), \tag{31}$$

where $T_n^{\nu m}\left(Q\right)$ are rotation coefficients depending on the rotation matrix Q. Due to the definition of the singular and regular solutions (5) and (10) and due to the fact that the modulus of the vector does not change with rotation of coordinates, we can write the expansion for the multipole in the rotated coordinate system as

$$S_n^m\left(\mathbf{r}_p\right) = \sum_{\nu=-n}^{n} T_n^{\nu m}\left(Q\right) S_n^{\nu}\left(\widehat{\mathbf{r}}_p\right), \qquad \left|\widehat{\mathbf{r}}_p\right| = \left|\mathbf{r}_p\right|, \tag{32}$$

$$R_n^m\left(\mathbf{r}_p\right) = \sum_{\nu=-n}^{n} T_n^{\nu m}\left(Q\right) R_n^{\nu}\left(\widehat{\mathbf{r}}_p\right), \qquad \left|\widehat{\mathbf{r}}_p\right| = \left|\mathbf{r}_p\right|, \tag{33}$$

where $\widehat{\mathbf{r}}_p$ is the radius-vector of the point in the rotated coordinate system.

Using the reexpansions (e.g. equation (12)) the sum (8) can be represented in the form

$$\psi\left(\mathbf{r}\right) = \sum_{n=0}^{\infty}\sum_{\nu=-n}^{n} C_n^{\nu} S_n^{\nu}\left(\widehat{\mathbf{r}}_p\right), \tag{34}$$

$$C_n^{\nu} = \sum_{p=1}^{N}\sum_{m=-n}^{m=n} T_n^{\nu m}\left(Q\right) A_n^{(p)m}.$$

The reason for particular consideration of rotations will be clear from the treatment of diagonalized multipole expansions below. Briefly, the rotations allow for efficient computation of multipole translations by decomposing them into a composition of rotations and coaxial translations.

4 Integral Representation of Translation Coefficients

Before considering the efficient evaluation of the reexpansion coefficients for translation $(S|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)$, we consider their evaluation using their definitions (5), (10), and (12) and the fact that spherical harmonics (6) form a complete orthonormal system. If we define a scalar product of two complex valued surface functions $f(\theta,\varphi)$ and $g(\theta,\varphi)$ in $L_2\left(S_u\right)$, where S_u is the surface of a unit sphere as

$$(f,g)=\int_{-\pi}^{\pi}d\varphi\int_0^{\pi}f(\theta,\varphi)\overline{g(\theta,\varphi)}\sin\theta d\theta=\overline{(g,f)}, \tag{35}$$

where the overbar denotes the complex conjugate, then

$$\left(Y_n^m,Y_\alpha^\beta\right)=\delta_{n\alpha}\delta_{m\beta}. \tag{36}$$

Therefore, from (5), (10), and (12) we have

$$\left(S_n^m\left(\mathbf{r}_p\right),Y_\alpha^\beta(\theta_q,\varphi_q)\right)=\sum_{l=0}^{\infty}\sum_{s=-l}^{l}(S|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)j_l(kr_q)\delta_{l\alpha}\delta_{s\beta}=(S|R)_{\alpha n}^{\beta m}\left(\mathbf{r}'_{pq}\right)j_\alpha(kr_q). \tag{37}$$

Therefore

$$\begin{aligned}(S|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)&=\frac{1}{j_l(kr_q)}\left(S_n^m\left(\mathbf{r}_p\right),Y_l^s(\theta_q,\varphi_q)\right)\\&=\frac{1}{j_l(kr_q)}\int_{-\pi}^{\pi}d\varphi_q\int_0^{\pi}h_n\left(kr_p\right)Y_n^m(\theta_p,\varphi_p)Y_l^{-s}(\theta_q,\varphi_q)\sin\theta_q d\theta_q,\quad r_q<\left|\mathbf{r}'_{pq}\right|,\end{aligned} \tag{38}$$

where we used the property of surface harmonics (see (6)):

$$\overline{Y_l^s(\theta_q,\varphi_q)}=Y_l^{-s}(\theta_q,\varphi_q). \tag{39}$$

Similarly, for the other reexpansion coefficients we have the explicit expressions

$$(R|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)=\frac{1}{j_l(kr_q)}\int_{-\pi}^{\pi}d\varphi_q\int_0^{\pi}j_n\left(kr_p\right)Y_n^m(\theta_p,\varphi_p)Y_l^{-s}(\theta_q,\varphi_q)\sin\theta_q d\theta_q, \tag{40}$$

$$(S|S)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)=\frac{1}{h_l(kr_q)}\int_{-\pi}^{\pi}d\varphi_q\int_0^{\pi}h_n\left(kr_p\right)Y_n^m(\theta_p,\varphi_p)Y_l^{-s}(\theta_q,\varphi_q)\sin\theta_q d\theta_q,\quad r_q>\left|\mathbf{r}'_{pq}\right|. \tag{41}$$

Of course these expressions will be relatively expensive to evaluate in the above form, and will not be used for practical multipole translations. Nevertheless they provide expressions that can be used to check the more efficient recursive relations that we derive.

5 Structure of Translation Coefficients

While the integral representation provides an explicit way to calculate the reexpansion coefficients, this approach is not practical as the integral must be evaluated numerically, making the method computationally expensive. Moreover, since the representations (38), (40), and (41) use coordinates of both the source point $\mathbf{p}$ and the target point $\mathbf{q}$, they are not useful for fast multipole methods. To be useful they would need to be rewritten in terms of the translation vector $\mathbf{r}'_{pq}$ alone.

According to (11) and (12) we have

$$S_n^m\left(\mathbf{r}_q+\mathbf{r}'_{pq}\right)=\sum_{l=0}^{\infty}\sum_{s=-l}^{l}(S|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)R_l^s\left(\mathbf{r}_q\right). \tag{42}$$

The function $S_n^m\left(\mathbf{r}_q+\mathbf{r}'_{pq}\right)$ is regular inside $\left|\mathbf{r}_q\right| \leqslant \left|\mathbf{r}'_{pq}\right|$ and satisfies the Helmholtz equation:

$$\left(\nabla^2+k^2\right) S_n^m\left(\mathbf{r}_q+\mathbf{r}'_{pq}\right)=0. \tag{43}$$

The Laplace operator here can be considered to be acting either at fixed $\mathbf{r}'_{pq}$ or at fixed $\mathbf{r}_q$. In the former case we have

$$\left(\nabla^2+k^2\right) R_l^s\left(\mathbf{r}_q\right)=0, \tag{44}$$

which also follows from the definition of R_l^s. In the latter case we have

$$\left(\nabla^2+k^2\right)(S|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)=0. \tag{45}$$

The solution of this equation can be sought in the form of a multipole expansion as

$$(S|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)=\sum_{\alpha=0}^{\infty}\sum_{\beta=-\alpha}^{\alpha}(s|r)_{\alpha ln}^{\beta sm} S_\alpha^\beta\left(\mathbf{r}'_{pq}\right). \tag{46}$$

Indeed, in the expansion we need to only use the functions $S_\alpha^\beta\left(\mathbf{r}'_{pq}\right)$, not $R_\alpha^\beta\left(\mathbf{r}'_{pq}\right)$ or combinations of $R_\alpha^\beta\left(\mathbf{r}'_{pq}\right)$ and $S_\alpha^\beta\left(\mathbf{r}'_{pq}\right)$, since as $\left|\mathbf{r}'_{pq}\right| \rightarrow \infty$, the solution should satisfy the Sommerfeld radiation conditions (see (42)), which is provided only by the functions S_α^β. The coefficients $(s|r)_{\alpha ln}^{\beta sm}$ are purely numerical and do not depend on the locations of the multipole or the center of expansion.

Note that these coefficients can be related to the Clebsch-Gordan coefficients due to the addition theorem for the scalar wave functions (Stein [14]), or to Wigner 3-j symbols [17], which are a more symmetrical form for the Clebsch-Gordan coefficients. In the paper of Epton & Dembart [7] the following expression for the reexpansion coefficients is provided (we rewrite it in our notation):

$$(S|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)=\sum_{\alpha=0}^{\infty}\sum_{\beta=-\alpha}^{\alpha}\left[\frac{(2n+1)(2l+1)(2\alpha+1)}{4\pi}\right]^{1/2} i^{l-n+\alpha} E\left(\begin{array}{ccc} m & -s & -\beta \\ n & l & \alpha \end{array}\right) S_\alpha^\beta\left(\mathbf{r}'_{pq}\right), \tag{47}$$

where the symbol E is defined as

$$E\left(\begin{array}{ccc} m & -s & -\beta \\ n & l & \alpha \end{array}\right)=4\pi\left[\frac{4\pi}{(2n+1)(2l+1)(2\alpha+1)}\right]^{1/2}\int_{-\pi}^{\pi} d\varphi \int_0^\pi Y_n^m(\theta,\varphi) Y_l^{-s}(\theta,\varphi) Y_\alpha^{-\beta}(\theta,\varphi)\sin\theta d\theta, \tag{48}$$

and is related to the Wigner 3-j symbols:

$$E\left(\begin{array}{ccc} m & -s & -\beta \\ n & l & \alpha \end{array}\right)=4\pi\epsilon_m\epsilon_{-s}\epsilon_{-\beta}\left(\begin{array}{ccc} n & l & \alpha \\ 0 & 0 & 0 \end{array}\right)\left(\begin{array}{ccc} n & l & \alpha \\ m & -s & -\beta \end{array}\right), \tag{49}$$

where

$$\epsilon_m=\left\{\begin{array}{cc} (-1)^m, & m \geqslant 0 \\ 1, & m \leqslant 0 \end{array}\right. . \tag{50}$$

Computation of the Wigner 3-j symbols, or E symbols requires summations over additional multiindices. We will not consider this way of obtaining the reexpansion coefficients and refer the reader to the paper of Epton & Dembart (1994) for details.

Comparing (47) with (46), we note that

$$(s|r)_{\alpha ln}^{\beta sm}=\left[\frac{(2n+1)(2l+1)(2\alpha+1)}{4\pi}\right]^{1/2} i^{l-n+\alpha} E\left(\begin{array}{ccc} m & -s & -\beta \\ n & l & \alpha \end{array}\right). \tag{51}$$

The above $E-$symbol has a multiplier $\delta_{\beta,m-s}$, which means that

$$(s|r)_{\alpha ln}^{\beta sm}=0, \text{ for } \beta \neq m-s. \tag{52}$$

It is also noteworthy that from the definition (48) and orthonormality of the spherical harmonics (36) we have

$$E\begin{pmatrix} 0 & -s & -\beta \\ 0 & l & \alpha \end{pmatrix} = 4\pi\left[\frac{1}{(2l+1)(2\alpha+1)}\right]^{1/2}\delta_{\beta,-s}\delta_{\alpha l}, \tag{53}$$

$$E\begin{pmatrix} m & 0 & -\beta \\ n & 0 & \alpha \end{pmatrix} = 4\pi\left[\frac{1}{(2n+1)(2\alpha+1)}\right]^{1/2}\delta_{\beta m}\delta_{\alpha n},$$

$$E\begin{pmatrix} m & -s & 0 \\ n & l & 0 \end{pmatrix} = 4\pi\left[\frac{1}{(2n+1)(2l+1)}\right]^{1/2}\delta_{sm}\delta_{ln},$$

leading to

$$(s|r)_{\alpha l0}^{\beta s0} = \sqrt{(4\pi)}\,(-1)^l\,\delta_{\beta,-s}\delta_{\alpha l}, \tag{54}$$

$$(s|r)_{\alpha 0n}^{\beta 0m} = \sqrt{(4\pi)}\delta_{\beta m}\delta_{\alpha n},$$

$$(s|r)_{0ln}^{0sm} = \sqrt{(4\pi)}\delta_{sm}\delta_{ln},$$

Substituting (46) into (42) we have the following expression

$$S_n^m\left(\mathbf{r}_q+\mathbf{r}'_{pq}\right) = \sum_{l=0}^{\infty}\sum_{s=-l}^{l}\sum_{\alpha=0}^{\infty}\sum_{\beta=-\alpha}^{\alpha}(s|r)_{\alpha ln}^{\beta sm}S_\alpha^\beta\left(\mathbf{r}'_{pq}\right)R_l^s\left(\mathbf{r}_q\right), \tag{55}$$

which is a form of the addition theorem for multipole solutions of the Helmholtz equation. Similar considerations for the other reexpansion pairs yields:

$$(R|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) = \sum_{\alpha=0}^{\infty}\sum_{\beta=-\alpha}^{\alpha}(r|r)_{\alpha ln}^{\beta sm}R_\alpha^\beta\left(\mathbf{r}'_{pq}\right), \tag{56}$$

$$(S|S)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) = \sum_{\alpha=0}^{\infty}\sum_{\beta=-\alpha}^{\alpha}(s|s)_{\alpha ln}^{\beta sm}R_\alpha^\beta\left(\mathbf{r}'_{pq}\right), \tag{57}$$

This leads to the following addition theorems

$$R_n^m\left(\mathbf{r}_q+\mathbf{r}'_{pq}\right) = \sum_{l=0}^{\infty}\sum_{s=-l}^{l}\sum_{\alpha=0}^{\infty}\sum_{\beta=-\alpha}^{\alpha}(r|r)_{\alpha ln}^{\beta sm}R_\alpha^\beta\left(\mathbf{r}'_{pq}\right)R_l^s\left(\mathbf{r}_q\right), \tag{58}$$

$$S_n^m\left(\mathbf{r}_q+\mathbf{r}'_{pq}\right) = \sum_{l=0}^{\infty}\sum_{s=-l}^{l}\sum_{\alpha=0}^{\infty}\sum_{\beta=-\alpha}^{\alpha}(s|s)_{\alpha ln}^{\beta sm}R_\alpha^\beta\left(\mathbf{r}'_{pq}\right)S_l^s\left(\mathbf{r}_q\right), \tag{59}$$

Comparing (59) with (55), we can notice that these are indeed the same expansions of $S_n^m\left(\mathbf{r}_q+\mathbf{r}'_{pq}\right)$. We can simply transform one to the other by exchanging $\mathbf{r}'_{pq}$ with $\mathbf{r}_q$ and subscripts α with l and β with s. Therefore,

$$(s|s)_{\alpha ln}^{\beta sm} = (s|r)_{l\alpha n}^{s\beta m}. \tag{60}$$

The numerical coefficients $(r|r)_{\alpha ln}^{\beta sm}$ can be also related to the Wigner symbols in a manner similar to the expression for $(s|r)_{\alpha ln}^{\beta sm}$ (51). As will follow from our analysis below,

$$(S|S)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) = (R|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right), \tag{61}$$

and thus from (56), (57), and (60) we have:

$$(r|r)_{\alpha ln}^{\beta sm} = (s|s)_{\alpha ln}^{\beta sm} = (s|r)_{l\alpha n}^{s\beta m}. \tag{62}$$

However, even if the Wigner's coefficients could be computed efficiently, calculation of the reexpansion coefficients $(S|R)_{ln}^{sm}$,$(R|R)_{ln}^{sm}$, and $(S|S)_{ln}^{sm}$ will require summation of these coefficients, which would be an expensive procedure, since the reexpansion coefficients are 4-dimensional (and numerical coefficients, such as $(s|r)_{\alpha ln}^{\beta sm}$ are 5-dimensional (taking into account the relation (52)). As an alternative method we develop a fast computational technique based on recurrent computation of the actual reexpansion coefficients.

6 Differentiation and Recurrence Relations for Multipoles

To derive recurrence relations for the reexpansion coefficients let us first consider differentiation of the multipoles. The spherical coordinates (r,θ,φ) are related to the Cartesian coordinates by

$$\begin{aligned} x &= r\cos\varphi\sqrt{1-\mu^2}, \\ y &= r\sin\varphi\sqrt{1-\mu^2}, \\ z &= r\mu, \quad \mu=\cos\theta. \end{aligned} \tag{63}$$

The following differential operators will be considered

$$\begin{aligned} \partial_z &\equiv \frac{\partial}{\partial z} = \mu\frac{\partial}{\partial r}+\frac{1-\mu^2}{r}\frac{\partial}{\partial\mu}, \\ \partial_{xy} &\equiv \frac{\partial}{\partial x}+i\frac{\partial}{\partial y} = \frac{e^{i\varphi}}{r\sqrt{1-\mu^2}}\left[\left(1-\mu^2\right)\left(r\frac{\partial}{\partial r}-\mu\frac{\partial}{\partial\mu}\right)+i\frac{\partial}{\partial\varphi}\right], \\ \overline{\partial_{xy}} &\equiv \frac{\partial}{\partial x}-i\frac{\partial}{\partial y} = \frac{e^{-i\varphi}}{r\sqrt{1-\mu^2}}\left[\left(1-\mu^2\right)\left(r\frac{\partial}{\partial r}-\mu\frac{\partial}{\partial\mu}\right)-i\frac{\partial}{\partial\varphi}\right], \\ \nabla &\equiv \mathbf{i}_x\frac{\partial}{\partial x}+\mathbf{i}_y\frac{\partial}{\partial y}+\mathbf{i}_z\frac{\partial}{\partial z} = \mathbf{i}_x\frac{1}{2}\left(\partial_{xy}+\overline{\partial_{xy}}\right)-\mathbf{i}_y\frac{i}{2}\left(\partial_{xy}-\overline{\partial_{xy}}\right)+\mathbf{i}_z\partial_z \\ &= \frac{1}{2}\left(\mathbf{i}_x-i\mathbf{i}_y\right)\partial_{xy}+\frac{1}{2}\left(\mathbf{i}_x+i\mathbf{i}_y\right)\overline{\partial_{xy}}+\mathbf{i}_z\partial_z, \end{aligned} \tag{64}$$

We also introduce the following notation for normalization factor of spherical harmonics:

$$N_n^m = N_n^{|m|} = (-1)^m\sqrt{\frac{2n+1}{4\pi}\frac{(n-|m|)!}{(n+|m|)!}}, \quad n=0,1,..., \quad m=-n,...,n. \tag{65}$$

So we have from (5), (6), and (10):

$$\begin{aligned} S_n^m(\mathbf{r}) &= N_n^m h_n(kr)\,P_n^{|m|}(\mu)\,e^{im\varphi}, \\ R_n^m(\mathbf{r}) &= N_n^m j_n(kr)\,P_n^{|m|}(\mu)\,e^{im\varphi}. \end{aligned} \tag{66}$$

Because the functions $h_n(kr)$ and $j_n(kr)$ have similar recurrence properties, we will use the notation

$$F_n^m(\mathbf{r}) = N_n^m f_n(kr)\,P_n^{|m|}(\mu)\,e^{im\varphi}, \qquad f=h,j; \qquad F=S,R.$$

to denote any of functions $S_n^m(\mathbf{r})$ or $R_n^m(\mathbf{r})$ and $h_n(kr)$ or $j_n(kr)$.

Theorem 1 *For $k\neq 0$ and integer n and m where*

$$\frac{1}{k}\partial_z F_n^m(\mathbf{r}) = a_{n-1}^m F_{n-1}^m(\mathbf{r}) - a_n^m F_{n+1}^m(\mathbf{r}), \qquad F=S,R. \tag{67}$$

$$\begin{aligned} a_n^m &= 0, \qquad \textit{for } n<|m| \\ a_n^m &= a_n^{|m|} = \frac{N_{n+1}^m}{N_n^m}\frac{n+1+|m|}{2n+3} = \sqrt{\frac{(n+1+|m|)(n+1-|m|)}{(2n+1)(2n+3)}}, \qquad \textit{for } n\geqslant|m|. \end{aligned} \tag{68}$$

Proof. Using the following relations for the associated Legendre functions:

$$\begin{aligned} \mu P_n^m(\mu) &= \frac{1}{2n+1}\left[(n+m)\,P_{n-1}^m(\mu)+(n-m+1)\,P_{n+1}^m(\mu)\right], \\ \left(1-\mu^2\right)\frac{dP_n^m(\mu)}{d\mu} &= \frac{1}{2n+1}\left[(n+1)(n+m)\,P_{n-1}^m(\mu)-n(n-m+1)\,P_{n+1}^m(\mu)\right], \end{aligned} \tag{69}$$

and for the spherical Bessel functions (where the prime denotes derivative):

$$f_{n-1}(kr) = \frac{n+1}{kr} f_n(kr) + f_n'(kr), \qquad (70)$$
$$f_{n+1}(kr) = \frac{n}{kr} f_n(kr) - f_n'(kr),$$

we have from definitions (64) and (66):

$$\frac{1}{k}\partial_z F_n^m(\mathbf{r}) = N_n^m e^{im\varphi}\left[\mu P_n^{|m|}(\mu)\, h_n'(kr) + \frac{f_n(kr)}{kr}\left(1-\mu^2\right)\frac{dP_n^{|m|}(\mu)}{d\mu}\right]$$
$$= \frac{N_n^m e^{im\varphi}}{2n+1}\left\{(n+|m|)\, P_{n-1}^{|m|}(\mu)\left[f_n'(kr) + \frac{n+1}{kr} f_n(kr)\right] - (n-|m|+1)\, P_{n+1}^{|m|}(\mu)\left[\frac{n}{kr} f_n(kr) - f_n'(kr)\right]\right\}$$
$$= \frac{kN_n^m e^{im\varphi}}{2n+1}\left\{(n+|m|)\, f_{n-1}(kr) P_{n-1}^{|m|}(\mu) - (n-|m|+1)\, P_{n+1}^{|m|}(\mu)\, f_{n+1}(kr)\right\}$$
$$= \begin{cases} -\frac{N_0^0}{N_1^0} F_1^0(\mathbf{r}), & n=0 \\ \frac{N_n^m}{2n+1}\left[\frac{n+|m|}{N_{n-1}^m} F_{n-1}^m(\mathbf{r}) - \frac{n-|m|+1}{N_{n+1}^m} F_{n+1}^m(\mathbf{r})\right], & n \geqslant 1 \end{cases}$$

The coefficients a_n^m can be defined as stated, since

$$P_n^{|m|}(\mu) = 0, \quad |m| > n. \qquad (71)$$

and for $n \geqslant 1$ according definitions (65):

$$\frac{N_n^m}{N_{n-1}^m}\frac{n+|m|}{2n+1} = \sqrt{\frac{(n+|m|)(n-|m|)}{(2n-1)(2n+1)}} = a_{n-1}^m,$$
$$\frac{N_n^m}{N_{n+1}^m}\frac{n-|m|+1}{2n+1} = \sqrt{\frac{(n+|m|+1)(n-|m|+1)}{(2n+1)(2n+3)}} = a_n^m.$$

■

Example 1 *To demonstrate the theorem practically, we evaluate the derivative on the left hand side of (67) using finite differences, and compare this evaluation with the result given by the right hand side. For example, let us consider the theorem for $k = 1$ and $\mathbf{r} = (0.1, -6, 1)$, .The finite difference evaluation using second order central differences and a grid size of 10^{-4} yields.*

$$\frac{1}{k}\left(\frac{\partial S_4^2(\mathbf{r})}{\partial z}\right) = -0.0277686 + 0.007371i.$$

Evaluation using the theorem yields

$$0.436436\; h_3(kr)\, Y_3^2(\theta,\phi) - 0.460566\; h_5(kr)\, Y_5^3(\theta,\phi) = -0.0277686 + 0.007371i,$$

demonstrating the theorem.

Theorem 2 *For $k \neq 0$ and integer m and n :*

$$\frac{1}{k}\partial_{xy} F_n^m(\mathbf{r}) = b_{n+1}^{-m-1} F_{n+1}^{m+1}(\mathbf{r}) - b_n^m F_{n-1}^{m+1}(\mathbf{r}), \qquad F = S, R. \qquad (72)$$

where

$$b_n^m = \begin{cases} \sqrt{\frac{(n-m-1)(n-m)}{(2n-1)(2n+1)}}, & 0 \leqslant m \leqslant n, \\ -\sqrt{\frac{(n-m-1)(n-m)}{(2n-1)(2n+1)}}, & -n \leqslant m < 0 \\ 0, & |m| > n, \end{cases}, \qquad (73)$$

Proof. To prove the theorem we use the following recurrence relations for the associated Legendre functions:

$$\sqrt{1-\mu^2}P_n^m(\mu) = \frac{1}{2n+1}\left[P_{n-1}^{m+1}(\mu) - P_{n+1}^{m+1}(\mu)\right], \quad 0 \leqslant m \leqslant n, \tag{74}$$

$$\sqrt{1-\mu^2}P_n^m(\mu) = \frac{1}{2n+1}\left[(n-m+1)(n-m+2)P_{n+1}^{m-1}(\mu) - (n+m-1)(n+m)P_{n-1}^{m-1}(\mu)\right], \quad 1 \leqslant m \leqslant n,$$

$$\mu\sqrt{1-\mu^2}\frac{dP_n^m(\mu)}{d\mu} + \frac{mP_n^m(\mu)}{\sqrt{1-\mu^2}} = -\frac{1}{2n+1}\left[(n+1)P_{n-1}^{m+1}(\mu) + nP_{n+1}^{m+1}(\mu)\right], \quad 0 \leqslant m \leqslant n,$$

$$\mu\sqrt{1-\mu^2}\frac{dP_n^m(\mu)}{d\mu} - \frac{mP_n^m(\mu)}{\sqrt{1-\mu^2}} = \frac{1}{2n+1}\left[(n+1)(n+m-1)(n+m)P_{n-1}^{m-1}(\mu) + n(n-m+1)(n-m+2)P_{n+1}^{m-1}(\mu)\right], 1 \leqslant m \leqslant n,$$

where one should set $P_n^m = 0$ in any case $n < m$.
Applying $k^{-1}\partial_{xy}$ to $F_n^m(\mathbf{r})$ (see (64)), we obtain

$$\frac{1}{k}\partial_{xy}F_n^m(\mathbf{r}) = e^{i(m+1)\varphi}N_n^{|m|}\left[\sqrt{1-\mu^2}P_n^{|m|}(\mu)f_n'(kr) - \left(\mu\sqrt{1-\mu^2}\frac{dP_n^{|m|}(\mu)}{d\mu} + \frac{mP_n^{|m|}(\mu)}{\sqrt{1-\mu^2}}\right)\frac{f_n(kr)}{kr}\right].$$

For $m \geqslant 0$ we have using (74) and (70):

$$\begin{aligned}\frac{1}{k}\partial_{xy}S_n^m(\mathbf{r}) &= \frac{N_n^m e^{i(m+1)\varphi}}{2n+1}\left\{\left[P_{n-1}^{m+1}(\mu) - P_{n+1}^{m+1}(\mu)\right]f_n'(kr) + \left[nP_{n+1}^{m+1}(\mu) + (n+1)P_{n-1}^{m+1}(\mu)\right]\frac{f_n(kr)}{kr}\right\} \\ &= \frac{N_n^m e^{i(m+1)\varphi}}{2n+1}\left[h_{n-1}(kr)P_{n-1}^{m+1}(\mu) + f_{n+1}(kr)P_{n+1}^{m+1}(\mu)\right].\end{aligned}$$

In case $n = m$ the first term in the last square brackets is zero (see (71)). Thus, using definition (66) we obtain the result of the theorem for all $m \geqslant 0$, since for $n \geqslant 1$ according definitions (65) and (73):

$$\begin{aligned}\frac{1}{2n+1}\frac{N_n^m}{N_{n-1}^{m+1}} &= -\sqrt{\frac{(n-m-1)(n-m)}{(2n-1)(2n+1)}} = -b_n^m, \\ \frac{1}{2n+1}\frac{N_n^m}{N_{n+1}^{m+1}} &= -\sqrt{\frac{(n+m+1)(n+m+2)}{(2n+1)(2n+3)}} = b_{n+1}^{-m-1},\end{aligned}$$

and for $n = 0$ we have $b_n^m = 0$.
For $m \leqslant -1$, $(m = -|m|)$ we have using (74) and (70):

$$\begin{aligned}\frac{1}{k}\partial_{xy}F_n^m(\mathbf{r}) = &\frac{N_n^{|m|}e^{i(m+1)\varphi}}{2n+1}\left\{\left[(n-|m|+1)(n-|m|+2)P_{n+1}^{|m|-1}(\mu) - (n+|m|-1)(n+|m|)P_{n-1}^{|m|-1}(\mu)\right]f_n'(kr) - \right. \\ &\left. - \left[(n+1)(n+|m|-1)(n+|m|)P_{n-1}^{|m|-1}(\mu) + n(n-|m|+1)(n-|m|+2)P_{n+1}^{|m|-1}(\mu)\right]\frac{f_n(kr)}{kr}\right\} \\ = -&\frac{N_n^m e^{i(m+1)\varphi}}{2n+1}\left[(n+|m|-1)(n+|m|)f_{n-1}(kr)P_{n-1}^{|m|-1}(\mu) + (n-|m|+1)(n-|m|+2)f_{n+1}(kr)P_{n+1}^{|m|-1}(\mu)\right].\end{aligned}$$

Thus, using definition (66) we obtain the result of the theorem for all $m < 0$, since for $n \geqslant 1$ according to definitions (65) and (73):

$$\begin{aligned}-\frac{(n+|m|-1)(n+|m|)}{2n+1}\frac{N_n^{|m|}}{N_{n-1}^{|m|-1}} &= \sqrt{\frac{(n-m-1)(n-m)}{(2n-1)(2n+1)}} = -b_n^m, \\ -\frac{(n-|m|+1)(n-|m|+2)}{2n+1}\frac{N_n^{|m|}}{N_{n+1}^{|m|-1}} &= \sqrt{\frac{(n+m+1)(n+m+2)}{(2n+1)(2n+3)}} = b_{n+1}^{-m-1}.\end{aligned}$$

■

Example 2 *We evaluate the theorem for $k = 1$ and $\mathbf{r} = (0.1, -6, 1)$, and S_3^2.Using central finite differences (with a step size of 10^{-4})*

$$\frac{1}{k}\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right) S_3^2(\mathbf{r}) = 0.001002 + 0.031406i$$

Using the theorem

$$b_4^{-3} S_4^3(\mathbf{r}) - b_3^2 S_2^3(\mathbf{r}) = 0.816497 h_4^3(kr) Y_4^3(\theta,\phi) - 0.h_2^3(kr) Y_2^3(\theta,\phi) = 0.001002 + 0.031406i,$$

demonstrating the theorem.

Theorem 3 *For $k \neq 0$ and integer n and m*

$$\frac{1}{k}\overline{\partial_{xy}} F_n^m(\mathbf{r}) = b_{n+1}^{m-1} F_{n+1}^{m-1}(\mathbf{r}) - b_n^{-m} F_{n-1}^{m-1}(\mathbf{r}), \qquad F = S, R. \tag{75}$$

where the coefficients b_n^m are defined by (73).

Proof. Since $j_n(kr)$ is a real function we have from definition (10) and relation for complex conjugates of surface harmonics (39)

$$\overline{R_n^m(\mathbf{r})} = R_n^{-m}(\mathbf{r}). \tag{76}$$

Thus, using the second equation (72) we have for $m' = -m$:

$$\frac{1}{k}\overline{\partial_{xy}} R_n^m(\mathbf{r}) = \overline{\frac{1}{k}\partial_{xy} R_n^{-m}(\mathbf{r})} = b_{n+1}^{m-1}\overline{R_{n+1}^{-m+1}(\mathbf{r})} - b_n^{-m}\overline{R_{n-1}^{-m+1}(\mathbf{r})} = b_{n+1}^{m-1} R_{n+1}^{m-1}(\mathbf{r}) - b_n^{-m} R_{n-1}^{m-1}(\mathbf{r}),$$

which proves the theorem for $R_n^m(\mathbf{r})$. For $S_n^m(\mathbf{r})$ the same relation holds since $h_n(kr)$ satisfies the same recurrence relations as $j_n(kr)$. ■

Example 3 *We evaluate the theorem for $k = 1$ and $\mathbf{r} = (0.1, -6, 1)$, and S_3^2.Using central finite differences (with a step size of 10^{-4})*

$$\frac{1}{k}\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right) S_3^2(\mathbf{r}) = -0.016306 - 0.017886i.$$

Using the theorem we get

$$b_4^1 S_4^1(\mathbf{r}) - b_3^{-2} S_2^1(\mathbf{r}) = 0.3086066 h_4(kr) Y_4^1 - 0.755929 h_2(kr) Y_2^1(\theta,\phi) = -0.016306 - 0.017886i,$$

demonstrating the theorem.

Theorem 4 *For $k \neq 0$ and integer n and m*

$$\begin{aligned}\frac{1}{k}\nabla F_n^m(\mathbf{r}) = {} & \frac{1}{2}(\mathbf{i}_x - i\mathbf{i}_y)\left[b_{n+1}^{-m-1} F_{n+1}^{m+1}(\mathbf{r}) - b_n^m F_{n-1}^{m+1}(\mathbf{r})\right] \\ & + \frac{1}{2}(\mathbf{i}_x + i\mathbf{i}_y)\left[b_{n+1}^{m-1} F_{n+1}^{m-1}(\mathbf{r}) - b_n^{-m} F_{n-1}^{m-1}(\mathbf{r})\right] \\ & + \mathbf{i}_z\left[a_{n-1}^m F_{n-1}^m(\mathbf{r}) - a_n^m F_{n+1}^m(\mathbf{r})\right], \\ F = {} & S, R.\end{aligned} \tag{77}$$

where the coefficients a_n^m and b_n^m are defined by (68) and (73).

Proof. Follows from definitions (64) and Theorems 1-3. ■

Example 4 *Since this theorem follows from a combination of the previous theorems, no example is needed.*

7 Recurrence Relations for Reexpansion Coefficients

Recurrence relations among the fundamental solutions of the Helmholtz equation produce recurrence relations for the reexpansion coefficients due to invariance of the differential operators $\partial/\partial z$, $\partial/\partial x \pm i\partial/\partial y$ with respect to translations of the origin of the reference frame. Since S_n^m and R_n^m satisfy the same recurrence relations, the reexpansion coefficients $(S|R)_{ln}^{sm}$, $(S|S)_{ln}^{sm}$ and $(R|R)_{ln}^{sm}$ also satisfy the same recurrence relations. To avoid repeating theorems and recurrence relations for every combination, we denote the generic translation coefficient as $(E|F)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)$ for any of the reexpansion coefficients $((E|F) = (S|R), (S|S)$ or $(R|R))$, i.e., E and F can be any of the functions S or R. Thus the following reexpansion holds:

$$E_n^m(\mathbf{r}_p) = E_n^m\left(\mathbf{r}_q + \mathbf{r}'_{pq}\right) = \sum_{l=0}^{\infty}\sum_{s=-l}^{l}(E|F)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)F_l^s(\mathbf{r}_q). \tag{78}$$

Denoting by D_p any of operators $\partial/\partial z_p$, $\partial/\partial x_p \pm i\partial/\partial y_p$ in the reference frame with the origin at $\mathbf{r}'_p$ and applying the operator to (78) at fixed $\mathbf{r}'_{pq}$, we have:

$$D_pE_n^m(\mathbf{r}_p) = D_qE_n^m\left(\mathbf{r}_q + \mathbf{r}'_{pq}\right) = \sum_{l=0}^{\infty}\sum_{s=-l}^{l}(E|F)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)D_qF_l^s(\mathbf{r}_q). \tag{79}$$

Theorem 5 *For $k \neq 0$ the following recurrence relation holds for $(E|F)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)$:*

$$a_{n-1}^m(E|F)_{l,n-1}^{sm}\left(\mathbf{r}'_{pq}\right) - a_n^m(E|F)_{l,n+1}^{sm}\left(\mathbf{r}'_{pq}\right) = a_l^s(E|F)_{l+1,n}^{sm}\left(\mathbf{r}'_{pq}\right) - a_{l-1}^s(E|F)_{l-1,n}^{sm}\left(\mathbf{r}'_{pq}\right), \tag{80}$$
$$l,n = 0,1,... \qquad s = -l,...,l, \qquad m = -n,...,n.$$

Proof. Consider $D_p = k^{-1}\partial/\partial z_p = k^{-1}\partial/\partial z_q = D_q$. Using Theorem 1, (67), and (78) we find

$$\begin{aligned}\frac{1}{k}\frac{\partial}{\partial z_p}E_n^m(\mathbf{r}_p) &= a_{n-1}^mE_{n-1}^m(\mathbf{r}_p) - a_n^mE_{n+1}^m(\mathbf{r}_p)\\ &= \sum_{l=0}^{\infty}\sum_{s=-l}^{l}\left[a_{n-1}^m(E|F)_{l,n-1}^{sm}\left(\mathbf{r}'_{pq}\right) - a_n^m(E|F)_{l,n+1}^{sm}\left(\mathbf{r}'_{pq}\right)\right]F_l^s(\mathbf{r}_q).\end{aligned}$$

On the other hand using the same Theorem 1 and definition we have

$$\begin{aligned}\frac{1}{k}\frac{\partial}{\partial z_p}E_n^m(\mathbf{r}_p) &= \sum_{l=0}^{\infty}\sum_{s=-l}^{l}(E|F)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)\frac{1}{k}\frac{\partial}{\partial z_q}F_l^s(\mathbf{r}_q)\\ &= \sum_{l=0}^{\infty}\sum_{s=-l}^{l}(E|F)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)\left[a_{l-1}^sF_{l-1}^s(\mathbf{r}_q) - a_l^sF_{l+1}^s(\mathbf{r}_q)\right]\\ &= \sum_{l=-1}^{\infty}\sum_{s=-l-1}^{l+1}a_l^s(E|F)_{l+1,n}^{sm}\left(\mathbf{r}'_{pq}\right)F_l^s(\mathbf{r}_q) - \sum_{l=1}^{\infty}\sum_{s=-l+1}^{l-1}a_{l-1}^s(E|F)_{l-1,n}^{sm}\left(\mathbf{r}'_{pq}\right)F_l^s(\mathbf{r}_q)\\ &= \sum_{l=0}^{\infty}\sum_{s=-l}^{l}\left[a_l^s(E|F)_{l+1,n}^{sm}\left(\mathbf{r}'_{pq}\right) - a_{l-1}^s(E|F)_{l-1,n}^{sm}\left(\mathbf{r}'_{pq}\right)\right]F_l^s(\mathbf{r}_q).\end{aligned}$$

The last equality holds due to according definition (68)

$$a_{-1}^s = a_l^{l+1} = a_l^{-l-1} = a_{l-1}^l = a_{l-1}^{-l} = 0. \tag{81}$$

Comparing these two expressions and using the orthogonality and completeness of the system of surface harmonics we obtain the statement of the theorem. ■

Consequences For $n = |m|$:

$$a_{|m|}^{m}\left(E|F\right)_{l,|m|+1}^{sm}\left(\mathbf{r}'_{pq}\right) = a_{l-1}^{s}\left(E|F\right)_{l-1,|m|}^{sm}\left(\mathbf{r}'_{pq}\right) - a_{l}^{s}\left(E|F\right)_{l+1,|m|}^{sm}\left(\mathbf{r}'_{pq}\right), \tag{82}$$
$$l = 0,1,... \qquad s = -l,...,l, \qquad m = 0,\pm 1,\pm 2,....$$

For $l = |s|$:

$$a_{|s|}^{s}\left(E|F\right)_{|s|+1,n}^{sm}\left(\mathbf{r}'_{pq}\right) = a_{n-1}^{m}\left(E|F\right)_{|s|,n-1}^{sm}\left(\mathbf{r}'_{pq}\right) - a_{n}^{m}\left(E|F\right)_{|s|,n+1}^{sm}\left(\mathbf{r}'_{pq}\right), \tag{83}$$
$$n = 0,1,... \qquad m = -n,...,n \qquad s = 0,\pm 1,\pm 2,....$$

For $n = |m|$ and $l = |s|$:

$$a_{|s|}^{s}\left(E|F\right)_{|s|+1,|m|}^{sm}\left(\mathbf{r}'_{pq}\right) = -a_{|m|}^{m}\left(E|F\right)_{|s|,|m|+1}^{sm}\left(\mathbf{r}'_{pq}\right), \tag{84}$$
$$m = 0,\pm 1,\pm 2,... \qquad s = 0,\pm 1,\pm 2,....$$

Theorem 6 *For $k \neq 0$ the following recurrence relation holds for $\left(E|F\right)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)$:*

$$b_{n}^{m}\left(E|F\right)_{l,n-1}^{s,m+1}\left(\mathbf{r}'_{pq}\right) - b_{n+1}^{-m-1}\left(E|F\right)_{l,n+1}^{s,m+1}\left(\mathbf{r}'_{pq}\right) = b_{l+1}^{s-1}\left(E|F\right)_{l+1,n}^{s-1,m}\left(\mathbf{r}'_{pq}\right) - b_{l}^{-s}\left(E|F\right)_{l-1,n}^{s-1,m}\left(\mathbf{r}'_{pq}\right), \tag{85}$$
$$l,n = 0,1,... \qquad s = -l,...,l, \qquad m = -n,...,n.$$

Proof. Consider $D_p = k^{-1}\left(\partial/\partial x_p + i\partial/\partial y_p\right) = k^{-1}\left(\partial/\partial x_q + i\partial/\partial y_q\right) = D_q$. Using Theorem 2, (72), and (78) we find:

$$\begin{aligned}\frac{1}{k}\left(\frac{\partial}{\partial x_p} + i\frac{\partial}{\partial y_p}\right)E_n^m\left(\mathbf{r}_p\right) &= b_{n+1}^{-m-1}E_{n+1}^{m+1}\left(\mathbf{r}_p\right) - b_n^m E_{n-1}^{m+1}\left(\mathbf{r}_p\right)\\ &= \sum_{l=0}^{\infty}\sum_{s=-l}^{l}\left[b_{n+1}^{-m-1}\left(E|F\right)_{l,n+1}^{s,m+1}\left(\mathbf{r}'_{pq}\right) - b_n^m\left(E|F\right)_{l,n-1}^{s,m+1}\left(\mathbf{r}'_{pq}\right)\right]F_l^s\left(\mathbf{r}_q\right).\end{aligned}$$

On the other hand using the same theorem and definition we have

$$\begin{aligned}\frac{1}{k}\left(\frac{\partial}{\partial x_p} + i\frac{\partial}{\partial y_p}\right)E_n^m\left(\mathbf{r}_p\right) &= \sum_{l=0}^{\infty}\sum_{s=-l}^{l}\left(E|F\right)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)\frac{1}{k}\left(\frac{\partial}{\partial x_q} + i\frac{\partial}{\partial y_q}\right)F_l^s\left(\mathbf{r}_q\right)\\ &= \sum_{l=0}^{\infty}\sum_{s=-l}^{l}\left(E|F\right)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)\left[b_{l+1}^{-s-1}F_{l+1}^{s+1}\left(\mathbf{r}_q\right) - b_l^s F_{l-1}^{s+1}\left(\mathbf{r}_q\right)\right]\\ &= \sum_{l=1}^{\infty}\sum_{s=-l+2}^{l} b_l^{-s}\left(E|F\right)_{l-1,n}^{s-1,m}\left(\mathbf{r}'_{pq}\right)F_l^s\left(\mathbf{r}_q\right) - \sum_{l=-1}^{\infty}\sum_{s=-l}^{l+2} b_{l+1}^{s-1}\left(E|F\right)_{l+1,n}^{s-1,m}\left(\mathbf{r}'_{pq}\right)F_l^s\left(\mathbf{r}_q\right)\\ &= \sum_{l=0}^{\infty}\sum_{s=-l}^{l}\left[b_l^{-s}\left(E|F\right)_{l-1,n}^{s-1,m}\left(\mathbf{r}'_{pq}\right) - b_{l+1}^{s-1}\left(E|F\right)_{l+1,n}^{s-1,m}\left(\mathbf{r}'_{pq}\right)\right]F_l^s\left(\mathbf{r}_q\right).\end{aligned}$$

The last equality holds due to $F_l^{l+1} = 0$ and according to definitions (73)

$$b_0^s = b_{l+1}^{l+1} = b_0^{-s} = b_l^{l-1} = b_l^l = 0.$$

Comparing these two expressions and using the orthogonality and completeness of the system of surface harmonics we obtain the statement of the theorem. ■

Consequences For $n = m$:

$$b_{m+1}^{-m-1}\left(E|F\right)_{l,m+1}^{s,m+1}\left(\mathbf{r}'_{pq}\right) = b_l^{-s}\left(E|F\right)_{l-1,m}^{s-1,m}\left(\mathbf{r}'_{pq}\right) - b_{l+1}^{s-1}\left(E|F\right)_{l+1,m}^{s-1,m}\left(\mathbf{r}'_{pq}\right), \tag{86}$$
$$l = 0,1,... \qquad s = -l,...,l, \qquad m = 0,1,2,....$$

For $l=|s|$, $s\leqslant 0$:

$$b_{|s|+1}^{-|s|-1}\left(E|F\right)_{|s|+1,n}^{-|s|-1,m}\left(\mathbf{r}_{pq}'\right)=b_n^m\left(E|F\right)_{|s|,n-1}^{-|s|,m+1}\left(\mathbf{r}_{pq}'\right)-b_{n+1}^{-m-1}\left(E|F\right)_{|s|,n+1}^{-|s|,m+1}\left(\mathbf{r}_{pq}'\right), \tag{87}$$
$$n=0,1,\ldots\qquad m=-n,\ldots,n\qquad s=0,-1,-2,\ldots.$$

For $n=m$ and $l=|s|$, $s\leqslant 0$:

$$b_{m+1}^{-m-1}\left(E|F\right)_{|s|,m+1}^{-|s|,m+1}\left(\mathbf{r}_{pq}'\right)=-b_{|s|+1}^{-|s|-1}\left(E|F\right)_{|s|+1,m}^{-|s|-1,m}\left(\mathbf{r}_{pq}'\right), \tag{88}$$
$$m=0,1,2,\ldots\qquad s=0,-1,-2,\ldots.$$

Theorem 7 *For $k\neq 0$ the following recurrence relation holds for $\left(E|F\right)_{ln}^{sm}\left(\mathbf{r}_{pq}'\right)$:*

$$b_{n+1}^{m-1}\left(E|F\right)_{l,n+1}^{s,m-1}\left(\mathbf{r}_{pq}'\right)-b_n^{-m}\left(E|F\right)_{l,n-1}^{s,m-1}\left(\mathbf{r}_{pq}'\right)=b_l^s\left(E|F\right)_{l-1,n}^{s+1,m}\left(\mathbf{r}_{pq}'\right)-b_{l+1}^{-s-1}\left(E|F\right)_{l+1,n}^{s+1,m}\left(\mathbf{r}_{pq}'\right), \tag{89}$$
$$l,n=0,1,\ldots\qquad s=-l,\ldots,l,\qquad m=-n,\ldots,n.$$

Proof. Consider $D_p=k^{-1}\left(\partial/\partial x_p-i\partial/\partial y_p\right)=k^{-1}\left(\partial/\partial x_q-i\partial/\partial y_q\right)=D_q$. Using Theorem 3, (75), and (78) we find:

$$\frac{1}{k}\left(\frac{\partial}{\partial x_p}-i\frac{\partial}{\partial y_p}\right)E_n^m\left(\mathbf{r}_p\right)=b_{n+1}^{m-1}E_{n+1}^{m-1}\left(\mathbf{r}_p\right)-b_n^{-m}E_{n-1}^{m-1}\left(\mathbf{r}_p\right)$$
$$=\sum_{l=0}^{\infty}\sum_{s=-l}^{l}\left[b_{n+1}^{m-1}\left(E|F\right)_{l,n+1}^{s,m-1}\left(\mathbf{r}_{pq}'\right)-b_n^{-m}\left(E|F\right)_{l,n-1}^{s,m-1}\left(\mathbf{r}_{pq}'\right)\right]F_l^s\left(\mathbf{r}_q\right).$$

On the other hand, using the same theorem and definition we have

$$\begin{aligned}\frac{1}{k}\left(\frac{\partial}{\partial x_p}-i\frac{\partial}{\partial y_p}\right)E_n^m\left(\mathbf{r}_p\right)&=\sum_{l=0}^{\infty}\sum_{s=-l}^{l}\left(E|F\right)_{ln}^{sm}\left(\mathbf{r}_{pq}'\right)\frac{1}{k}\left(\frac{\partial}{\partial x_q}-i\frac{\partial}{\partial y_q}\right)F_l^s\left(\mathbf{r}_q\right)\\&=\sum_{l=0}^{\infty}\sum_{s=-l}^{l}\left(E|F\right)_{ln}^{sm}\left(\mathbf{r}_{pq}'\right)\left[b_{l+1}^{s-1}F_{l+1}^{s-1}\left(\mathbf{r}_q\right)-b_l^{-s}F_{l-1}^{s-1}\left(\mathbf{r}_q\right)\right]\\&=\sum_{l=1}^{\infty}\sum_{s=-l}^{l-2}b_l^s\left(E|F\right)_{l-1,n}^{s+1,m}\left(\mathbf{r}_{pq}'\right)F_l^s\left(\mathbf{r}_q\right)-\sum_{l=-1}^{\infty}\sum_{s=-l-2}^{l}b_{l+1}^{-s-1}\left(E|F\right)_{l+1,n}^{s+1,m}\left(\mathbf{r}_{pq}'\right)F_l^s\left(\mathbf{r}_q\right)\\&=\sum_{l=0}^{\infty}\sum_{s=-l}^{l}\left[b_l^s\left(E|F\right)_{l-1,n}^{s+1,m}\left(\mathbf{r}_{pq}'\right)-b_{l+1}^{-s-1}\left(E|F\right)_{l+1,n}^{s+1,m}\left(\mathbf{r}_{pq}'\right)\right]F_l^s\left(\mathbf{r}_q\right).\end{aligned}$$

The last equality holds due to $F_l^{-l-1}=0$ and according definition (73)

$$b_0^s=b_{l+1}^{l+1}=b_l^{l-1}=b_{l-1}^{l-1}=0.$$

Comparing these two expressions and using the orthogonality and completeness of the system of surface harmonics we obtain the statement of the theorem. ■

Consequences For $n=|m|$, $m\leqslant 0$:

$$b_{|m|+1}^{-|m|-1}\left(E|F\right)_{l,|m|+1}^{s,-|m|-1}\left(\mathbf{r}_{pq}'\right)=b_l^s\left(E|F\right)_{l-1,|m|}^{s+1,-|m|}\left(\mathbf{r}_{pq}'\right)-b_{l+1}^{-s-1}\left(E|F\right)_{l+1,|m|}^{s+1,-|m|}\left(\mathbf{r}_{pq}'\right), \tag{90}$$
$$l=0,1,\ldots\qquad s=-l,\ldots,l,\qquad m=0,-1,-2,\ldots.$$

For $l=s$:

$$b_{s+1}^{-s-1}\left(E|F\right)_{s+1,n}^{s+1,m}\left(\mathbf{r}_{pq}'\right)=b_n^{-m}\left(E|F\right)_{s,n-1}^{s,m-1}\left(\mathbf{r}_{pq}'\right)-b_{n+1}^{m-1}\left(E|F\right)_{s,n+1}^{s,m-1}\left(\mathbf{r}_{pq}'\right), \tag{91}$$
$$n=0,1,\ldots\qquad m=-n,\ldots,n\qquad s=0,1,2,\ldots.$$

For $n=|m|$, $m\leqslant 0$ and $l=s$:

$$b_{|m|+1}^{-|m|-1}\left(E|F\right)_{s,|m|+1}^{s,-|m|-1}\left(\mathbf{r}_{pq}'\right)=-b_{s+1}^{-s-1}\left(E|F\right)_{s+1,|m|}^{s+1,-|m|}\left(\mathbf{r}_{pq}'\right),\quad m=0,-1,-2,\ldots\quad s=0,1,2,\ldots. \tag{92}$$

8 Recurrence Relations for Rotation Coefficients

Theorem 8 *The following recurrence relations holds for* $T_n^{\nu m}(Q)$:

$$\frac{1}{2}(\mathbf{i}_x - i\mathbf{i}_y)b_{n+1}^{-m-1}T_{n+1}^{\nu,m+1} + \frac{1}{2}(\mathbf{i}_x + i\mathbf{i}_y)b_{n+1}^{m-1}T_{n+1}^{\nu,m-1} - \mathbf{i}_z a_n^m T_{n+1}^{\nu m} = \frac{1}{2}(\mathbf{i}_{\hat{x}} - i\mathbf{i}_{\hat{y}})b_{n+1}^{-\nu}T_n^{\nu-1,m} + \frac{1}{2}(\mathbf{i}_{\hat{x}} + i\mathbf{i}_{\hat{y}})b_{n+1}^{\nu}T_n^{\nu+1,m} - \mathbf{i}_{\hat{z}} a_n^{\nu} T_n^{\nu m}, \tag{93}$$

where $n = 0, 1, 2, ..., m = -n, ..., n, \nu = -n-1, ..., n+1,$ *and*

$$\frac{1}{2}(\mathbf{i}_x - i\mathbf{i}_y)b_n^m T_{n-1}^{\nu,m+1} + \frac{1}{2}(\mathbf{i}_x + i\mathbf{i}_y)b_n^{-m}T_{n-1}^{\nu,m-1} - \mathbf{i}_z a_{n-1}^m T_{n-1}^{\nu m} = \frac{1}{2}(\mathbf{i}_{\hat{x}} - i\mathbf{i}_{\hat{y}})\, b_n^{\nu-1}T_n^{\nu-1,m} + \frac{1}{2}(\mathbf{i}_{\hat{x}} + i\mathbf{i}_{\hat{y}})\, b_n^{-\nu-1}T_n^{\nu+1,m} - \mathbf{i}_{\hat{z}} a_{n-1}^{\nu} T_n^{\nu m}. \tag{94}$$

where $n = 0, 1, 2, ..., m = -n, ..., n, \nu = -n+1, ..., n-1.$

Proof. Let us apply operator $k^{-1}\nabla$ to any of the relations (32) or (33):

$$k^{-1}\nabla F_n^m(\mathbf{r}_p) = \sum_{\nu=-n}^{n} T_n^{\nu m}(Q)\, k^{-1}\nabla F_n^{\nu}(\widehat{\mathbf{r}}_p), \qquad |\widehat{\mathbf{r}}_p| = |\mathbf{r}_p|, \qquad F = S, R. \tag{95}$$

Due to independence of the operator ∇ from the selection of the reference frame, particularly to rotations, $\nabla = \widehat{\nabla}$, we can use (77), to represent the left and right hand sides of (95). So, for the left hand side we have using definitions (32) or (33)

$$\begin{aligned}\frac{1}{k}\nabla F_n^m(\mathbf{r}_p) &= \frac{1}{2}(\mathbf{i}_x - i\mathbf{i}_y)\left[b_{n+1}^{-m-1}F_{n+1}^{m+1}(\mathbf{r}_p) - b_n^m F_{n-1}^{m+1}(\mathbf{r}_p)\right] \\ &+ \frac{1}{2}(\mathbf{i}_x + i\mathbf{i}_y)\left[b_{n+1}^{m-1}F_{n+1}^{m-1}(\mathbf{r}_p) - b_n^{-m}F_{n-1}^{m-1}(\mathbf{r}_p)\right] + \mathbf{i}_z\left[a_{n-1}^m F_{n-1}^m(\mathbf{r}_p) - a_n^m F_{n+1}^m(\mathbf{r}_p)\right]\end{aligned} \tag{96}$$

$$\begin{aligned}&= \sum_{\nu=-n-1}^{n+1}\left[\frac{1}{2}(\mathbf{i}_x - i\mathbf{i}_y)\, b_{n+1}^{-m-1}T_{n+1}^{\nu,m+1} + \frac{1}{2}(\mathbf{i}_x + i\mathbf{i}_y)\, b_{n+1}^{m-1}T_{n+1}^{\nu,m-1} - \mathbf{i}_z a_n^m T_{n+1}^{\nu m}\right]F_{n+1}^{\nu}(\widehat{\mathbf{r}}_p) \\ &- \sum_{\nu=-n+1}^{n-1}\left[\frac{1}{2}(\mathbf{i}_x - i\mathbf{i}_y)\, b_n^m T_{n-1}^{\nu,m+1} + \frac{1}{2}(\mathbf{i}_x + i\mathbf{i}_y)\, b_n^{-m}T_{n-1}^{\nu,m-1} - \mathbf{i}_z a_{n-1}^m T_{n-1}^{\nu m}\right]F_{n-1}^{\nu}(\widehat{\mathbf{r}}_p).\end{aligned}$$

The right hand side can be expanded as

$$\sum_{\nu=-n}^{n} T_n^{\nu m} k^{-1} \nabla F_n^{\nu}(\widehat{\mathbf{r}}_p) = \sum_{\nu=-n}^{n} T_n^{\nu m} \left\{ \frac{1}{2} (\mathbf{i}_{\hat{x}} - i\mathbf{i}_{\hat{y}}) \left[b_{n+1}^{-\nu-1} F_{n+1}^{\nu+1}(\widehat{\mathbf{r}}_p) - b_n^{\nu} F_{n-1}^{\nu+1}(\widehat{\mathbf{r}}_p) \right] + \right. \tag{97}$$

$$\left. \frac{1}{2} (\mathbf{i}_{\hat{x}} + i\mathbf{i}_{\hat{y}}) \left[b_{n+1}^{\nu-1} F_{n+1}^{\nu-1}(\widehat{\mathbf{r}}_p) - b_n^{-\nu} F_{n-1}^{\nu-1}(\widehat{\mathbf{r}}_p) \right] + \mathbf{i}_{\hat{z}} \left[a_{n-1}^{\nu} F_{n-1}^{\nu}(\widehat{\mathbf{r}}_p) - a_n^{\nu} F_{n+1}^{\nu}(\widehat{\mathbf{r}}_p) \right] \right\}$$

$$= \frac{1}{2} (\mathbf{i}_{\hat{x}} - i\mathbf{i}_{\hat{y}}) \sum_{\nu=-n}^{n} T_n^{\nu m} b_{n+1}^{-\nu-1} F_{n+1}^{\nu+1}(\widehat{\mathbf{r}}_p) + \frac{1}{2} (\mathbf{i}_{\hat{x}} + i\mathbf{i}_{\hat{y}}) \sum_{\nu=-n}^{n} T_n^{\nu m} b_{n+1}^{\nu-1} F_{n+1}^{\nu-1}(\widehat{\mathbf{r}}_p) - \mathbf{i}_{\hat{z}} \sum_{\nu=-n}^{n} T_n^{\nu m} a_n^{\nu} F_{n+1}^{\nu}(\widehat{\mathbf{r}}_p)$$

$$- \left[\frac{1}{2} (\mathbf{i}_{\hat{x}} - i\mathbf{i}_{\hat{y}}) \sum_{\nu=-n}^{n} T_n^{\nu m} b_n^{\nu} F_{n-1}^{\nu+1}(\widehat{\mathbf{r}}_p) + \frac{1}{2} (\mathbf{i}_{\hat{x}} + i\mathbf{i}_{\hat{y}}) \sum_{\nu=-n}^{n} T_n^{\nu m} b_n^{-\nu} F_{n-1}^{\nu-1}(\widehat{\mathbf{r}}_p) - \mathbf{i}_{\hat{z}} \sum_{\nu=-n}^{n} T_n^{\nu m} a_{n-1}^{\nu} F_{n-1}^{\nu}(\widehat{\mathbf{r}}_p) \right]$$

$$= \frac{1}{2} (\mathbf{i}_{\hat{x}} - i\mathbf{i}_{\hat{y}}) \sum_{\nu=-n+1}^{n+1} b_{n+1}^{-\nu} T_n^{\nu-1,m} F_{n+1}^{\nu}(\widehat{\mathbf{r}}_p) + \frac{1}{2} (\mathbf{i}_{\hat{x}} + i\mathbf{i}_{\hat{y}}) \sum_{\nu=-n-1}^{n-1} b_{n+1}^{\nu} T_n^{\nu+1,m} F_{n+1}^{\nu}(\widehat{\mathbf{r}}_p) - \mathbf{i}_{\hat{z}} \sum_{\nu=-n}^{n} a_n^{\nu} T_n^{\nu m} F_{n+1}^{\nu}(\widehat{\mathbf{r}}_p)$$

$$- \left[\frac{1}{2} (\mathbf{i}_{\hat{x}} - i\mathbf{i}_{\hat{y}}) \sum_{\nu=-n+1}^{n+1} b_n^{\nu-1} T_n^{\nu-1,m} F_{n-1}^{\nu}(\widehat{\mathbf{r}}_p) + \frac{1}{2} (\mathbf{i}_{\hat{x}} + i\mathbf{i}_{\hat{y}}) \sum_{\nu=-n-1}^{n-1} b_n^{-\nu-1} T_n^{\nu+1,m} F_{n-1}^{\nu}(\widehat{\mathbf{r}}_p) - \mathbf{i}_{\hat{z}} \sum_{\nu=-n}^{n} a_{n-1}^{\nu} T_n^{\nu m} F_{n-1}^{\nu}(\widehat{\mathbf{r}}_p) \right]$$

$$= \sum_{\nu=-n-1}^{n+1} \left[\frac{1}{2} (\mathbf{i}_{\hat{x}} - i\mathbf{i}_{\hat{y}}) b_{n+1}^{-\nu} T_n^{\nu-1,m} + \frac{1}{2} (\mathbf{i}_{\hat{x}} + i\mathbf{i}_{\hat{y}}) b_{n+1}^{\nu} T_n^{\nu+1,m} - \mathbf{i}_{\hat{z}} a_n^{\nu} T_n^{\nu m} \right] F_{n+1}^{\nu}(\widehat{\mathbf{r}}_p)$$

$$- \sum_{\nu=-n+1}^{n-1} \left[\frac{1}{2} (\mathbf{i}_{\hat{x}} - i\mathbf{i}_{\hat{y}}) b_n^{\nu-1} T_n^{\nu-1,m} + \frac{1}{2} (\mathbf{i}_{\hat{x}} + i\mathbf{i}_{\hat{y}}) b_n^{-\nu-1} T_n^{\nu+1,m} - \mathbf{i}_{\hat{z}} a_{n-1}^{\nu} T_n^{\nu m} \right] F_{n-1}^{\nu}(\widehat{\mathbf{r}}_p).$$

The last equality holds due to $b_n^{n-1} = b_n^n = a_{n-1}^n = a_{n-1}^{-n} = 0$ (see (68) and (73)).Comparing (96) and (97) with a notice that F_{n+1}^{ν} and F_{n-1}^{ν} are linearly independent, we have the statement of the theorem. ■

Theorem 9 *The following recurrence relations holds for* $T_n^{\nu m}(Q)$:

$$b_{n+1}^{-m-1} T_{n+1}^{\nu,m+1} + b_{n+1}^{m-1} T_{n+1}^{\nu,m-1} = W_{11} b_{n+1}^{-\nu} T_n^{\nu-1,m} + W_{12} b_{n+1}^{\nu} T_n^{\nu+1,m} + W_{13} a_n^{\nu} T_n^{\nu m}, \tag{98}$$

$$b_{n+1}^{-m-1} T_{n+1}^{\nu,m+1} - b_{n+1}^{m-1} T_{n+1}^{\nu,m-1} = W_{21} b_{n+1}^{-\nu} T_n^{\nu-1,m} + W_{22} b_{n+1}^{\nu} T_n^{\nu+1,m} + W_{23} a_n^{\nu} T_n^{\nu m}, \tag{99}$$

$$a_n^m T_{n+1}^{\nu m} = W_{31} b_{n+1}^{-\nu} T_n^{\nu-1,m} + W_{32} b_{n+1}^{\nu} T_n^{\nu+1,m} + W_{33} a_n^{\nu} T_n^{\nu m}, \tag{100}$$

where $n = 0, 1, 2, \ldots$, $m = -n, \ldots, n$, $\nu = -n-1, \ldots, n+1$, *and* $W_{\alpha\beta}$ *are components of the following complex rotation matrix*

$$\mathbf{W} = \begin{pmatrix} \mathbf{i}_x \cdot (\mathbf{i}_{\hat{x}} - i\mathbf{i}_{\hat{y}}) & \mathbf{i}_x \cdot (\mathbf{i}_{\hat{x}} + i\mathbf{i}_{\hat{y}}) & -2\mathbf{i}_x \cdot \mathbf{i}_{\hat{z}} \\ i\mathbf{i}_y \cdot (\mathbf{i}_{\hat{x}} - i\mathbf{i}_{\hat{y}}) & i\mathbf{i}_y \cdot (\mathbf{i}_{\hat{x}} + i\mathbf{i}_{\hat{y}}) & -2i\mathbf{i}_y \cdot \mathbf{i}_{\hat{z}} \\ -\frac{1}{2}\mathbf{i}_z \cdot (\mathbf{i}_{\hat{x}} - i\mathbf{i}_{\hat{y}}) & -\frac{1}{2}\mathbf{i}_z \cdot (\mathbf{i}_{\hat{x}} + i\mathbf{i}_{\hat{y}}) & \mathbf{i}_z \cdot \mathbf{i}_{\hat{z}} \end{pmatrix}, \tag{101}$$

Proof. Taking scalar product of both sides of (93) with $\mathbf{i}_x, i\mathbf{i}_y$, and $\mathbf{i}_z$, we obtain the statement of the theorem. ■

Consequences: Summing and subtracting relations (98) and (99) we have

$$2b_{n+1}^{-m-1} T_{n+1}^{\nu,m+1} = (W_{11} + W_{21}) b_{n+1}^{-\nu} T_n^{\nu-1,m} + (W_{12} + W_{22}) b_{n+1}^{\nu} T_n^{\nu+1,m} + (W_{13} + W_{23}) a_n^{\nu} T_n^{\nu m}, \tag{102}$$

$$2b_{n+1}^{m-1} T_{n+1}^{\nu,m-1} = (W_{11} - W_{21}) b_{n+1}^{-\nu} T_n^{\nu-1,m} + (W_{12} - W_{22}) b_{n+1}^{\nu} T_n^{\nu+1,m} + (W_{13} - W_{23}) a_n^{\nu} T_n^{\nu m}, \tag{103}$$

For $\nu = n+1$ we have

$$2b_{n+1}^{-m-1} T_{n+1}^{n+1,m+1} = (W_{11} + W_{21}) b_{n+1}^{-n-1} T_n^{nm}, \tag{104}$$

$$2b_{n+1}^{m-1}T_{n+1}^{n+1,m-1} = (W_{11} - W_{21})\, b_{n+1}^{-n-1}T_n^{nm}, \tag{105}$$

$$a_n^m T_{n+1}^{n+1,m} = W_{31} b_{n+1}^{-n-1} T_n^{nm}, \tag{106}$$

For $\nu = -n-1$ we have

$$2b_{n+1}^{-m-1}T_{n+1}^{-n-1,m+1} = (W_{12} + W_{22})\, b_{n+1}^{-n-1}T_n^{-n,m}, \tag{107}$$

$$2b_{n+1}^{m-1}T_{n+1}^{-n-1,m-1} = (W_{12} - W_{22})\, b_{n+1}^{-n-1}T_n^{-n,m}, \tag{108}$$

$$a_n^m T_{n+1}^{-n-1,m} = W_{32} b_{n+1}^{-n-1} T_n^{-n,m}. \tag{109}$$

Theorem 10 *The following recurrence relations holds for* $T_n^{\nu m}(Q)$:

$$b_n^m T_{n-1}^{\nu,m+1} + b_n^{-m} T_{n-1}^{\nu,m-1} = W_{11} b_n^{\nu-1} T_n^{\nu-1,m} + W_{12} b_n^{-\nu-1} T_n^{\nu+1,m} + W_{13} a_{n-1}^{\nu} T_n^{\nu m} \tag{110}$$

$$b_n^m T_{n-1}^{\nu,m+1} - b_n^{-m} T_{n-1}^{\nu,m-1} = W_{21} b_n^{\nu-1} T_n^{\nu-1,m} + W_{22} b_n^{-\nu-1} T_n^{\nu+1,m} + W_{23} a_{n-1}^{\nu} T_n^{\nu m}. \tag{111}$$

$$a_{n-1}^m T_{n-1}^{\nu m} = W_{31} b_n^{\nu-1} T_n^{\nu-1,m} + W_{32} b_n^{-\nu-1} T_n^{\nu+1,m} + W_{33} a_{n-1}^{\nu} T_n^{\nu m}. \tag{112}$$

where $n = 0,1,2,...,$ $m = -n,...,n,$ $\nu = -n+1,...,n-1,$ *and* $W_{\alpha\beta}$ *are components of complex rotation matrix (101).*

Proof. Taking scalar product of both sides of (93) with $\mathbf{i}_x, i\mathbf{i}_y$, and $\mathbf{i}_z$, we obtain the statement of the theorem. ■

Consequences Summing and subtracting relations (110) and (111) we have

$$2b_n^m T_{n-1}^{\nu,m+1} = (W_{11} + W_{21})\, b_n^{\nu-1} T_n^{\nu-1,m} + (W_{12} + W_{22})\, b_n^{-\nu-1} T_n^{\nu+1,m} + (W_{13} + W_{23})\, a_{n-1}^{\nu} T_n^{\nu m}, \tag{113}$$

$$2b_n^{-m} T_{n-1}^{\nu,m-1} = (W_{11} - W_{21})\, b_n^{\nu-1} T_n^{\nu-1,m} + (W_{12} - W_{22})\, b_n^{-\nu-1} T_n^{\nu+1,m} + (W_{13} - W_{23})\, a_{n-1}^{\nu} T_n^{\nu m}, \tag{114}$$

For $m = n$ we have

$$(W_{11} + W_{21})\, b_n^{\nu-1} T_n^{\nu-1,n} + (W_{12} + W_{22})\, b_n^{-\nu-1} T_n^{\nu+1,n} + (W_{13} + W_{23})\, a_{n-1}^{\nu} T_n^{\nu n} = 0, \tag{115}$$

$$W_{31} b_n^{\nu-1} T_n^{\nu-1,n} + W_{32} b_n^{-\nu-1} T_n^{\nu+1,n} + W_{33} a_{n-1}^{\nu} T_n^{\nu n} = 0. \tag{116}$$

For $m = -n$ we have

$$(W_{11} - W_{21})\, b_n^{\nu-1} T_n^{\nu-1,-n} + (W_{12} - W_{22})\, b_n^{-\nu-1} T_n^{\nu+1,-n} + (W_{13} - W_{23})\, a_{n-1}^{\nu} T_n^{\nu,-n}, \tag{117}$$

$$W_{31} b_n^{\nu-1} T_n^{\nu-1,-n} + W_{32} b_n^{-\nu-1} T_n^{\nu+1,-n} + W_{33} a_{n-1}^{\nu} T_n^{\nu,-n} = 0. \tag{118}$$

9 Particular Values of Translation Coefficients

9.1 (S|R) Coefficients

Expression (55) reveals a particular value of the reexpansion coefficients $(S|R)_{ln}^{sm}$. Setting $\mathbf{r}_q = \mathbf{0}$ we have

$$R_l^s(\mathbf{0}) = \sqrt{\frac{1}{4\pi}}\,\delta_{l0}\delta_{s0}, \tag{119}$$

$$S_n^m\left(\mathbf{r}'_{pq}\right)=\sqrt{\frac{1}{4\pi}}\sum_{\alpha=0}^{\infty}\sum_{\beta=-\alpha}^{\alpha}(s|r)_{\alpha 0n}^{\beta 0m}S_\alpha^\beta\left(\mathbf{r}'_{pq}\right),\qquad p\neq q. \tag{120}$$

Due to the orthogonality of surface functions we obtain then

$$(s|r)_{\alpha 0n}^{\beta 0m}=\sqrt{(4\pi)}\delta_{\alpha n}\delta_{\beta m}. \tag{121}$$

This value also can be obtained directly from (54). Substituting this expression into (46), we have

$$(S|R)_{0n}^{0m}\left(\mathbf{r}'_{pq}\right)=\sqrt{(4\pi)}S_n^m\left(\mathbf{r}'_{pq}\right),\qquad n=0,1,...,\quad m=-n,...,n. \tag{122}$$

Another particular value can be found from well-known expansion of fundamental solution $G\left(\mathbf{r}_p\right)$ of the Helmholtz equation (see e.g. Morse & Feshbach [4]) into a series of spherical harmonics:

$$G_k\left(\mathbf{r}_p\right)=ik\sum_{l=0}^{\infty}\sum_{s=-l}^{s=l}S_l^{-s}\left(-\mathbf{r}'_{pq}\right)R_l^s\left(\mathbf{r}_q\right),\qquad \left|\mathbf{r}_q\right|\leqslant\left|\mathbf{r}'_{pq}\right|, \tag{123}$$

In fact the fundamental solution is a monopole

$$G_k\left(\mathbf{r}_p\right)=\frac{e^{ikr_p}}{4\pi r_p}=\frac{ik}{4\pi}h_0(kr_p)=\frac{ik}{\sqrt{(4\pi)}}S_0^0\left(\mathbf{r}_q+\mathbf{r}'_{pq}\right). \tag{124}$$

Thus, comparing (123) and (124) with (42), we obtain the following value for the reexpansion coefficients:

$$(S|R)_{l0}^{s0}\left(\mathbf{r}'_{pq}\right)=\sqrt{(4\pi)}S_l^{-s}\left(-\mathbf{r}'_{pq}\right)=\sqrt{(4\pi)}\,(-1)^l\,S_l^{-s}\left(\mathbf{r}'_{pq}\right),\qquad l=0,1,...,\quad s=-l,...,l. \tag{125}$$

The last equality holds due to

$$\begin{aligned}S_l^{-s}\left(-\mathbf{r}'_{pq}\right)&=h_l(kr'_{pq})Y_l^{-s}(\pi-\theta'_{pq},\varphi'_{pq}+\pi)=h_l(kr'_{pq})\sqrt{\frac{2l+1}{4\pi}\frac{(l-|s|)!}{(l+|s|)!}}P_l^{|s|}(-\cos\theta'_{pq})e^{-is\varphi'_{pq}} \qquad (126)\\&=(-1)^{l+s}\,h_l(kr'_{pq})\sqrt{\frac{2l+1}{4\pi}\frac{(l-|s|)!}{(l+|s|)!}}P_l^{|s|}(\cos\theta'_{pq})e^{-is\varphi'_{pq}}=(-1)^l\,S_l^{-s}\left(\mathbf{r}'_{pq}\right),\end{aligned}$$

where we used the fact that $P_l^{|s|}(-\mu)=(-1)^{l+s}\,P_l^{|s|}(\mu)$. Comparing (125) with (46), we have:

$$(s|r)_{\alpha l0}^{\beta s0}=\sqrt{(4\pi)}(-1)^l\delta_{\alpha l}\delta_{\beta,-s}, \tag{127}$$

which is consistent with (54).

Note, that formulae (122) and (125) are consistent in terms that they both provide the value of $(S|R)_{00}^{00}\left(\mathbf{r}'_{pq}\right)$:

$$(S|R)_{00}^{00}\left(\mathbf{r}'_{pq}\right)=\sqrt{(4\pi)}S_0^0\left(\mathbf{r}'_{pq}\right)=h_0(kr'_{pq}). \tag{128}$$

It is also worth mentioning that once $(S|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)$ is known, the coefficients $(S|R)_{ln}^{sm}\left(\mathbf{r}'_{qp}\right)$ representing reexpansion of multipoles near point p:

$$S_n^m\left(\mathbf{r}_q\right)=\sum_{l=0}^{\infty}\sum_{s=-l}^{l}(S|R)_{ln}^{sm}\left(\mathbf{r}'_{qp}\right)R_l^s\left(\mathbf{r}_p\right),\qquad p\neq q.$$

can be determined due to a symmetry relation. Indeed, changing the sign of the radius vector in (42) we have:

$$\begin{aligned}\sum_{l=0}^{\infty}\sum_{s=-l}^{l}(S|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)R_l^s\left(\mathbf{r}_q\right)&=S_n^m\left(\mathbf{r}_q+\mathbf{r}'_{pq}\right)=(-1)^nS_n^m\left(-\mathbf{r}_q-\mathbf{r}'_{pq}\right)\\=(-1)^n\sum_{l=0}^{\infty}\sum_{s=-l}^{l}(S|R)_{ln}^{sm}\left(-\mathbf{r}'_{pq}\right)R_l^s\left(-\mathbf{r}_q\right)&=\sum_{l=0}^{\infty}\sum_{s=-l}^{l}(-1)^{n+l}(S|R)_{ln}^{sm}\left(\mathbf{r}'_{qp}\right)R_l^s\left(\mathbf{r}_q\right).\end{aligned}$$

Due to orthogonality of surface harmonics we obtain:

$$(S|R)_{ln}^{sm}\left(\mathbf{r}'_{qp}\right) = (-1)^{n+l}(S|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right), \qquad p \neq q, \tag{129}$$
$$n, l = 0, 1, ..., \qquad m = -n, ..., n, \quad l = -s, ..., s.$$

We also can find using (42) and

$$S_n^m = 0, \quad R_n^m = 0, \quad \text{for } |m| > n, \tag{130}$$

that

$$(S|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) = 0, \quad \text{for } |m| > n \text{ or } |s| > l. \tag{131}$$

9.2 (R|R) Coefficients

Setting $\mathbf{r}_q = \mathbf{0}$ in (58) and using (119) we have

$$R_n^m\left(\mathbf{r}'_{pq}\right) = \sqrt{\frac{1}{4\pi}} \sum_{\alpha=0}^{\infty} \sum_{\beta=-\alpha}^{\alpha} (r|r)_{\alpha 0n}^{\beta 0m} R_\alpha^\beta\left(\mathbf{r}'_{pq}\right). \tag{132}$$

Due to the orthogonality of surface functions we obtain then

$$(r|r)_{\alpha 0n}^{\beta 0m} = \sqrt{(4\pi)}\delta_{\alpha n}\delta_{\beta m}. \tag{133}$$

Substituting this expression into (56), we have

$$(R|R)_{0n}^{0m}\left(\mathbf{r}'_{pq}\right) = \sqrt{(4\pi)} R_n^m\left(\mathbf{r}'_{pq}\right), \qquad n = 0, 1, ..., \quad m = -n, ..., n. \tag{134}$$

In (58) we also can set $\mathbf{r}'_{pq} = \mathbf{0}$. In this case from (119) we have

$$R_n^m\left(\mathbf{r}_q\right) = \sqrt{\frac{1}{4\pi}} \sum_{l=0}^{\infty} \sum_{s=-l}^{l} (r|r)_{0ln}^{0sm} R_l^s\left(\mathbf{r}_q\right), \tag{135}$$

This yields

$$(r|r)_{0ln}^{0sm} = \sqrt{(4\pi)}\delta_{ln}\delta_{sm}. \tag{136}$$

Both values (133) and (136) are consistent with those following from the particular values of the Wigner symbols (54). Generally, we notice that (58) is symmetrical with respect to the exchange of $\mathbf{r}_q$ and $\mathbf{r}'_{pq}$, which shows the following symmetry:

$$(r|r)_{\alpha ln}^{\beta sm} = (r|r)_{l\alpha n}^{s\beta m}. \tag{137}$$

To obtain the value of $(S|R)_{l0}^{s0}\left(\mathbf{r}'_{pq}\right)$ we notice that the spherical Bessel and Hankel functions of the first kind are related via

$$j_n(kr) = \frac{1}{2}\left[h_n(kr) + \overline{h_n(kr)}\right]. \tag{138}$$

Particularly this results in

$$R_0^0(\mathbf{r}_q) = \frac{1}{2}\left[S_0^0(\mathbf{r}_q) + \overline{S_0^0(\mathbf{r}_q)}\right]. \tag{139}$$

Using this relation and the expansion of the fundamental solution (123), (124), and (126) we obtain:

$$R_0^0(\mathbf{r}_q) = \frac{1}{2}\sqrt{(4\pi)}\left\{\sum_{l=0}^{\infty}\sum_{s=-l}^{s=l}(-1)^l S_l^{-s}\left(\mathbf{r}'_{pq}\right)R_l^s\left(\mathbf{r}_q\right) + \sum_{l=0}^{\infty}\sum_{s=-l}^{s=l}(-1)^l \overline{S_l^{-s}\left(\mathbf{r}'_{pq}\right)R_l^s\left(\mathbf{r}_q\right)}\right\} \tag{140}$$
$$= \frac{1}{2}\sqrt{(4\pi)}\left\{\sum_{l=0}^{\infty}\sum_{s=-l}^{s=l}(-1)^l S_l^{-s}\left(\mathbf{r}'_{pq}\right)R_l^s\left(\mathbf{r}_q\right) + \sum_{l=0}^{\infty}\sum_{s=-l}^{s=l}(-1)^l \frac{\overline{h_l(kr'_{pq})}}{h_l(kr'_{pq})}S_l^s\left(\mathbf{r}'_{pq}\right)R_l^{-s}\left(\mathbf{r}_q\right)\right\}$$
$$= \sqrt{(4\pi)}\sum_{l=0}^{\infty}\sum_{s=-l}^{s=l}(-1)^l\frac{1}{2}\left[h_l(kr'_{pq}) + \overline{h_l(kr'_{pq})}\right]\frac{1}{h_l(kr'_{pq})}S_l^{-s}\left(\mathbf{r}'_{pq}\right)R_l^s\left(\mathbf{r}_q\right)$$
$$= \sqrt{(4\pi)}\sum_{l=0}^{\infty}\sum_{s=-l}^{s=l}(-1)^l R_l^{-s}\left(\mathbf{r}'_{pq}\right)R_l^s\left(\mathbf{r}_q\right).$$

Comparing this expansion with (14) and using the orthogonality of the surface harmonics, we obtain

$$(R|R)_{l0}^{s0}\left(\mathbf{r}'_{pq}\right) = \sqrt{(4\pi)}(-1)^l R_l^{-s}\left(\mathbf{r}'_{pq}\right), \qquad l = 0,1,..., \quad s = -l,...,l. \tag{141}$$

In the same way as for $(S|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)$ (see (129) and (131)) we can show that

$$(R|R)_{ln}^{sm}\left(\mathbf{r}'_{qp}\right) = (-1)^{n+l}(R|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right), \tag{142}$$
$$n,l = 0,1,..., \qquad m = -n,...,n, \quad l = -s,...,s.$$

and

$$(R|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) = 0, \quad \text{for } |m| > n \text{ or } |s| > l. \tag{143}$$

Note that to obtain the above values and properties of coefficients $(S|R)_{ln}^{sm}$ and $(R|R)_{ln}^{sm}$ there is no need to use Wigner's or Clebsch-Gordan coefficients.

9.3 (S|S) Coefficients

Due to (60) particular values of $(S|S)_{ln}^{sm}$ coefficients can be found using properties of the $(s|r)_{l\alpha n}^{s\beta m}$ symbols, which are stated earlier (see also (54)). Using (57) and comparing with (134) and (141) we obtain

$$(S|S)_{l0}^{s0}\left(\mathbf{r}'_{pq}\right) = \sqrt{(4\pi)}(-1)^l R_l^{-s}\left(\mathbf{r}'_{pq}\right) = (R|R)_{l0}^{s0}\left(\mathbf{r}'_{pq}\right). \tag{144}$$

$$(S|S)_{0n}^{0m}\left(\mathbf{r}'_{pq}\right) = \sqrt{(4\pi)}R_n^m\left(\mathbf{r}'_{pq}\right) = (R|R)_{0n}^{0m}\left(\mathbf{r}'_{pq}\right). \tag{145}$$

In the same way as was shown for $(S|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)$ (see (129) and (131)) we can show that

$$(S|S)_{ln}^{sm}\left(\mathbf{r}'_{qp}\right) = (-1)^{n+l}(S|S)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right), \quad n,l = 0,1,..., \quad m = -n,...,n, \quad l = -s,...,s. \tag{146}$$

and

$$(S|S)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) = 0, \quad \text{for } |m| > n \text{ or } |s| > l. \tag{147}$$

10 Sectorial Translation Coefficients

In analogy with the surface spherical harmonics we will call reexpansion coefficients of type $(E|F)_{l|m|}^{sm}$ and $(E|F)_{|s|n}^{sm}$ as "sectorial reexpansion coefficients", since they involve reexpansion of sectorial harmonics or represent coefficients near sectorial harmonics in reexpansions. For such coefficients we will use simplified notation

$$(E|F)_{l,}^{sm} = (E|F)_{l|m|}^{sm}, \quad (E|F)_{,n}^{sm} = (E|F)_{|s|n}^{sm}. \tag{148}$$

Particularly we have from (122) and (125), (134) and (141), and (144) and (145) :

$$(S|R)_{l,}^{s0}\left(\mathbf{r}'_{pq}\right)=\sqrt{(4\pi)}\,(-1)^l\,S_l^{-s}\left(\mathbf{r}'_{pq}\right),\quad (S|R)_{,n}^{0m}\left(\mathbf{r}'_{pq}\right)=\sqrt{(4\pi)}S_n^m\left(\mathbf{r}'_{pq}\right), \tag{149}$$
$$(R|R)_{l,}^{s0}\left(\mathbf{r}'_{pq}\right)=(S|S)_{l,}^{s0}\left(\mathbf{r}'_{pq}\right)=\sqrt{(4\pi)}\,(-1)^l\,R_l^{-s}\left(\mathbf{r}'_{pq}\right),\quad (R|R)_{,n}^{0m}\left(\mathbf{r}'_{pq}\right)=(S|S)_{,n}^{0m}\left(\mathbf{r}'_{pq}\right)=\sqrt{(4\pi)}R_n^m\left(\mathbf{r}'_{pq}\right).$$

We will call also coefficients $(E|F)_{|s||m|}^{sm}$ “double sectorial reexpansion coefficients” and simplify notation as

$$(E|F)^{sm}=(E|F)_{|s||m|}^{sm}. \tag{150}$$

Particularly, (149) provides:

$$(S|R)^{s0}\left(\mathbf{r}'_{pq}\right)=\sqrt{(4\pi)}\,(-1)^s\,S_l^{-s}\left(\mathbf{r}'_{pq}\right),\quad (S|R)^{0m}\left(\mathbf{r}'_{pq}\right)=\sqrt{(4\pi)}S_n^m\left(\mathbf{r}'_{pq}\right), \tag{151}$$
$$(R|R)^{s0}\left(\mathbf{r}'_{pq}\right)=(S|S)^{s0}\left(\mathbf{r}'_{pq}\right)=\sqrt{(4\pi)}\,(-1)^s\,R_l^{-s}\left(\mathbf{r}'_{pq}\right),\quad (R|R)^{0m}\left(\mathbf{r}'_{pq}\right)=(S|S)^{0m}\left(\mathbf{r}'_{pq}\right)=\sqrt{(4\pi)}R_n^m\left(\mathbf{r}'_{pq}\right).$$

The reason why we pay special attention to the sectorial reexpansion coefficients is that they can be computed by simplified recurrence relations, or explicitly, and they provide “boundary conditions” for the recursive computation of the tesseral reexpansion coefficients $(E|F)_{ln}^{sm}$.

10.1 Computation of Sectorial Translation Coefficients

The sectorial reexpansion coefficients can be computed independently from the other coefficients, since the initial values (149) and recurrence relations (86)-(87) and (90)-(91) include only sectorial coefficients and are sufficient for their computation. These relations can be rewritten in the form:

$$b_{m+1}^{-m-1}\,(E|F)_{l,}^{s,m+1}=b_l^{-s}\,(E|F)_{l-1,}^{s-1,m}-b_{l+1}^{s-1}\,(E|F)_{l+1,}^{s-1,m}, \tag{152}$$
$$l=0,1,...\qquad s=-l,...,l,\qquad m=0,1,2,....$$

$$b_{m+1}^{-m-1}\,(E|F)_{l,}^{s,-m-1}=b_l^{s}\,(E|F)_{l-1,}^{s+1,-m}-b_{l+1}^{-s-1}\,(E|F)_{l+1,}^{s+1,-m}, \tag{153}$$
$$l=0,1,...\qquad s=-l,...,l,\qquad m=0,1,2,....$$

$$b_{s+1}^{-s-1}\,(E|F)_{,n}^{-s-1,m}=b_n^{m}\,(E|F)_{,n-1}^{-s,m+1}-b_{n+1}^{-m-1}\,(E|F)_{,n+1}^{-s,m+1}, \tag{154}$$
$$n=0,1,...\qquad m=-n,...,n\qquad s=0,1,2,....$$

$$b_{s+1}^{-s-1}\,(E|F)_{,n}^{s+1,m}=b_n^{-m}\,(E|F)_{,n-1}^{s,m-1}-b_{n+1}^{m-1}\,(E|F)_{,n+1}^{s,m-1}, \tag{155}$$
$$n=0,1,...\qquad m=-n,...,n\qquad s=0,1,2,....$$

Relations (152) and (153) provide values of coefficients $(E|F)_{l,}^{sm}$ for layers with increasing $|m|$. This process starts with known values $(E|F)_{l,}^{s0}$ (149). Similarly, relations 154) and (155) provide values of coefficients $(E|F)_{,n}^{sm}$ for layers with increasing $|s|$. This process starts with known values $(E|F)_{,n}^{0m}$ (149).

An important consequence of the symmetry is that

$$(S|S)_{l,}^{sm}=(R|R)_{l,}^{sm},\quad (S|S)_{,n}^{sm}=(R|R)_{,n}^{sm}, \tag{156}$$
$$l,n=0,1,2,...,\qquad s=-l,...,l,\qquad m=-n,...,n.$$

Indeed, sectorial coefficients $(S|S)$ and $(R|R)$ have the same initial values (149) and satisfy the same recurrence relations. Keeping this in mind, further we can consider only $(R|R)$ coefficients.

Note also the following relation for the sectorial reexpansion coefficients following from (84)

$$a_{|s|}^{s}\,(E|F)_{|s|+1,}^{sm}=-a_{|m|}^{m}\,(E|F)_{,|m|+1}^{sm}, \tag{157}$$
$$m=0,\pm1,\pm2,...\qquad s=0,\pm1,\pm2,....$$

10.2 Symmetries of Sectorial Translation Coefficients

The reexpansion coefficients obey many symmetry properties, which can be a subject for a separate investigation. The symmetry relations are very important for efficient computation and enable substantial savings of computer resources. They are also important for developing fast numerical methods. Here we note just a few symmetries, which immediately follow from the recurrence relations and initial values of the sectorial coefficients.

Theorem 11 *S0: The following symmetry holds*

$$(E|F)_{l,}^{sm} = (-1)^{l+m} (E|F)_{,l}^{-m,-s}, \qquad (158)$$
$$l = 0,1,2,..., \qquad s = -l,...,l, \qquad m = -n,...,n.$$

Proof. According (149) for $m = 0$ we have

$$(E|F)_{l,}^{s0} = (-1)^l (E|F)_{,l}^{0,-s}.$$

Assume that this holds for $l = 0,1,...; s = -l,...,l; |m| = 0,...,M$. Let us prove that it also holds for $l = 0,1,...; s = -l,...,l; |m| = 0,...,M+1$.
Consider $m > 0$. According the assumption of induction and (152), we have

$$b_{M+1}^{-M-1}(E|F)_{l,}^{s,M+1} = b_l^{-s}(E|F)_{l-1,}^{s-1,M} - b_{l+1}^{s-1}(E|F)_{l+1,}^{s-1,M} = (-1)^{l+M+1}\left(b_l^{-s}(E|F)_{,l-1}^{-M,-s+1} - b_{l+1}^{s-1}(E|F)_{,l+1}^{-M,-s+1}\right).$$

The expression in the former brackets coincides with the right hand side of (154) if we replace s with $-m$ and l with n. Thus,

$$b_l^{-s}(E|F)_{,l-1}^{M,-s+1} - b_{l+1}^{s-1}(E|F)_{,l+1}^{M,-s+1} = b_{M+1}^{-M-1}(E|F)_{,l}^{-M-1,-s},$$

and

$$b_{M+1}^{-M-1}(E|F)_{l,}^{s,M+1} = (-1)^{l+M+1} b_{M+1}^{-M-1}(E|F)_{,l}^{-M-1,-s},$$

which proves the theorem for $m > 0$, since $b_m^{-m} \neq 0$ for $m > 0$ by (73).

For $m \leqslant 0$ we have from (153),(155) and the assumption of induction

$$b_{M+1}^{-M-1}(E|F)_{l,}^{s,-M-1} = b_l^{s}(E|F)_{l-1,}^{s+1,-M} - b_{l+1}^{-s-1}(E|F)_{l+1,}^{s+1,-M} = (-1)^{l+M+1}\left(b_l^{s}(E|F)_{,l-1}^{M,-s-1} - b_{l+1}^{-s-1}(E|F)_{,l+1}^{M,-s-1}\right)$$
$$= (-1)^{l+M+1} b_{M+1}^{-M-1}(E|F)_{,l}^{M+1,-s}.$$

which proves the theorem for this case as well. ■

Theorem 12 *S1: The following symmetry holds*

$$(R|R)_{l,}^{sm} = \overline{(R|R)_{l,}^{-s,-m}}, \qquad (159)$$
$$l = 0,1,2,..., \qquad s = -l,...,l, \qquad m = 0,\pm1,\pm2,...$$

Proof. This relation obviously holds for $m = 0$ (see (149) and (76)). It is also clear that we can consider only non-negative $m = 0,1,2,...$, since for negative m we can take complex conjugate of the equality (159) and change $-m$ to m. Assume now that it holds for $m = M$, and prove that in this case it holds for $m = M+1$. Replacing m with M in (152) we have

$$b_{M+1}^{-M-1}(R|R)_{l,}^{s,M+1} = b_l^{-s}(R|R)_{l-1,}^{s-1,M} - b_{l+1}^{s-1}(R|R)_{l+1,}^{s-1,M}.$$

According to the induction assumption the right hand side can be rewritten as

$$b_l^{-s}(R|R)_{l-1,}^{s-1,M} - b_{l+1}^{s-1}(R|R)_{l+1,}^{s-1,M} = \overline{b_l^{-s}(R|R)_{l-1,}^{-s+1,-M} - b_{l+1}^{s-1}(R|R)_{l+1,}^{-s+1,-M}} = b_{M+1}^{-M-1}\overline{(R|R)_{l,}^{-s,-M-1}},$$

where the last equality holds due to (153), in which one should replace m with M and s with $-s$. This proves the statement of the theorem for $m = M+1$. ■

Theorem 13 *S2: The following symmetry holds*

$$(R|R)_{,n}^{sm} = \overline{(R|R)_{,n}^{-s,-m}}, \qquad (160)$$
$$l = 0,1,2,..., \qquad s = -l,...,l, \qquad m = 0,\pm1,\pm2,...$$

Proof. Follows from (159) and (158). ■

10.3 Particular Values of Double Sectorial Translation Coefficients

Using the notation of (150) we can rewrite relation (88) in the form

$$b_{m+1}^{-m-1}(E|F)^{-s,m+1} = -b_{s+1}^{-s-1}(E|F)^{-s-1,m}, \quad m,s = 0,1,2,... \qquad (161)$$

So we have for $m \geqslant 1$:

$$(E|F)^{-s,m} = \frac{b_{s+1}^{-s-1}}{-b_m^{-m}}(E|F)^{-s-1,m-1} = ... = \frac{b_{s+1}^{-s-1}...b_{s+m}^{-s-m}}{\left(-b_m^{-m}\right)...\left(-b_1^{-1}\right)}(E|F)^{-s-m,0}, \quad m = 1,2,..., \quad s = 0,1,2,...$$

Using (73), we have

$$\frac{b_{s+1}^{-s-1}...b_{s+m}^{-s-m}}{\left(-b_m^{-m}\right)...\left(-b_1^{-1}\right)} = (-1)^m \frac{(s+m)!}{s!m!}\sqrt{\frac{(2m+1)!(2s+1)!}{(2s+2m+1)!}} \qquad (162)$$

and from (151):

$$(S|R)^{-s,m}\left(\mathbf{r}'_{pq}\right) = (-1)^s \frac{(s+m)!}{s!m!}\sqrt{\frac{4\pi(2m+1)!(2s+1)!}{(2s+2m+1)!}}S_{s+m}^{s+m}\left(\mathbf{r}'_{pq}\right), \qquad (163)$$
$$(R|R)^{-s,m}\left(\mathbf{r}'_{pq}\right) = (S|S)^{-s,m}\left(\mathbf{r}'_{pq}\right) = (-1)^s \frac{(s+m)!}{s!m!}\sqrt{\frac{4\pi(2m+1)!(2s+1)!}{(2s+2m+1)!}}R_{s+m}^{s+m}\left(\mathbf{r}'_{pq}\right),$$
$$m = 0,1,2,... \qquad s = 0,1,2,....$$

Relation (92) can be rewritten in the form

$$-b_{m+1}^{-m-1}(E|F)^{s,-m-1} = b_{s+1}^{-s-1}(E|F)^{s+1,-m}, \quad m,s = 0,1,2,... \qquad (164)$$

So we have

$$(E|F)^{s,-m} = \frac{b_{s+1}^{-s-1}}{-b_m^{-m}}(E|F)^{s+1,-m+1} = ... = \frac{b_{s+1}^{-s-1}...b_{s+m}^{-s-m}}{\left(-b_m^{-m}\right)...\left(-b_1^{-1}\right)}(E|F)_{s+m,0}^{s+m,0}, \quad m = 1,2,..., \quad s = 0,1,2,...$$

Using (162) and (151) we obtain

$$(S|R)^{s,-m}\left(\mathbf{r}'_{pq}\right) = (-1)^s \frac{(s+m)!}{s!m!}\sqrt{\frac{4\pi(2m+1)!(2s+1)!}{(2s+2m+1)!}}S_{s+m}^{-s-m}\left(\mathbf{r}'_{pq}\right), \qquad (165)$$
$$(R|R)^{s,-m}\left(\mathbf{r}'_{pq}\right) = (S|S)^{-s,m}\left(\mathbf{r}'_{pq}\right) = (-1)^s \frac{(s+m)!}{s!m!}\sqrt{\frac{4\pi(2m+1)!(2s+1)!}{(2s+2m+1)!}}R_{s+m}^{-s-m}\left(\mathbf{r}'_{pq}\right),$$
$$m = 0,1,2,... \qquad s = 0,1,2,....$$

11 Zonal Translation Coefficients

Using terminology, similar to that used for spherical surface harmonics (zonal, sectorial and tesseral harmonics) we can call the coefficients

$$(E|F)_{ln}\left(\mathbf{r}'_{pq}\right) = (E|F)^{00}_{ln}\left(\mathbf{r}'_{pq}\right), \quad l,n = 0,1,2,... \tag{166}$$

"zonal" reexpansion coefficients.

Particularly we have from (122) and (125), (134) and (141), and (144) and (145) :

$$(S|R)_{l0}\left(\mathbf{r}'_{pq}\right) = \sqrt{(4\pi)}\,(-1)^l\, S^0_l\left(\mathbf{r}'_{pq}\right), \quad (S|R)_{0n}\left(\mathbf{r}'_{pq}\right) = \sqrt{(4\pi)}S^0_n\left(\mathbf{r}'_{pq}\right), \tag{167}$$

$$(R|R)_{l0}\left(\mathbf{r}'_{pq}\right) = (S|S)_{l0}\left(\mathbf{r}'_{pq}\right) = \sqrt{(4\pi)}\,(-1)^l\, R_l\left(\mathbf{r}'_{pq}\right), \quad (R|R)_{0n}\left(\mathbf{r}'_{pq}\right) = (S|S)_{0n}\left(\mathbf{r}'_{pq}\right) = \sqrt{(4\pi)}R^m_n\left(\mathbf{r}'_{pq}\right).$$

As sectorial coefficients, the zonal reexpansion coefficients can be computed independently on the other coefficients using (80), which can be rewritten as

$$a^0_{n-1}\,(E|F)_{l,n-1} - a^0_n\,(E|F)_{l,n+1} = a^0_l\,(E|F)_{l+1,n} - a^0_{l-1}\,(E|F)_{l-1,n}, \quad l,n = 0,1,... \tag{168}$$

11.1 Symmetry of Zonal Translation Coefficients

Note the following symmetry relation, which can be useful for computation of the zonal reexpansion coefficients.

Theorem 14 *The following symmetry relation holds*

$$(E|F)_{ln} = (-1)^{n+l}\,(E|F)_{nl}, \quad l,n = 0,1,... \tag{169}$$

Proof. First we notice that according (149) this relation holds for $n = 0$ and any $l = 0,1,...$, which provides a basis for induction. The induction assumption is that it is true for all $n \leqslant N$ and any $l = 0,1,....$ We prove then that it is also holds for $n = N+1$ and any $l = 0,1,.....$

From (80) we have

$$a^0_N\,(E|F)^{00}_{l,N+1} = a^0_{N-1}\,(E|F)^{00}_{l,N-1} - a^0_l\,(E|F)^{00}_{l+1,N} + a^0_{l-1}\,(E|F)^{00}_{l-1,N}, \quad l = 0,1,...$$

According to the induction assumption the right hand side of this expression can be rewritten as

$$a^0_{N-1}\,(E|F)^{00}_{l,N-1} - a^0_l\,(E|F)^{00}_{l+1,N} + a^0_{l-1}\,(E|F)^{00}_{l-1,N} = (-1)^{N+1+l}\left[a^0_{N-1}\,(E|F)^{00}_{N-1,l} - a^0_l\,(E|F)^{00}_{N,l+1} + a^0_{l-1}\,(E|F)^{00}_{N,l-1}\right].$$

Since (80) holds for any $l,n \geqslant 0$ we have :

$$a^0_l\,(E|F)^{00}_{N,l+1} = a^0_{N-1}\,(E|F)^{00}_{N-1,l} - a^0_N\,(E|F)^{00}_{N+1,l} + a^0_{l-1}\,(E|F)^{00}_{N,l-1}$$

Substituting this expression into the previous ones, we obtain:

$$(E|F)^{00}_{l,N+1} = (-1)^{N+1+l}\,(E|F)^{00}_{N+1,l}.$$

■

12 Computation of Translation Coefficients

As soon as the sectorial reexpansion are computed, so the values $(E|F)^{sm}_{l|m|}$, $l = |s|, |s|+1, ...$ and $(E|F)^{sm}_{|s|n}$, $n = |m|, |m|+1, ...$ are known, coefficients $(E|F)^{sm}_{ln}$ for all pairs (l,n) can be computed using recurrence relation (80) (note that $(E|F)^{sm}_{ln} = 0$, for $l < |s|$ or for $n < |m|$).

Another method can be to compute first the zonal coefficients $(E|F)^{00}_{ln}$, $l,n = 0,1,2,...$ and then use recurrence relations (85) and (89) to propagate with respect to orders m and s in positive and negative directions.

Note that since the obtained recurrence procedure enables computation of all reexpansion coefficients and they are determined by their initial values and recurrence relations uniquely, we have

$$(S|S)^{sm}_{ln} = (R|R)^{sm}_{ln}, \qquad l,n = 0,1,2,..., \quad s = -l,...,l, \quad m = -n,...,n. \tag{170}$$

which proves (61) and (62).

12.1 Symmetry of Translation Coefficients

Theorem 15 *The following symmetry relation holds:*

$$(E|F)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) = (-1)^{n+l}\,(E|F)_{nl}^{-m,-s}\left(\mathbf{r}'_{pq}\right), \qquad (171)$$
$$l,n = 0,1,... \qquad s=-l,...,l, \qquad m=-n,...,n.$$

Proof. First we notice that according (149) this relation holds for $n = 0$ $(m = -n, ..., n = 0)$ and any $l = 0,1,...,s=-l,...,l$, which provides a basis for induction. The inductional assumption is that it is true for all $n \leqslant N$ $(m=-n,...,n)$ and any $l=0,1,...,s=-l,...,l$. We prove then that it is also holds for $n = N+1$ $(m=-n,...,n)$. Consider first case $n=N+1$, $m=-N,...,N$. From (80) we have

$$a_N^m\,(E|F)_{l,N+1}^{sm} = a_{N-1}^m\,(E|F)_{l,N-1}^{sm} - a_l^s\,(E|F)_{l+1,N}^{sm} + a_{l-1}^s\,(E|F)_{l-1,N}^{sm},$$
$$l=0,1,... \qquad s=-l,...,l, \qquad m=-N,...,N.$$

According the inductional assumption the right hand side of this expression can be rewritten as

$$a_{N-1}^m(E|F)_{l,N-1}^{sm} - a_l^s\,(E|F)_{l+1,N}^{sm} + a_{l-1}^s\,(E|F)_{l-1,N}^{sm} = (-1)^{N+1+l}\left[a_{N-1}^m\,(E|F)_{N-1,l}^{-m,-s} - a_l^s\,(E|F)_{N,l+1}^{-m,-s} + a_{l-1}^s\,(E|F)_{N,l-1}^{-m,-s}\right].$$

Since (80) holds for any $l,n \geqslant 0$ and corresponding ranges of s and m, we have :

$$a_l^s\,(E|F)_{N,l+1}^{-m,-s} = a_{N-1}^m\,(E|F)_{N-1,l}^{-m,-s} - a_N^m\,(E|F)_{N+1,l}^{-m,-s} + a_{l-1}^s\,(E|F)_{N,l-1}^{-m,-s}$$

Here we took into account $a_n^m = a_n^{|m|} = a_n^{-m}$(68). Substituting this expression into the previous ones, we obtain:

$$(E|F)_{l,N+1}^{sm} = (-1)^{N+1+l}\,(E|F)_{N+1,l}^{-m,-s}.$$

The case $n=N+1$, $|m|=N+1$ can be proved easily, since from (158) we have immediately

$$(E|F)_{l|m|}^{sm} = (-1)^{l+|m|}\,(E|F)_{|m|l}^{-m,-s},$$
$$l=0,1,2,..., \qquad s=-l,...,l, \qquad |m|=N+1.$$

So this property is proved. ■

12.2 Structure of Recurrence Relations

For efficient computation of the reexpansion coefficients it is important to make clear the structure of the recurrence relations.

Consider first how the recurrence relation (80) works. A diagram shown in Figure 6 shows that for given three values at lower l or at lower n reexpansion coefficients can be computed for larger l or n at the same s and m. Such diagrams can be called the diagrams of recurrence propagation of the values of the coefficients in the l and in the n directions, respectively. Therefore, if say the values of $(E|F)_{ln}^{sm}$ are known for $l=|s|$ and all n, $N_1 < n < N_2$, relation (80) enables computation of $(E|F)_{ln}^{sm}$ in a triangular domain in the plane (l,n) up to $l = |s| + \left[\frac{1}{2}(N_2 - N_1)\right]$ for fixed s and m (see Figure 7). The same holds for propagation in n direction, where $(E|F)_{ln}^{sm}$ can be computed based on the values of sectorial coefficients $n=|m|$ and all l with $L_1 < l < L_2$, and relation (80) in triangular domain in plane (l,n) up to $n = |m| + \left[\frac{1}{2}(L_2 - L_1)\right]$ (see Figure 7).

Assume now that the sectorial reexpansion coefficients are known for given s and m and consider the ranges for n and l that are required to compute all other (tesseral) reexpansion coefficients $(E|F)_{ln}^{sm}$ for $l=|s|,|s|+1,...,N_t$ and, $n=|m|,|m|+1,...,N_t$, where N_t is the truncation number (the degree of the highest harmonics in the series that we want to take into account). Thus $(E|F)_{ln}^{sm}$ must be computed in a rectangular domain in the (l,n) plane. Since the filling of the domain occurs in triangular fashion we will compute some reexpansion coefficients only for intermediate purposes, which are specified at points in the (l,n) plain outside the rectangular domain. Optimization of the computational procedure, which will be the subject of future studies, will consider the problem of reduction

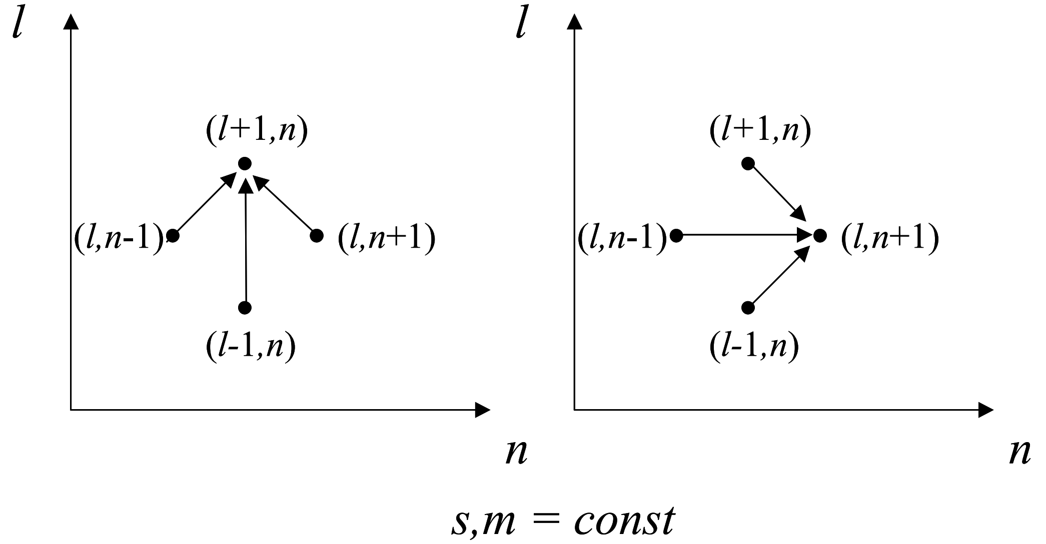


Figure 6: A diagram showing how the reccurence relation (80) enables recursive computation (propagation) of the values of the reexpansion coefficients for increasing $l > |s|$ and $n > |m|$ at fixed s and m. For $l = |s|$ or $n = |m|$ coefficients corresponding to "coordinates" $(l-1, n)$ or $(l, n-1)$ can be dropped, since the values of the corresponding reexpansion coefficients at these points are zero (respectively for $l = |s|$ or $n = |m|$).

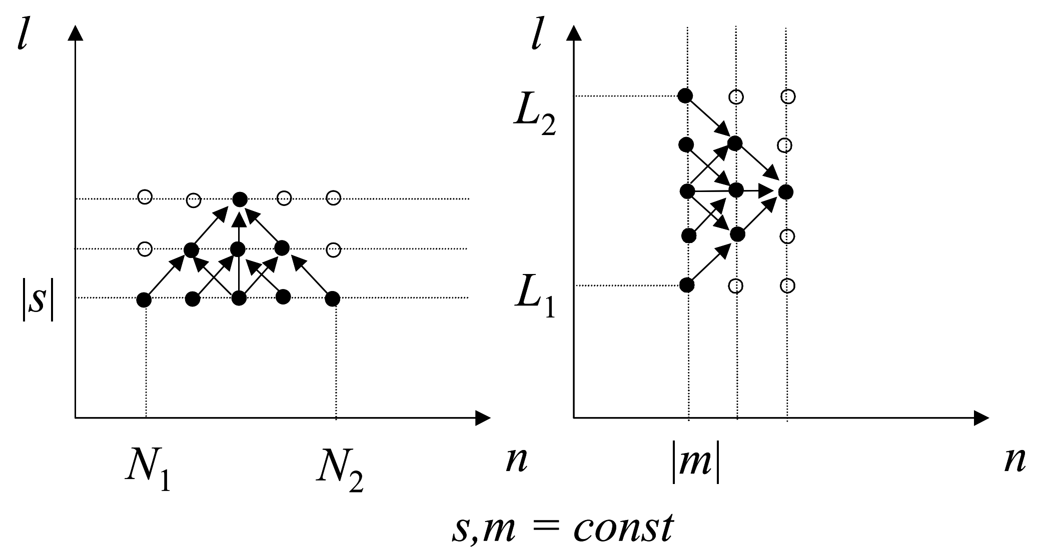


Figure 7: A diagram showing that the reexpansion coefficients can be computed using the recursive relation (80) at points marked by dark circles if the values of sectorial reexpansion coefficients are known for some range of n and l. For computation of the values at points marked by light circles additional data is needed.

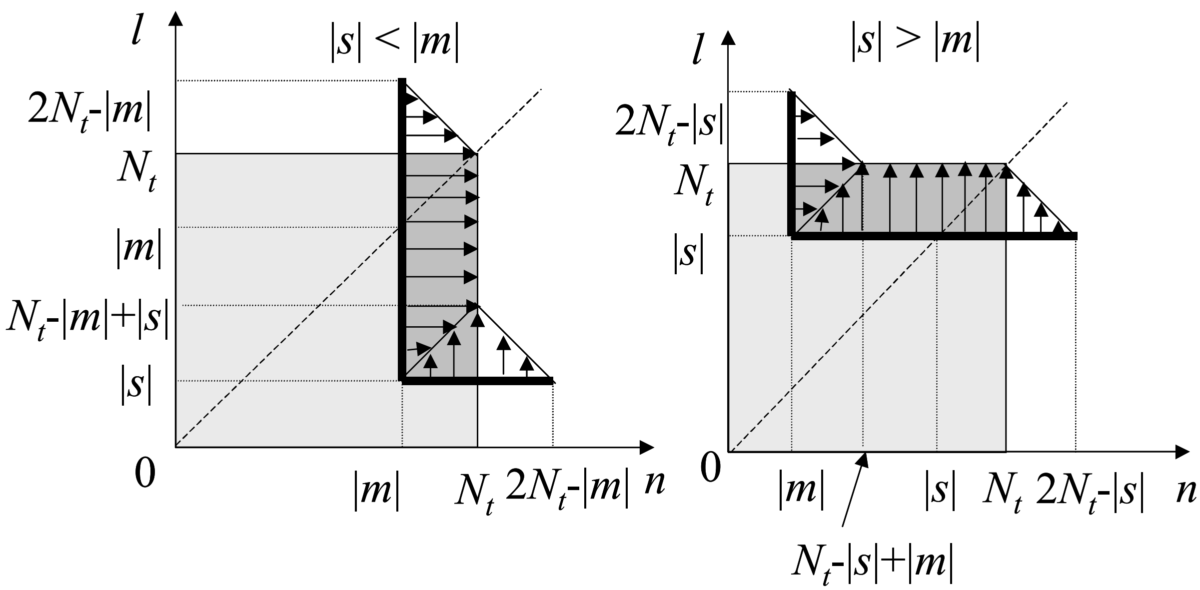


Figure 8: A diagram showing how the values of the tesseral reexpansion coefficients can be computed recursively inside a rectange in the index space shown in dark grey using the values of the sectorial coefficients specified at the bold lines.

of computation of reexpansion coefficient outside the domain. The following method of computation of the required coefficients may be considered as preliminary.

Consider first the case $|s| \leqslant |m|$. In the square $N_t \times N_t$ shown in light gray in the left of Figure 8 all reexpansion coefficients are zero, except for the coefficients inside the rectangle shaded by dark grey. To compute them with the aid of recurrence relation (80) we can propagate the "boundary values" (or the values of the sectorial coefficients shown by thick lines in the figure.) in the l and n directions as shown by arrows. This allows us to fill the trapezoidal and the triangular domains, which cover the dark grey rectangle. For this purpose the sectorial coefficients $(E|F)_{|s|n}^{sm}$ are needed for $n = |m|, ..., 2N_t - |m|$, while $(E|F)_{l|m|}^{sm}$ are needed for $l = |s|, ..., 2N_t - |m|$.

A similar situation holds for the case $|s| \geqslant |m|$ shown in the right Figure 8. In this case for computation of the tesseral coefficients we need the values of sectorial coefficients $(E|F)_{|s|,n}^{sm}$ for $n = |m|, ..., 2N_t - |s|$, while $(E|F)_{l|m|}^{sm}$ are needed for $l = |s|, ..., 2N_t - |s|$. Both cases $|s| \leqslant |m|$ and $|s| \geqslant |m|$ will be covered if $(E|F)_{|s|n}^{sm}$ are provided for $n = |m|, ..., 2N_t - \max(|m|, |s|)$, and $(E|F)_{l|m|}^{sm}$ are provided for $l = |s|, ..., 2N_t - \max(|m|, |s|)$.

Consider now the computation of the sectorial coefficients $(E|F)_{l,}^{sm} = (E|F)_{l|m|}^{sm}$. The left diagram in Figure 9 shows how the recurrence relation (152) enables computation of $(E|F)_{l,}^{sm}$ $(m \geqslant 0)$, based on the known initial values of $(E|F)_{l,}^{s0}$. To compute $(E|F)_{l,}^{sm}$ two values $(E|F)_{l-1,}^{s-1,m-1}$ and $(E|F)_{l+1,}^{s-1,m-1}$ are required. The propagation occurs in the plane passing through the line $(0, s-m)$ in the (m,s)-plane and through the point (m,s,l). Therefore, to compute $(E|F)_{l,}^{sm}$ initial values $(E|F)_{\alpha,}^{s-m,0}$, $\alpha = l-m, ..., l+m$ are required. Since for the computation of the tesseral coefficients at given s and m the values of the sectorial coefficients for $l = |s|, ..., 2N_t - \max(m, |s|)$ are needed, this shows that $(E|F)_{\alpha,}^{s-m,0}$, $\alpha = |s| - m, ..., 2N_t - \max(m, |s|) + m$ should be provided for this purpose. Since $(E|F)_{\alpha,}^{s-m,0} = 0$ for $\alpha < |s-m|$ then the lower bound of α is $\alpha = |s-m| \geqslant |s| - m$.

Similar consideration can be given for computation of $(E|F)_{l,}^{sm}$ $(m < 0)$, where recurrence relation (153) can be employed. This case is shown in the right diagram in Figure 9. Diagrams for computation of sectorial coefficients $(E|F)_{,n}^{sm} = (E|F)_{|s|n}^{sm}$ using the relations (154) and (155) are shown in Figure 10.

It is clear that in all cases it is sufficient to provide initial values $(E|F)_{l,}^{s0}$ for $l = 0, ..., 2N_t$, $|s| = 0, ..., l$, and $(E|F)_{,n}^{0m}$ for $n = 0, ..., 2N_t$, $|m| = 0, ..., n$.

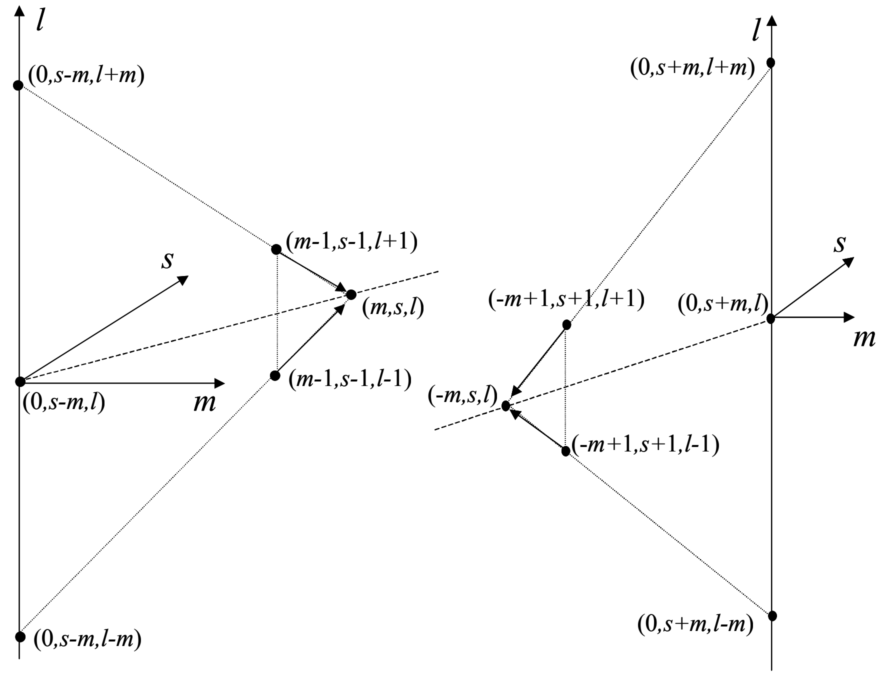


Figure 9: A diagram showing reccurent propagation of the sectorial coefficients in 3-dimensional space of indices with respect to m.

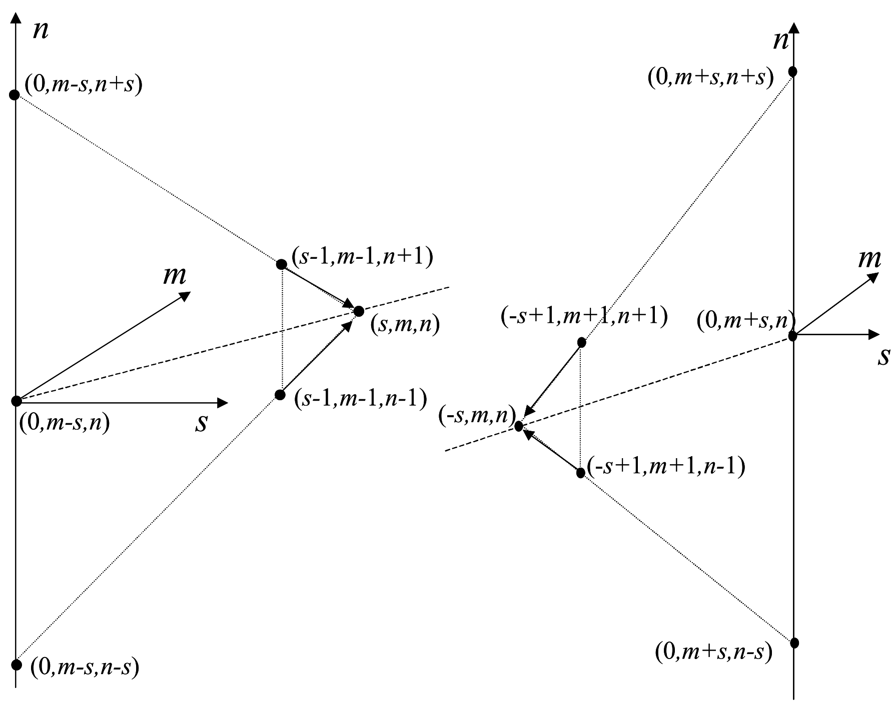


Figure 10: The same as in Figure 9 but with respect to s.

12.3 Example

As an example consider computation of $S_5^2(\mathbf{r}_p)$ for $k = 1$ and $\mathbf{r}_p = (1, -6, 1)$ using multipole reexpansion near $\mathbf{r}_q = (-1, 1, 0)$. We have $\mathbf{r}'_{pq} = \mathbf{r}_p - \mathbf{r}_q = (2, -7, 1)$ .The reexpansion may be written as

$$S_5^2(\mathbf{r}_p) = \sum_{l=0}^{N_t} \sum_{s=-l}^{l} (S|R)_{l5}^{s2} \left(\mathbf{r}'_{pq}\right) R_l^s(\mathbf{r}_q).$$

Direct computation yields

$$S_5^2(\mathbf{r}_p) = h_5\left(kr_p\right) Y_5^2\left(\theta_p, \phi_p\right) = 0.049626 - 0.019882i.$$

For computation of $(S|R)_{l5}^{s2}\left(\mathbf{r}'_{pq}\right)$ we used the above recurrence relations and $R_l^s(\mathbf{r}_q)$ are computed directly. The table below provides the values of the sum with increasing truncation number N_t and the relative error (in percents) between the exact and approximate values of $\left|S_5^2(\mathbf{r}_p)\right|$:

N_t	$Exact$	Sum	$Error$,%
0	$0.049626 - 0.019882i$	$0.020196 + 0.013655i$	83
2	$0.049626 - 0.019882i$	$0.049166 - 0.014885i$	9.4
4	$0.049626 - 0.019882i$	$0.049805 - 0.019548i$	0.71
6	$0.049626 - 0.019882i$	$0.049643 - 0.019875i$	0.034
8	$0.049626 - 0.019882i$	$0.049627 - 0.019883i$	0.0015

In this example the error decays exponentially and a good accuracy can be achieved at relatively low N_t.

13 Reciprocity of Translation Coefficients

Reciprocity relations for the reexpansion coefficients can be obtained if we reexpand the reexpansion back at the original point. Particularly, we have

$$R_n^m\left(\mathbf{r}_p\right) = \sum_{l=0}^{\infty} \sum_{s=-l}^{l} (R|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) R_l^s\left(\mathbf{r}_q\right) = \sum_{l=0}^{\infty} \sum_{s=-l}^{l} \sum_{\alpha=0}^{\infty} \sum_{\beta=-\alpha}^{\alpha} (R|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) (R|R)_{\alpha l}^{\beta s}\left(\mathbf{r}'_{qp}\right) R_\alpha^\beta\left(\mathbf{r}_p\right)$$

$$= \sum_{l=0}^{\infty} \sum_{s=-l}^{l} \sum_{\alpha=0}^{\infty} \sum_{\beta=-\alpha}^{\alpha} (-1)^{\alpha+l} (R|R)_{\alpha l}^{\beta s}\left(\mathbf{r}'_{pq}\right) (R|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) R_\alpha^\beta\left(\mathbf{r}_p\right). \tag{172}$$

$$\sum_{l=0}^{\infty} \sum_{s=-l}^{l} (-1)^{\alpha+l} (R|R)_{\alpha l}^{\beta s}\left(\mathbf{r}'_{pq}\right) (R|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) = \delta_{n\alpha}\delta_{m\beta}, \tag{173}$$

or in matrix form:

$$(\mathbf{R}|\mathbf{R})^2 = \mathbf{I}, \quad (\mathbf{R}|\mathbf{R}) = \left\{(-1)^\alpha (R|R)_{\alpha l}^{\beta s}\right\}. \tag{174}$$

This relation is valid inside the finite domain, where the regular reexpansion holds. It is interesting to notice that substituting into (173) values $(R|R)_{0l}^{0s}\left(\mathbf{r}'_{pq}\right)$ and $(R|R)_{l0}^{s0}\left(\mathbf{r}'_{pq}\right)$ from (134) and (141) and using the fact that $R_l^{-s}\left(\mathbf{r}'_{pq}\right) = \overline{R_l^s\left(\mathbf{r}'_{pq}\right)}$, we obtain the following fundamental theorem for the regular elementary solutions:

Theorem 16

$$4\pi \sum_{l=0}^{\infty} \sum_{s=-l}^{l} \left|R_l^s\left(\mathbf{r}'_{pq}\right)\right|^2 = 1. \tag{175}$$

Note that the reciprocity relations show that the matrix of the reexpansion coefficients $(\mathbf{R}|\mathbf{R})$ is non-singular and

$$(\mathbf{R}|\mathbf{R}) = (\mathbf{R}|\mathbf{R})^{-1}. \tag{176}$$

This matrix also has symmetry properties following from (171) and (159).

14 Coaxial (Diagonal) Translation Coefficients

The consideration given above treats a general three-dimensional problem in arbitrary reference frames. For some problems proper selection of the reference frame enables substantial simplification including reduction in computation of the reexpansion coefficients. Indeed, we can introduce the reference frame in such a way that its axis z is directed from point $\mathbf{r}'_p$ to the center of reexpansion $\mathbf{r}'_q$ (or from $\mathbf{r}'_q$ to $\mathbf{r}'_p$). Since the reexpansion coefficients depend only on $\mathbf{r}'_{pq}$, there will be no angular dependence of these coefficients for such selection of the frame orientation. In these particular cases general reexpansion formulae (12)-(14) simplify considerably to:

$$S_n^m(\mathbf{r}_p) = \sum_{l=|m|}^{\infty} (S|R)_{ln}^m \left(r'_{pq}\right) R_l^s(\mathbf{r}_q), \qquad |\mathbf{r}_q| < \left|\mathbf{r}'_{pq}\right|, \tag{177}$$

$$S_n^m(\mathbf{r}_p) = \sum_{l=|m|}^{\infty} (S|S)_{ln}^m \left(r'_{pq}\right) S_l^s(\mathbf{r}_q), \qquad |\mathbf{r}_q| > \left|\mathbf{r}'_{pq}\right|, \tag{178}$$

$$R_n^m(\mathbf{r}_p) = \sum_{l=|m|}^{\infty} (R|R)_{ln}^m \left(r'_{pq}\right) R_l^s(\mathbf{r}_q). \tag{179}$$

Since the coefficients are now only three dimensional, we can say that they correspond to a "diagonalization" of the 4-D case. To comply with the general practice in the literature, henceforth we will refer to these coefficients as "diagonal." The coefficients

$$(E|F)_{ln}^m \left(r'_{pq}\right) = (E|F)_{ln}^{mm} \left(\mathbf{r}'_{pq}\right), \quad l,n = 0,1,..., \quad m = -n,...,n, \quad (E|F) = (S|R),(S|S),(R|R) \tag{180}$$

satisfy general recurrence relations and can be computed using the general algorithm. However, the simpler relations provide an advantage in their fast computation. First we consider such relations.

14.1 Recurrence Relations and Properties of Diagonal Translation Coefficients

In this subsection we will drop argument r'_{pq} for the reexpansion coefficients to simplify notation. The recurrence formula (80) does not act on the orders of the reexpansion coefficients, so putting there $s = m$ we have

$$a_{n-1}^m (E|F)_{l,n-1}^m - a_n^m (E|F)_{l,n+1}^m = a_l^m (E|F)_{l+1,n}^m - a_{l-1}^m (E|F)_{l-1,n}^m, \tag{181}$$
$$l,n = 0,1,... \qquad m = -n,...,n.$$

In relation (85) we set $s = m+1$ to obtain

$$b_n^m (E|F)_{l,n-1}^{m+1} - b_{n+1}^{-m-1} (E|F)_{l,n+1}^{m+1} = b_{l+1}^m (E|F)_{l+1,n}^m - b_l^{-m-1} (E|F)_{l-1,n}^m, \tag{182}$$
$$l,n = 0,1,... \qquad m = -n,...,n.$$

Now it is obvious that we can start from $m = 0$ and $(E|F)_{ln}^0$ to compute $(E|F)_{ln}^m$ and $(E|F)_{ln}^{-m}$ for $m = 1,2,...$ by using (182) and obtain all coefficients. Since the recurrence coefficients in (182) for propagation in positive and negative directions of m are the same, we come to conclusion that

$$(E|F)_{ln}^m = (E|F)_{ln}^{-m} = (E|F)_{ln}^{|m|}, \quad l,n = 0,1,..., \qquad m = -n,...,n. \tag{183}$$

Therefore computation of $(E|F)_{ln}^m$ is required only for non-negative m and formulae (181) and (182) are sufficient for this purpose. Due to (171) we also have the following symmetry property:

$$(E|F)_{ln}^m = (-1)^{n+l} (E|F)_{nl}^m, \tag{184}$$
$$l,n = 0,1,... \qquad m = -n,...,n.$$

14.2 Computation of Diagonal Translation Coefficients

Due to the symmetry relations $(E|F)_{ln}^{m}$ can be computed only for $l \geqslant n \geqslant m \geqslant 0$. The process of recurrent filling of the matrix $\{(E|F)_{ln}^{m}\}$ can be organized by filling the layers, with respect to the degrees l and n followed by advancement with respect to the order m. If such a filling procedure is selected then the first step is filling of the layer $m=0$. If the axis z is directed from point q to point p (so $\theta'_{pq}=\pi$), we have according (180) and (149):

$$(S|R)_{l0}^{0}\left(r'_{pq}\right)=(S|R)_{l0}^{00}\left(\mathbf{r}'_{pq}\right)=\sqrt{(4\pi)}(-1)^{l}S_{l}^{0}\left(\mathbf{r}'_{pq}\right)=(-1)^{l}\sqrt{(2l+1)}h_{l}(kr'_{pq})P_{l}(\cos\theta'_{pq}|_{\theta'_{pq}=\pi})=\sqrt{(2l+1)}h_{l}(kr'_{pq}), \tag{185}$$

$$(R|R)_{l0}^{0}\left(r'_{pq}\right)=(S|S)_{l0}^{0}\left(r'_{pq}\right)=\sqrt{(2l+1)}j_{l}(kr'_{pq}),$$

all other $(E|F)_{ln}^{0}$ can be obtained using (181) and (184). For the opposite direction of the axis z, we have $\theta'_{pq}=0$, and

$$\begin{aligned}(S|R)_{l0}^{0}\left(r'_{pq}\right)&=(-1)^{l}\sqrt{(2l+1)}h_{l}(kr'_{pq}),\\ (R|R)_{l0}^{0}\left(r'_{pq}\right)&=(S|S)_{l0}^{0}\left(r'_{pq}\right)=(-1)^{l}\sqrt{(2l+1)}j_{l}(kr'_{pq})\end{aligned} \tag{186}$$

For advancement with respect to m it is convenient to use (182) for $n=m$:

$$b_{m+1}^{-m-1}(E|F)_{l,m+1}^{m+1}=b_{l}^{-m-1}(E|F)_{l-1,m}^{m}-b_{l+1}^{m}(E|F)_{l+1,m}^{m}, \quad l=m+1,m+2,... \tag{187}$$

and obtain other $(E|F)_{ln}^{m+1}$ using (181) and (184) in the same way as $(E|F)_{ln}^{0}$ are computed.

Formulae (187) and (185) employ sectorial coefficients of type $(E|F)_{lm}^{m}$, which can conveniently be denoted as

$$(E|F)_{l}^{m}=(E|F)_{lm}^{m}, \quad l=m,m+1,... \tag{188}$$

which satisfy the relations

$$(S|R)_{l}^{0}=(\pm1)^{l}\sqrt{(2l+1)}h_{l}(kr'_{pq}), \quad (R|R)_{l}^{0}\left(r'_{pq}\right)=(S|S)_{l}^{0}\left(r'_{pq}\right)=(\pm1)^{l}\sqrt{(2l+1)}j_{l}(kr'_{pq}) \tag{189}$$

$$\begin{aligned}b_{m+1}^{-m-1}(E|F)_{l}^{m+1}&=b_{l}^{-m-1}(E|F)_{l-1}^{m}-b_{l+1}^{m}(E|F)_{l+1}^{m}, \quad l=m+1,m+2,...,\\ (E|F)&=(S|R),(S|S),(R|R).\end{aligned}$$

Here the sign depends on the orientation of the reference frame and equal to $-\cos\theta'_{pq}$ (see (185) and (186)).

Note that for computation of the reexpansion coefficients inside an (l,n,m) cube of size (N_t,N_t,N_t) coefficients $(E|F)_{l0}^{0}$ should be computed for $l=0,...,2N_t$. This is due to the recurrence relations for increase of n (181) and for increase of l (189) require $(E|F)_{l+1,n}^{m}$ for computation of $(E|F)_{l,n+1}^{m}$ and $(E|F)_{ln}^{m+1}$. Therefore in these relations each step requires increase of the $l-$dimension of the array by one, i.e. to reach $m=N_t, n=N_t$, we need to have $(E|F)_{l0}^{0}$ of twice length with respect to l.

15 Computation of Translation Operators

Theorem 17 *Computation of multipole reexpansion, or translation, coefficients $(E|F)_{ln}^{sm}(\mathbf{r}_{pq})$ for all values of $l=0,...,N_t$, $s=-l,...,l$, $n=0,...,N_t$, $m=-n,...,n$ can be performed within $O(N_t^4)$ operations.*

Proof. First we notice that the total number of coefficients $(E|F)_{ln}^{sm}$, $l=0,...,N_t$, $s=-l,...,l$, $n=0,...,N_t$, $m=-n,...,n$, is $(N_t+1)^4=O(N_t^4)$. So if at least one operation is required for computation of each coefficient the total number of operations will be $O(N_t^4)$. Computation of the initial values $(E|F)_{l0}^{s0}$ and $(E|F)_{0n}^{0m}$ requires $O(N_t)$ operations. Computation of the sectorial coefficients $(E|F)_{l|m|}^{sm}$ and $(E|F)_{|s|n}^{sm}$ using the initial values and recurrence relations, which include not more than 2 multiplications and one addition to produce a new value requires $O(N_t^3)$ operations, since the total number of the sectorial coefficients is $O(N_t^3)$. Computation of the tesseral coefficients $(E|F)_{ln}^{sm}$ using the values of the sectorial coefficients recurrence relations which include not more than 3 multiplications and 2 additions requires $O(N_t^4)$ operations. In the recurrence process additional values of $(E|F)_{ln}^{sm}$ for $l>N_t$ and $n>N_t$ can be required. However the maximum size of l and n is limited by $2N_t$, which is provided constructively by the above algorithms. Therefore the total number of operations is limited by $O(N_t^4)$. ■

Theorem 18 *Computation of coaxial (diagonal) multipole reexpansion, or translation, coefficients* $(E|F)_{ln}^{m}(r_{pq})$ *for all values of* $l = 0, ..., N_t$, $n = 0, ..., N_t$, $m = -n, ..., n$ *can be performed within* $O(N_t^3)$ *operations.*

Proof. The proof follows from the algorithm provided above. ■

16 Rotation-Translation Operation

As is clear from the above theorem, the computation of the coaxial coefficients can be performed in $O(N_t^3)$ operations as opposed to $O(N_t^4)$ operations required for the general case. To take advantage of this fact for the general case we will consider the rotation of the coordinate system to make the axis $\mathbf{i}_{\hat{z}}$ directed from point p to point q (so $\theta'_{pq} = \pi$) and then apply the theory for coaxial coefficients. Such a rotation occurs in the plane determined by vectors $\mathbf{i}_z$ and $\mathbf{i}_{\hat{z}} = \mathbf{r}'_{pq}/\left|\mathbf{r}'_{pq}\right| = -\mathbf{r}'_{qp}/\left|\mathbf{r}'_{pq}\right|$, and therefore can be specified by a single angle γ'_{pq} :

$$\cos\gamma'_{pq} = \mathbf{i}_z \cdot \mathbf{i}_{\hat{z}} = \frac{\mathbf{i}_z \cdot \mathbf{r}'_{pq}}{\left|\mathbf{r}'_{pq}\right|} = \frac{z'_q - z'_p}{r'_{pq}}, \tag{190}$$

where z'_q and z'_p are $z-$coordinates of points q and p in the original coordinate system. The matrix of rotation Q to achieve this rotation was derived as Equation (23).

Equations (32) and (33) can be rewritten as

$$E_n^m(\mathbf{r}_p) = \sum_{\nu=-n}^{n} T_n^{\nu m}\left(Q'_{pq}\right) E_n^{\nu}(\widehat{\mathbf{r}}_p), \qquad |\widehat{\mathbf{r}}_p| = |\mathbf{r}_p|, \qquad E = S, R. \tag{191}$$

where $\widehat{\mathbf{r}}_p$ is the radius-vector of the point in the rotated coordinate system.

Functions $E_n^j(\widehat{\mathbf{r}}_p)$ then can be translated/reexpanded near the reexpansion point q according to (177)-(179):

$$E_n^{\nu}(\widehat{\mathbf{r}}_p) = \sum_{l=|\nu|}^{\infty} (E|F)_{ln}^{\nu}\left(r'_{pq}\right) F_l^{\nu}(\widehat{\mathbf{r}}_q), \qquad F, E = S, R, \tag{192}$$

where $\widehat{\mathbf{r}}_p$ is the radius vector centered in point q in the rotated coordinate system. To return to initial coordinates we rotate coordinates back, so we perform rotation of coordinate system, specified by the rotation matrix $Q'^{*}_{pq} = Q'^{-1}_{pq}$:

$$F_l^{\nu}(\widehat{\mathbf{r}}_q) = \sum_{s=-l}^{l} T_l^{s\nu}\left(Q'^{*}_{pq}\right) F_l^{s}(\mathbf{r}_q), \qquad |\widehat{\mathbf{r}}_q| = |\mathbf{r}_q|, \qquad E = S, R. \tag{193}$$

Combining (191) and (193) we obtain:

$$E_n^m(\mathbf{r}_p) = \sum_{\nu=-n}^{n} \sum_{l=|\nu|}^{\infty} \sum_{s=-l}^{l} T_l^{s\nu}\left(Q'^{*}_{pq}\right) T_n^{\nu m}\left(Q'_{pq}\right) (E|F)_{ln}^{\nu}\left(r'_{pq}\right) F_l^{s}(\mathbf{r}_q), \qquad E = S, R. \tag{194}$$

Changing the order of summation of l and ν, we obtain

$$E_n^m(\mathbf{r}_p) = \sum_{l=0}^{\infty} \sum_{s=-l}^{l} \sum_{\nu=-\min(l,n)}^{\min(l,n)} T_l^{s\nu}\left(Q'^{*}_{pq}\right) T_n^{\nu m}\left(Q'_{pq}\right) (E|F)_{ln}^{\nu}\left(r'_{pq}\right) F_l^{s}(\mathbf{r}_q), \qquad E = S, R.. \tag{195}$$

On the other hand we have the representation (78), which yields:

$$(E|F)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) = \sum_{\nu=-\min(l,n)}^{\min(l,n)} (E|F)_{ln}^{\nu}\left(r'_{pq}\right) T_l^{s\nu}\left(Q'^{*}_{pq}\right) T_n^{\nu m}\left(Q'_{pq}\right), \qquad E = S, R. \tag{196}$$

Note that $T_l^{s\nu}\left(Q'^{*}_{pq}\right) T_n^{\nu m}\left(Q'_{pq}\right)$ depends only on the spherical polar angles of $\mathbf{r}'_{pq}$:

$$T_l^{s\nu}\left(Q'^{*}_{pq}\right) T_n^{\nu m}\left(Q'_{pq}\right) = \mathbb{T}_{ln}^{s\nu m}(\theta'_{pq}, \varphi'_{pq}) \tag{197}$$

and form (196) is a separation of the angular and distance variables for translation reexpansion coefficients. It must be noted that this product is only conceptual, and in practice it would be used for computation of the translation reexpansion coefficients $(E|F)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)$ by a composition of successive products (thereby avoiding matrix-matrix products). The computational advantage of this form for the solution of the Helmholtz equation is that one can perform the rotation operation (which requires $O(N_t^3)$ operations), and then the coaxial translation, which also can be performed for $O(N_t^3)$ operations, and then (if needed), rotation that can again be made for $O(N_t^3)$ operations. So the total number of operations for such a procedure is $O(N_t^3)$ opposed to $O(N_t^4)$ operations required for a general translation. The practical value of these rotations (in comparison with the efficient recursions developed in this report) is a matter that must be investigated. We note that αN_t^3 operations with large α can be less efficient than βN_t^4 with small β, since for most fat multipole methods we expect that N_t will be small due to the quickly convergent series.

17 Computation of Rotation Coefficients

To complete a set of recurrence algorithms for computation of the reexpansion coefficients, we just briefly describe the procedure for computation of rotation coefficients $T_n^{\nu m}\left(Q'_{pq}\right)$. It is noteworthy that these coefficients are not a property of the Helmholtz equation but purely a property of spherical harmonics, which has been studied in much more depth, than the translation coefficients for the Helmholtz equation (see e.g. Stein [14] for addition theorems, and explicit relations to Wigner's symbols). However this classical problem is still of interest, and only recently in the literature have there appeared algorithms (for use in computational quantum chemistry) for stable and rapid computation of the rotation coefficients based on the recurrence relations for real spherical harmonics (Ivanic & Ruedenberg [18]) and general complex case (Choi et al. [19]). Our derivation of the recurrence relations differs from those in the cited papers and uses different definitions of spherical harmonics (so care should be taken when comparing the results). Due to their dependence only on the angular part, these results should be the same for the Laplace, Schrödinger, heat etc. equations.

17.1 Initial Values

Consider (31) for $m = 0$:

$$Y_n^0(\theta,\varphi) = \sqrt{\frac{2n+1}{4\pi}} P_n(\cos\theta) = \sum_{\nu=-n}^{n} T_n^{\nu 0}(Q)\, Y_n^{\nu}\left(\widehat{\theta},\widehat{\varphi}\right). \tag{198}$$

A well-known addition theorem for spherical harmonics (it is reproduced e.g., in Ref. [3]) yields:

$$P_n(\cos\theta) = \frac{4\pi}{2n+1} \sum_{\nu=-n}^{n} Y_n^{-\nu}\left(\theta',\varphi'\right) Y_n^{\nu}\left(\widehat{\theta},\widehat{\varphi}\right), \tag{199}$$

where θ is the angle between points with spherical coordinates $\left(\theta',\varphi'\right)$ and $\left(\widehat{\theta},\widehat{\varphi}\right)$ on a unit sphere. Comparing (198) and (199) we obtain

$$T_n^{\nu 0}(Q) = \sqrt{\left(\frac{4\pi}{2n+1}\right)} Y_n^{-\nu}\left(\theta',\varphi'\right), \quad n = 0,1,..., \quad \nu = -n,...,n. \tag{200}$$

Note that θ' and φ' are nothing but the spherical polar angles of the axis $\mathbf{i}_z$ in the reference frame $(\mathbf{i}_{\widehat{x}},\mathbf{i}_{\widehat{y}},\mathbf{i}_{\widehat{z}})$ and formulae (27) and (29) provide explicit expressions for components of Q through these angles.

17.2 Symmetry of Rotation Coefficients

Theorem 19 *The following symmetry holds*

$$\begin{aligned} T_n^{-\nu,-m}(Q) &= \overline{T_n^{\nu m}(Q)}, \\ n &= 0,1,..., \qquad \nu, m = -n,...,n. \end{aligned} \tag{201}$$

Proof. Since $Y_n^{-\nu} = \overline{Y_n^{\nu}}$ for any $n = 0, 1, ..., \nu = -n, ..., n$, we have from (31):

$$Y_n^m(\theta,\varphi) = \overline{Y_n^{-m}(\theta,\varphi)} = \sum_{\nu=-n}^{n} \overline{T_n^{\nu,-m}(Q)\, Y_n^{\nu}\left(\widehat{\theta},\widehat{\varphi}\right)} = \sum_{\nu=-n}^{n} \overline{T_n^{\nu,-m}(Q)} Y_n^{-\nu}\left(\widehat{\theta},\widehat{\varphi}\right) = \sum_{\nu=-n}^{n} \overline{T_n^{-\nu,-m}(Q)} Y_n^{\nu}\left(\widehat{\theta},\widehat{\varphi}\right). \tag{202}$$

Comparing this result with expansion of $Y_n^m(\theta,\varphi)$ (31) we obtain the statement of the theorem, since $Y_n^{\nu}\left(\widehat{\theta},\widehat{\varphi}\right)$ is orthonormal and representation (31) is unique. ■

17.3 Computational Procedure

Since $T_n^{\nu 0}(Q)$ are known explicitly for arbitrary $n = 0, 1, 2, ...$ and $v = -n, ..., n$, we need perform only one-dimensional recursive propagation for $T_n^{\nu m}$ for increasing m ($m > 0$) and decreasing m ($m < 0$). The recurrence for negative m can be dropped due to $T_n^{\nu m}$ for such m can be simply found using symmetry relation (201). For non-negative m we can use any of relations (102) or (113).

For example, using the following relation between the elements of matrices W (101) and Q (17):

$$\begin{aligned} W_{11} + W_{21} &= Q_{11} + Q_{22} + i\left(Q_{12} - Q_{21}\right), \\ W_{12} + W_{22} &= Q_{11} - Q_{22} + i\left(Q_{12} + Q_{21}\right), \\ W_{13} + W_{23} &= -2\left(Q_{31} + iQ_{32}\right), \end{aligned} \tag{203}$$

and expressions for elements of Q through the polar angles (27), we obtain from (113) the following recurrence relation explicitly expressing the recurrence coefficients through the reference frame rotation angles θ', φ' and χ :

$$\begin{aligned} T_{n-1}^{\nu,m+1} &= \frac{e^{i\chi}}{b_n^m}\left\{\frac{1}{2}\left[b_n^{-\nu-1}e^{i\varphi'}\left(1-\cos\theta'\right)T_n^{\nu+1,m} - b_n^{\nu-1}\left(1+\cos\theta'\right)e^{-i\varphi'}T_n^{\nu-1,m}\right] - a_{n-1}^{\nu}\sin\theta' T_n^{\nu m}\right\}, \\ n &= 2,3,..., \quad \nu = -n+1,...,n-1, \quad m = 0,...,n-2, \end{aligned} \tag{204}$$

which enables computation of all $T_n^{\nu m}$ for positive m.This requires $O(N_t^3)$ operations for rotating a multipole series truncated at $n = N_t$ (i.e., for $O\left(N_t^2\right)$ coefficients).

17.4 Example

As an example consider computation of $Y_3^2(\theta,\varphi)$ for $\theta = 36°$ and $\varphi = 60°$ using reexpansion for rotation $\theta' = 35°, \varphi' = 165°$, and $\chi = 10°$. In this case we have $\widehat{\theta} = 28.42795°$ and $\widehat{\varphi} = 93.9431°$, so the reexpansion may be written as

$$Y_3^2(\theta,\varphi) = \sum_{\nu=-3}^{3} T_3^{\nu 2}(Q)\, Y_3^{\nu}\left(\widehat{\theta},\widehat{\varphi}\right).$$

Straight-forward computation yields

$$Y_3^2(\theta,\varphi) = -0.14283 + 0.24738i.$$

For computation of we used recurrence relation (204) with initial values provided by (200) and $Y_3^{\nu}\left(\widehat{\theta},\widehat{\varphi}\right)$ were computed directly. The computed values are shown in the table below.

ν	$\mathrm{Re}\{T_3^{\nu 2}(Q)\}$	$\mathrm{Im}\{T_3^{\nu 2}(Q)\}$	$\mathrm{Re}\left\{Y_3^{\nu}\left(\widehat{\theta},\widehat{\varphi}\right)\right\}$	$\mathrm{Im}\left\{Y_3^{\nu}\left(\widehat{\theta},\widehat{\varphi}\right)\right\}$
-3	-0.00521	0.00243	-0.05567	-0.05567
-2	0.03589	-0.00633	0.23852	0.13771
-1	-0.14123	-0.01236	-0.42168	-0.11299
0	0.34676	0.12621	0.10853	0.00000
1	0.49241	0.34479	-0.42168	0.11299
2	0.24327	0.28992	0.23852	-0.13771
3	-0.24562	-0.52673	-0.05567	0.05567

Summation of the products $T_3^{\nu 2}(Q)\, Y_3^{\nu}\left(\widehat{\theta},\widehat{\varphi}\right)$ with the index ν varying over -3 to 3 yields $Y_3^2(\theta,\varphi)$, which coincides with the straight-forward computation.

18 Conclusions and Future Work

We have presented a method for fast computation of the multipole translation and rotation coefficients for the 3-D Helmholtz equation based on recurrence relations, which we derive. This method enables computation of the full matrix of translation coefficients truncated by N_t terms in multipole expansion for $O(N_t^4)$ operations, opposed to $O(N_t^5)$ operations required for computations using the Wigner or Clebsch-Gordan summations. We provided an algorithm realizing $O(N_t^4)$ number of operations and proved recurrence theorems for translation operators and translation coefficients. These theorems also were checked numerically by comparing of the exact values of multipoles and the values computed using multipole reexpansions. Using an explicit rotation of the multipoles, the full set of translation coefficient of multipoles can be computed in $O(N_t^3)$ operations, if coaxial coefficients are used. Since we provide explicit relations, the constants multiplying the order symbols for all our algorithms are small.

The results presented have an advantage compared to computation of the translation coefficients based on computation of integral representations, because it requires much fewer operations, and does not introduce additional errors due to numerical discretization and approximation of integrals.

As a future work the following problems are of interest:

1. Optimize the computational algorithm. This includes optimal use of recurrence relations and symmetries of the translation and rotation coefficients, which may substantially reduce the number of coefficients that are need to be computed outside the domain limited by the truncation.
2. Evaluate the errors due to the recurrence procedures. While the series converge extremely quickly, we need to provide explicit theorems for this.
3. Evaluate the behavior of the translation coefficients of large degrees and orders, to provide error bounds (some similar work has already been done by Koc et al [12] for the approximate diagonal forms). Evaluate combined errors of truncation and recurrence procedures.
4. Apply the method for solution of particular problems and compare with the other methods.

From a theoretical point of view, it can also be interesting to obtain more insight to the structure of the reexpansion coefficients of the Helmholtz equation. For example, further reciprocity relations and symmetry properties of the matrices of the reexpansion coefficients can lead to substantial speedups of computations of the coefficients.

It must be also noted that the recurrence relations are valid not only for multipole translations, but also for computation of regular solutions inside finite domains. This can be used for solution of the boundary value problems for the Helmholtz equation in 3-D domains.

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A The Helmholtz Equation in Spherical Coordinates

A.1 Spherical Coordinates

The mutual transformations between spherical coordinates and Cartesian coordinates with a common origin

$$(x, y, z) \to (r, \theta, \varphi), \tag{205}$$

are given by

$$\begin{aligned} x &= r \sin\theta \cos\varphi, \\ y &= r \sin\theta \sin\varphi, \\ z &= r \cos\theta. \end{aligned} \tag{206}$$

and

$$\begin{aligned} r &= \sqrt{x^2+y^2+z^2}, \qquad r \geqslant 0, \\ \theta &= \arccos \frac{z}{\sqrt{x^2+y^2+z^2}}, \qquad 0 \leqslant \theta \leqslant \pi, \\ \varphi &= \begin{cases} \arccos \frac{x}{\sqrt{x^2+y^2}}, & 0 \leqslant \varphi \leqslant \pi, \\ 2\pi - \arccos \frac{x}{\sqrt{x^2+y^2}}, & \pi \leqslant \varphi \leqslant 2\pi. \end{cases} \end{aligned} \tag{207}$$

The gradient of an arbitrary scalar function Ψ in spherical coordinates is

$$\nabla\Psi = \mathbf{i}_r \frac{\partial\Psi}{\partial r} + \mathbf{i}_\theta \frac{1}{r}\frac{\partial\Psi}{\partial\theta} + \mathbf{i}_\varphi \frac{1}{r\sin\theta}\frac{\partial\Psi}{\partial\varphi}, \tag{208}$$

where $(\mathbf{i}_r, \mathbf{i}_\theta, \mathbf{i}_\varphi)$ is a right-oriented orthonormal basis in spherical coordinates.

The Laplacian of a scalar function Ψ is:

$$\nabla^2\Psi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\Psi}{\partial\varphi^2}. \tag{209}$$

A.2 Separation of Variables

The Helmholtz equation

$$\nabla^2\Psi + k^2\Psi = 0 \tag{210}$$

in the spherical coordinates has the factored solution:

$$\Psi(r,\theta,\varphi) = R(r)\Theta(\theta)\Phi(\varphi), \tag{211}$$

where the function Θ is periodic with a period π and Φ is periodic with a period 2π.

Substituting (211) into the Helmholtz equation and multiplying by $r^2\sin^2\theta/\Psi$ we obtain:

$$\sin^2\theta\left[\frac{\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)}{R} + k^2r^2\right] + \sin\theta\frac{\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)}{\Theta} + \frac{\frac{d^2\Phi}{d\varphi^2}}{\Phi} = 0. \tag{212}$$

A.2.1 Equation with Respect to the Angle φ

Since neither the first, nor the second term in the left hand side depend on φ the third term there also must not depend on φ. Therefore, we have

$$\frac{d^2\Phi}{d\varphi^2} = \lambda\Phi, \tag{213}$$

where λ is a separation constant. Due to the period of Φ being 2π this separation constant must be

$$\lambda = -m^2, \qquad m = 0, 1, 2, \ldots \tag{214}$$

where m is a non-negative integer number.

In this case solution of Eq. (213) becomes

$$\Phi = C_1 e^{im\varphi} + C_2 e^{-im\varphi}, \tag{215}$$

or

$$\Phi = B_1 \sin m\varphi + B_2 \cos m\varphi, \tag{216}$$

where B_1, B_2, C_1, and C_2 are arbitrary constants of integration (remember, that Ψ can be complex and so these constants also can be complex).

A.2.2 Equation with Respect to the Angle θ

Using Equations (213) and (214) we can rewrite Equation (43) now in the form:

$$\frac{\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)}{R} + k^2r^2 = \frac{m^2}{\sin^2\theta} - \frac{\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)}{\Theta}. \tag{217}$$

The left hand side of this equation is a function of r only, while the right hand side can depend only on Θ. This may occur only both the left hand side and the right hand side are constants. As before let λ denote the separation constant. So we have:

$$\frac{m^2}{\sin^2\theta} - \frac{\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)}{\Theta} = \lambda, \tag{218}$$

$$\frac{\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)}{R} + k^2r^2 = \lambda. \tag{219}$$

Consider the first equation. Denoting

$$\mu = \cos\theta, \tag{220}$$

we have:

$$\frac{d\Theta}{d\theta} = \frac{d\Theta}{d\mu}\frac{d\mu}{d\theta} = -\frac{d\Theta}{d\mu}\sin\theta, \tag{221}$$

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) = \frac{1}{\sin\theta}\frac{d}{d\mu}\left(\sin\theta\frac{d\Theta}{d\theta}\right)\frac{d\mu}{d\theta}$$

$$= \frac{d}{d\mu}\left(\sin^2\theta\frac{d\Theta}{d\mu}\right) = \frac{d}{d\mu}\left[\left(1-\mu^2\right)\frac{d\Theta}{d\mu}\right].$$

Thus, the first equation can be rewritten in the form

$$\frac{d}{d\mu}\left[\left(1-\mu^2\right)\frac{d\Theta}{d\mu}\right] + \left[\lambda - \frac{m^2}{1-\mu^2}\right]\Theta = 0. \tag{222}$$

General solution of this equation, which is known as the *associated Legendre differential equation* is a superposition of two special functions – Legendre functions of the first and the second kind. However, we are interested only with solutions Θ periodic in π. Such solutions are realized only if

$$\lambda = n(n+1), \qquad n = 0, 1, 2, ..., \tag{223}$$

where n is a non-negative integer number. In this case the nonsingular periodic solution is

$$\Theta = CP_n^m(\mu), \tag{224}$$

where C is the constant of integration and $P_n^m(\mu)$ are the associated Legendre functions. These functions can be represented in the form:

$$P_n^m(\mu) = \left(1-\mu^2\right)^{m/2}\frac{d^mP_n(\mu)}{d\mu^m}, \tag{225}$$

where $P_n(\mu) = P_n^0(\mu)$ are the Legendre polynomials.

A.2.3 Equation with Respect to the Distance r

With λ from Eq. (223) equation for the radial coordinate (121) becomes

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \left[k^2r^2 - n(n+1)\right]R = 0. \tag{226}$$

Denoting

$$\rho = kr, \qquad v(\rho) = R(r), \tag{227}$$

we have the following differential equation for $v(\rho)$:

$$\rho^2v'' + 2\rho v' + \left[\rho^2 - n(n+1)\right]v = 0. \tag{228}$$

This is the *Spherical Bessel equation.* Particular solutions are the *Spherical Bessel functions of the first kind*

$$j_n(\rho) = \sqrt{\frac{\pi}{2\rho}} J_{n+1/2}(\rho), \tag{229}$$

the *Spherical Bessel functions of the second kind*

$$y_n(\rho) = \sqrt{\frac{\pi}{2\rho}} Y_{n+1/2}(\rho), \tag{230}$$

and the *Spherical Bessel functions of the third kind*

$$h_n^{(1)}(\rho) = j_n(\rho) + iy_n(\rho) = \sqrt{\frac{\pi}{2\rho}} H_{n+1/2}^{(1)}(\rho), \tag{231}$$

$$h_n^{(2)}(\rho) = j_n(\rho) - iy_n(\rho) = \sqrt{\frac{\pi}{2\rho}} H_{n+1/2}^{(2)}(\rho). \tag{232}$$

Functions $J_{n+1/2}(\rho)$ and $Y_{n+1/2}(\rho)$ are the *Bessel and Neumann functions of fractional order*, and $H_{n+1/2}^{(1)}(\rho)$ and $H_{n+1/2}^{(2)}(\rho)$ are the *Hankel functions of fractional order.* The pairs $j_n(\rho), y_n(\rho)$ and $h_n^{(1)}(\rho), h_n^{(2)}(\rho)$ are linearly independent solutions for every n.

It is very noticeable that the spherical Bessel functions can be expressed through elementary transcendental functions. This is clear from the following *Rayleigh's formulas*:

$$j_n(\rho) = \rho^n \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)^n \frac{\sin\rho}{\rho}, \tag{233}$$

$$y_n(\rho) = -\rho^n \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)^n \frac{\cos\rho}{\rho}, \qquad n = 0, 1, 2, ... \tag{234}$$

These formulas for spherical Bessel functions of the third kind become:

$$h_n^{(1)}(\rho) = \rho^n \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)^n \frac{\sin\rho - i\cos\rho}{\rho} = -i\rho^n \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)^n \frac{e^{i\rho}}{\rho}, \tag{235}$$

$$h_n^{(2)}(\rho) = \rho^n \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)^n \frac{\sin\rho + i\cos\rho}{\rho} = i\rho^n \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)^n \frac{e^{-i\rho}}{\rho}. \tag{236}$$

A.3 Spherical Harmonics

Solutions for angular variables usually are combined into the *Spherical Harmonics*:

$$Y_n^m(\theta, \varphi) = (-1)^m \sqrt{\frac{2n+1}{4\pi}\frac{(n-|m|)!}{(n+|m|)!}} P_n^{|m|}(\cos\theta) e^{im\varphi}, \tag{237}$$
$$n = 0, 1, 2, ...; \qquad m = -n, ..., n.$$

The spherical harmonics are also called sometimes *Surface Harmonics of the First Kind*, *Tesseral* for $m < n$ and *Sectorial* for $m = n$.

The spherical harmonics form a complete orthonormal system in $L^2(S_u)$, where S_u is the surface of the unit sphere $x^2 + y^2 + z^2 = 1$. By definition of the norm of an arbitrary function $F(\theta, \varphi)$ in $L^2(S_u)$ we have

$$\|F\|^2 = (F, F) = \int_{S_u} F\bar{F} dS = \int_{S_u} |F|^2 dS = \int_0^\pi \sin\theta d\theta \int_0^{2\pi} |F(\theta, \varphi)|^2 d\varphi. \tag{238}$$

where the $\bar{F}$ denotes the complex conjugate of F. Therefore, the scalar product of two spherical harmonics in $L^2(S_u)$ is

$$
\begin{aligned}
\left(Y_n^m, Y_j^l\right) &= \int_0^\pi \sin\theta d\theta \int_0^{2\pi} Y_n^m(\theta,\varphi)\bar{Y}_j^l(\theta,\varphi)d\varphi \\
&= (-1)^{m+l}\frac{1}{4\pi}\sqrt{(2n+1)\frac{(n-|m|)!}{(n+|m|)!}(2j+1)\frac{(j-|l|)!}{(j+|l|)!}}\int_0^\pi P_n^{|m|}(\cos\theta)P_j^{|l|}(\cos\theta)\sin\theta d\theta\int_0^{2\pi} e^{i(m-l)\varphi}d\varphi \\
&= \delta_{ml}\frac{1}{2}\sqrt{(2n+1)\frac{(n-|m|)!}{(n+|m|)!}(2j+1)\frac{(j-|m|)!}{(j+|m|)!}}\int_0^\pi P_n^{|m|}(\cos\theta)P_j^{|m|}(\cos\theta)\sin\theta d\theta \\
&= \delta_{ml}\delta_{nj}\left(n+\frac{1}{2}\right)\frac{(n-|m|)!}{(n+|m|)!}\int_{-1}^1\left[P_n^{|m|}(\mu)\right]^2 d\mu = \delta_{ml}\delta_{nj},
\end{aligned}
\tag{239}
$$

where δ_{ml} is the Kronecker delta. This proves orthonormality of the system. A proof of the completeness of the system of the spherical harmonics can be found elsewhere.

Consider now expansion of an arbitrary function $F(\theta,\varphi)$ using the basis of spherical harmonics:

$$
F(\theta,\varphi) = \sum_{n=0}^{\infty}\sum_{m=-n}^{m=n} F_n^m Y_n^m(\theta,\varphi). \tag{240}
$$

The scalar product of F and the spherical harmonic $Y_j^l(\theta,\varphi)$ is

$$
\left(F, Y_j^l\right) = \int_0^\pi \sin\theta d\theta\int_0^{2\pi} F(\theta,\varphi)\bar{Y}_j^l(\theta,\varphi)d\varphi. \tag{241}
$$

At the same time we have using (240) and (239):

$$
\left(F, Y_j^l\right) = \sum_{n=0}^{\infty}\sum_{m=-n}^{m=n} F_n^m\left(Y_n^m, Y_j^l\right) = \sum_{n=0}^{\infty}\sum_{m=-n}^{m=n} F_n^m\delta_{ml}\delta_{nj} = F_j^l. \tag{242}
$$

Therefore

$$
F_j^l = \int_0^\pi \sin\theta d\theta\int_0^{2\pi} F(\theta,\varphi)\bar{Y}_j^l(\theta,\varphi)d\varphi \tag{243}
$$

and coefficients in representation (240) can be determined using (243).

A.4 Superposition of Factored Solutions

Due to the linearity a particular solution of the Helmholtz equation can be represented as a sum of factored solutions:

$$
\Psi(r,\theta,\varphi) = \sum_{n=0}^{\infty}\sum_{m=-n}^{m=n}\left[A_n^m j_n(kr) + B_n^m y_n(kr)\right]Y_n^m(\theta,\varphi), \tag{244}
$$

where A_n^m and B_n^m are arbitrary constants. Functions $j_n(kr)$ are non-singular at real kr, while $y_n(kr)$ have singularity at $r = 0$. Thus for non-singular solutions in a bounded domain containing the origin of coordinates we must set $B_n^m = 0$. In this case solution in spherical coordinates becomes:

$$
\Psi(r,\theta,\varphi) = \sum_{n=0}^{\infty}\sum_{m=-n}^{m=n} A_n^m j_n(kr)Y_n^m(\theta,\varphi). \tag{245}
$$

For solutions outside a bounded domain it is more convenient to use representation of Ψ using spherical Bessel functions of the third kind:

$$
\Psi(r,\theta,\varphi) = \sum_{n=0}^{\infty}\sum_{m=-n}^{m=n}\left[A_n^m h_n^{(1)}(kr) + B_n^m h_n^{(2)}(kr)\right]Y_n^m(\theta,\varphi). \tag{246}
$$

Coefficients A_n^m and B_n^m should be selected to satisfy boundary conditions and Sommerfeld condition (3) of radiation.

Note that according Eq. (235) and (236) the third kind Bessel spherical functions can be represented in the form

$$h_n^{(1)}(\rho) = f(\rho)e^{i\rho}, \qquad h_n^{(2)}(\rho) = \bar{h}_n^{(1)}(\rho) = f(\rho)e^{-i\rho}, \qquad f(\rho) = O(\rho^{-1})$$

Thus, we have

$$\lim_{r\to\infty} r\left(\frac{dh_n^{(1)}(kr)}{dr} - ikh_n^{(1)}(kr)\right) = \lim_{\rho\to\infty} \rho\left(\frac{dh_n^{(1)}(\rho)}{d\rho} - ih_n^{(1)}(\rho)\right) = \lim_{\rho\to\infty}\left(\rho\frac{df}{d\rho}e^{i\rho}\right) = 0. \tag{247}$$

$$\lim_{r\to\infty} r\left(\frac{dh_n^{(2)}(kr)}{dr} - ikh_n^{(2)}(kr)\right) = \lim_{\rho\to\infty} \rho\left(\frac{dh_n^{(2)}(\rho)}{d\rho} - ih_n^{(2)}(\rho)\right) = \lim_{\rho\to\infty} \rho\left(\frac{df}{d\rho} - 2if(\rho)\right)e^{-i\rho}$$
$$= -2i\lim_{\rho\to\infty} \rho f(\rho)e^{-i\rho} \neq 0.$$

This shows that only $h_n^{(1)}(kr)$ is the radiating solution and B_n^m should be set to zero in an infinite region (due to the linear independence of the spherical harmonics the Sommerfeld condition should hold for each mode):

$$\Psi(r,\theta,\varphi) = \sum_{n=0}^{\infty}\sum_{m=-n}^{m=n} A_n^m h_n^{(1)}(kr)Y_n^m(\theta,\varphi). \tag{248}$$