SIAM J. SCI. COMPUT.
Vol. 25, No. 4, pp. 1344–1381

RECURSIONS FOR THE COMPUTATION OF MULTIPOLE TRANSLATION AND ROTATION COEFFICIENTS FOR THE 3-D HELMHOLTZ EQUATION*

NAIL A. GUMEROV† AND RAMANI DURAISWAMI†

Abstract. We develop exact expressions for the coefficients of series representations of translations and rotations of local and multipole fundamental solutions of the Helmholtz equation in spherical coordinates. These expressions are based on the derivation of recurrence relations, some of which, 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, although we compare our results with methods that use these to prove their accuracy. For evaluating an N_t term truncation of the translated series (involving $O(N_t^2)$ multipoles), our expressions require $O(N_t^3)$ evaluations, compared to previous exact expressions that require $O(N_t^5)$ operations.

Key words. Helmholtz equation, multipole solutions, translation and rotation coefficients, fast evaluation

AMS subject classifications. 33C55, 33C10, 35J05, 65N38, 65N99, 65Y20

DOI. 10.1137/S1064827501399705

1. Introduction.

In several scientific computing applications, the solution to the Helmholtz and Maxwell equations is expressed in terms of the singular (multipole) and regular solutions of the Helmholtz equation in spherical coordinates, centered at various points. Series of such solutions (see (2.16)) in one coordinate system must be expressed in terms of series of singular or regular solutions in another coordinate system. Such expressions are guaranteed to exist by the completeness of the functions on a sphere. Addition theorems [5, 15] provide the expressions for the coefficients of the series in the shifted coordinates, in terms of the original coefficients. The paper by Epton and Dembart [8] provides an introduction to expressions of the coefficients. Chew [22] applied differentiation theorems for spherical functions, similar to those in this paper, to obtain recursions for the translation coefficients.

One important area of scientific computing in which there is a need for such expressions is the fast multipole method (FMM) solution of the Helmholtz and Maxwell equations [9, 27, 10]. The FMM algorithm [4, 12] was referred to in [1] as one of the most important algorithms of the 20th century. Here, the complexity of the translation expressions on the one hand, and the numerical accuracy achievable on the other, are key barriers to the use of these methods in more complicated problems that are of interest, and thus these barriers comprise an area of active research. Other areas of scientific computing in which there is a need for such translation theorems are the solution of boundary value problems of scatterings from many spheres [24] and the use of the T-matrix method for solution of scattering problems from many scatterers [14]. Note that in some multipole methods (e.g., [24]) computation of each entry of the translation matrix is needed. In this case the recursive computation of the

*Received by the editors December 15, 2001; accepted for publication (in revised form) June 30, 2003; published electronically December 19, 2003. This research was supported by NSF awards 0086075 and 0219681.
http://www.siam.org/journals/sisc/25-4/39970.html
†Perceptual Interfaces and Reality Laboratory, Institute for Advanced Computer Studies, University of Maryland, College Park, MD 20742 (gumerov@umiacs.umd.edu, ramani@umiacs.umd.edu).

matrix elements provides the algorithm which has a theoretical minimum of asymptotic complexity. For specific applications we refer the reader to [14, 24].

In this paper we follow and extend the approach of [22] to develop general recursive methods for obtaining translation and rotation coefficients. We also derive recursions for a particular type of translation coefficients, which we call "coaxial" translation coefficients. An algorithm for fast and exact computation of the latter coefficients together with the rotation coefficients yields a translation algorithm based on a rotation-coaxial translation decomposition with the lower asymptotic complexity. While the relations are derived here for the Helmholtz equation with real k in (2.1) below, they are in fact applicable for arbitrary complex nonzero k and appear in the modified Helmholtz equation describing screened coulombic ("Yukawa") interactions, and in the equation obtained on the Fourier transform of the heat conduction equation, the telegraph, or the wave equation describing propagation of waves in media with relaxation, dispersion, and dissipation.

For similar reasons, there is also a need for development of translation expressions for other equations of mathematical physics, such as the Laplace and linearized Poisson–Boltzmann equations. The approach we follow in deriving the translation is rather general and might be useful in obtaining similar recursions for these other equations. Finally, rotations on a sphere, and the spherical harmonics, play important roles in many areas of scientific computation. In quantum chemistry, they occur, for instance, as factors of atomic orbitals and as factors in multipole expansions. The recursion that we develop for computation of the rotation coefficients is different from those used in this field (see, e.g., [18, 19]). A computationally efficient recursion for rotation coefficients that deals with real numbers is presented here.

2. Background. We consider the Helmholtz equation in three dimensions for the complex function $\psi(\mathbf{r})$, given by

$$\nabla^2\psi + k^2\psi = 0, \tag{2.1}$$

where ∇^2 is the Laplace operator $\nabla \cdot (\nabla)$, and k is a real scalar (the wavenumber). The transformation between spherical coordinates and Cartesian coordinates with a common origin $(x, y, z) \to (r, \theta, \varphi)$ is given by

$$x = r\sin\theta\cos\varphi, \quad y = r\sin\theta\sin\varphi, \quad z = r\cos\theta. \tag{2.2}$$

The gradient and Laplacian of a function ψ in spherical coordinates are

$$\nabla\psi = \mathbf{i}_r\frac{\partial\psi}{\partial r} + \mathbf{i}_\theta\frac{1}{r}\frac{\partial\psi}{\partial\theta} + \mathbf{i}_\varphi\frac{1}{r\sin\theta}\frac{\partial\psi}{\partial\varphi}, \tag{2.3}$$
$$\nabla\cdot(\nabla\psi) = \nabla^2\psi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2},$$

where $(\mathbf{i}_r, \mathbf{i}_\theta, \mathbf{i}_\varphi)$ is a right-handed orthonormal basis in spherical coordinates. Solutions of the Helmholtz equation in spherical coordinates can be expressed in the factored form ("separation of variables")

$$\psi_n^m(r,\theta,\varphi) = \Pi_n(r)\Theta_n^m(\theta)\Phi^m(\varphi), \tag{2.4}$$

where the function Θ_n^m is periodic with period π and Φ^m is periodic with period 2π. The spherical harmonics provide such a periodic basis

(2.5)
$$\Theta_n^m(\theta)\Phi^m(\varphi) = Y_n^m(\theta,\varphi) = (-1)^m \sqrt{\frac{2n+1}{4\pi}\frac{(n-|m|)!}{(n+|m|)!}} P_n^{|m|}(\mu) e^{im\varphi}, \quad \mu = \cos\theta,$$
$$n = 0,1,2,\dots; \qquad m = -n,\dots,n,$$

where $P_n^{|m|}(\mu)$ are the associated Legendre functions [6]. The spherical harmonics are also sometimes called surface harmonics of the first kind, tesseral for $m < n$ and sectorial for $m = n$. We will use the definition of the associated Legendre function $P_n^m(\mu)$ which is consistent with the value on the cut $(-1,1)$ of the hypergeometric function $P_n^m(z)$ (see Abramowitz and Stegun [6]). These functions can be obtained from the Legendre polynomials $P_n(\mu)$ via the Rodrigues formula

(2.6)
$$P_n^m(\mu) = (-1)^m \left(1-\mu^2\right)^{m/2} \frac{d^m}{d\mu^m} P_n(\mu), \quad P_n(\mu) = \frac{1}{2^n n!}\frac{d^n}{d\mu^n}\left(\mu^2-1\right)^n.$$

Our definition of spherical harmonics coincides with that of Epton and Dembart [8], except for a factor $\sqrt{(2n+1)/4\pi}$, which we include to make them an orthonormal basis over the sphere. As remarked in [8] the definition of spherical harmonics has an important bearing on developing an efficient multipole translation theory and needs to be further researched.

The spherical harmonics defined by (2.5) form a complete orthonormal system on $L^2(S_u)$, where S_u is the surface of the unit sphere $x^2+y^2+z^2=1$:

(2.7)
$$\begin{aligned}(Y_n^m, Y_l^s) &= \int_0^\pi \sin\theta d\theta \int_0^{2\pi} Y_n^m(\theta,\varphi)\bar{Y}_l^s(\theta,\varphi)d\varphi \\ &= \int_0^\pi \sin\theta d\theta \int_0^{2\pi} Y_n^m(\theta,\varphi)Y_l^{-s}(\theta,\varphi)d\varphi = \delta_{nl}\delta_{ms},\end{aligned}$$

where δ_{nl} is the Kronecker delta. An arbitrary surface function $F(\theta,\varphi)$ can be expanded over this orthonormal basis as

(2.8)
$$F(\theta,\varphi) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} F_n^m Y_n^m(\theta,\varphi),$$

where the coefficients of the expansion F_n^m are given by

(2.9)
$$F_n^m = (F, Y_n^m) = \int_0^\pi \sin\theta d\theta \int_0^{2\pi} F(\theta,\varphi)Y_n^{-m}(\theta,\varphi)d\varphi.$$

The dependence of the function Π_n on the radial coordinate in (2.4) is described by

(2.10)
$$\frac{d}{dr}\left(r^2\frac{d\Pi_n}{dr}\right) + \left[k^2r^2 - n(n+1)\right]\Pi_n = 0,$$

which is the spherical Bessel equation. Particular solutions are the spherical Bessel functions of the first and second kinds, j_n and y_n, related, respectively, to the Bessel and Neumann functions of fractional order, $J_{n+1/2}$ and $Y_{n+1/2}$:

(2.11)
$$\Pi_n = j_n(kr) = \sqrt{\frac{\pi}{2kr}}J_{n+1/2}(kr), \quad \Pi_n = y_n(kr) = \sqrt{\frac{\pi}{2kr}}Y_{n+1/2}(kr).$$

When problems are posed on infinite domains, linear combinations of these solutions, called the spherical Hankel functions of the first and second kinds, are used since they can be used to represent outgoing and incoming waves

$$h_n^{(1)}(kr) = j_n(kr) + iy_n(kr), \quad h_n^{(2)}(kr) = j_n(kr) - iy_n(kr). \tag{2.12}$$

In the problems we are interested in, we will need functions which either are regular at the origin or satisfy the Sommerfeld condition

$$\lim_{r\to\infty} r\left(\frac{\partial\psi}{\partial r} - ik\psi\right) = 0 \tag{2.13}$$

at infinity. These functions, respectively, are $j_n(kr)$ (regular as $r \to 0$) and $h_n^{(1)}(kr)$ (outgoing waves). Accordingly, we can express the general solutions of the Helmholtz equation in terms of either the "elementary regular solutions" R_n^m or the "elementary singular solutions" S_n^m, defined by

$$R_n^m(\mathbf{r}) = j_n(kr)Y_n^m(\theta,\varphi), \quad S_n^m(\mathbf{r}) = h_n^{(1)}(kr)Y_n^m(\theta,\varphi), \quad n = 0,1,2,\ldots; \quad m = -n,\ldots,n, \tag{2.14}$$

and which are linearly independent. The singular solution $S_n^m(\mathbf{r})$ sometimes is called the multipole of *order* m and *degree* n centered at the origin (in some papers the multipoles are introduced as derivatives of the Green function). Since only the functions $h_n^{(1)}(kr)$ will be considered below, we will drop the superscript (1) for notational simplicity.

Because the functions $h_n(kr)$ and $j_n(kr)$ have similar recurrence properties, and when an expression applies to both types of functions, we will use the notation

$$F_n^m(\mathbf{r}) = f_n(kr)Y_n^m, \qquad f = h, j, \quad F = S, R. \tag{2.15}$$

2.1. Reexpansions of elementary solutions. Solutions of the Helmholtz equation, ψ, in a finite or an infinite domain can be expressed in terms of the functions S_n^m and R_n^m as (see, e.g., [5])

$$\psi(\mathbf{r}) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\left[A_n^m S_n^m(\mathbf{r}) + B_n^m R_n^m(\mathbf{r})\right], \tag{2.16}$$

where A_n^m and B_n^m are expansion coefficients. In particular, for $A_n^m = 0$ such series describe any regular solution inside a sphere, for $B_n^m = 0$ any radiating solution in the space exterior to a sphere circumscribing a scatterer, and for $A_n^m \neq 0$ and $B_n^m \neq 0$ any regular solution in a spherical layer. These series also can be considered as centered at different locations, and sums of such functions provide solutions to the Helmholtz equation in multiply connected domains, such as those appearing in multiple scattering problems, or in domains with complex boundaries. In these cases, the series centered at different locations should be "translated" to provide local or far field expansions, and the coefficients of the translated series should be evaluated. These coefficients could be obtained by taking appropriate scalar products, resulting in integral expressions for the coefficients, which, absent analytical expressions, must be evaluated numerically via quadrature, and are thus inefficient. "Translation theorems" provide explicit ways for evaluating the coefficients, and are thus more efficient. The translation theorem expression for the monopole source centered at the origin is well

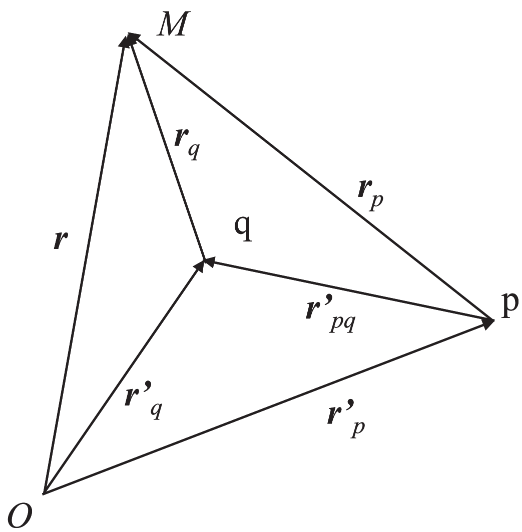

FIG. 1. *Coordinates of points in various reference frames.*

known and given in many textbooks (see, e.g., [5]). The monopole can be expanded in a series of spherical harmonics centered about a point q using the identity

$$G(\mathbf{r}) = \frac{e^{ik|\mathbf{r}|}}{4\pi|\mathbf{r}|} = ik\sum_{n=0}^{\infty}\sum_{m=-n}^{n} R_n^{-m}\left(-\mathbf{r}'_q\right) S_n^m(\mathbf{r}_q), \qquad \left|\mathbf{r}'_q\right| \leqslant |\mathbf{r}_q|, \tag{2.17}$$

where $\mathbf{r}_q$ is the radius-vector of the field point in the reference frame centered at q and $\mathbf{r}'_q$ is the radius-vector of the point q in the original reference frame. Thus in this expression the multipole of order zero, centered at the origin, has been translated into a series of multipoles centered at a point q, and the series has coefficients $ikR_n^{-m}\left(-\mathbf{r}'_q\right)$. If the outer summation of the series (2.17) is truncated at $n = N_t$, the series has $O\left(N_t+1\right)^2$ terms, and the monopole can be translated to a new location in $O(N_t^2)$ operations.

Such succinct expressions are usually not available for higher order multipoles. Exact expressions for multipole translations for the Helmholtz equation have been presented in [8]. However, these expressions are relatively cumbersome, as they use the Wigner or Clebsch–Gordan coefficients, and are relatively expensive to compute, requiring $O(N_t^5)$ operations to evaluate the $O(N_t^2)$ terms.

2.2. Translations. We wish to represent $S_n^m(\mathbf{r}_p)$ and $R_n^m(\mathbf{r}_p)$ as sums of singular or regular elementary solutions with the center of expansion specified at 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

$$\mathbf{r} = \mathbf{r}_p + \mathbf{r}'_p = \mathbf{r}_q + \mathbf{r}'_q, \quad \mathbf{r}_p = \mathbf{r}_q + \mathbf{r}'_{pq}, \quad \mathbf{r}'_{pq} = \mathbf{r}'_q - \mathbf{r}'_p = \mathbf{r}_p - \mathbf{r}_q, \tag{2.18}$$

where the vector $\mathbf{r}'_{pq}$ is directed from point p to point q (see Figure 1). This vector determines the radius of reexpansion $r'_{pq} = \left|\mathbf{r}'_{pq}\right|$. Inside the sphere with radius r'_{pq},

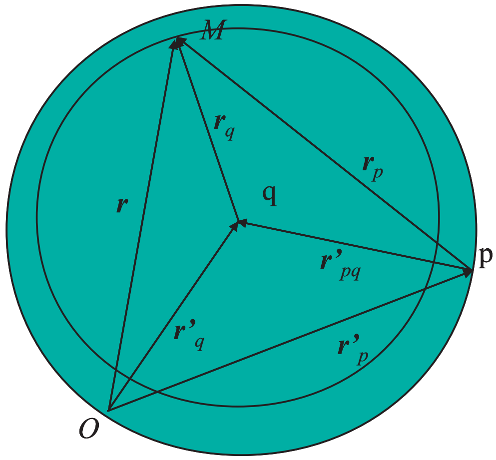

FIG. 2. *Illustration of the reexpansion of the singular to regular solution* (2.19). *Such reexpansion can be performed inside the dark sphere. It can be used for a field point* M*, since the distance to this point from point* q *is smaller than the radius of the dark sphere.*

centered at $\mathbf{r} = \mathbf{r}'_q$ (see Figure 2), the solution is regular and can be represented as

$$S_n^m(\mathbf{r}_p) = \sum_{l=0}^{\infty} \sum_{s=-l}^{l} (S|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) R_l^s(\mathbf{r}_q), \qquad |\mathbf{r}_q| < \left|\mathbf{r}'_{pq}\right|, \quad p \neq q. \tag{2.19}$$

The singular elementary solution outside this sphere (see Figure 3) satisfies the radiation conditions, and therefore we can represent S_n^m in a series of multipole solutions:

$$S_n^m(\mathbf{r}_p) = \sum_{l=0}^{\infty} \sum_{s=-l}^{l} (S|S)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) S_l^s(\mathbf{r}_q), \qquad |\mathbf{r}_q| > \left|\mathbf{r}'_{pq}\right|. \tag{2.20}$$

The regular elementary solutions inside a finite domain can be reexpanded in a series of regular elementary solutions near an arbitrary point, so that

$$R_n^m(\mathbf{r}_p) = \sum_{l=0}^{\infty} \sum_{s=-l}^{l} (R|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) R_l^s(\mathbf{r}_q). \tag{2.21}$$

In expansions (2.19)–(2.21) the symbols $(S|R), (S|S)$, and $(R|R)$ denote that the singular (S) and regular (R) elementary solutions are reexpanded in 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 of 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.

With such translations of the basis functions the coefficients in sums of type (2.16) also can be translated via multiplication of corresponding translation matrices by the vectors of coefficients. For example, if we have a far field expansion of a radiating

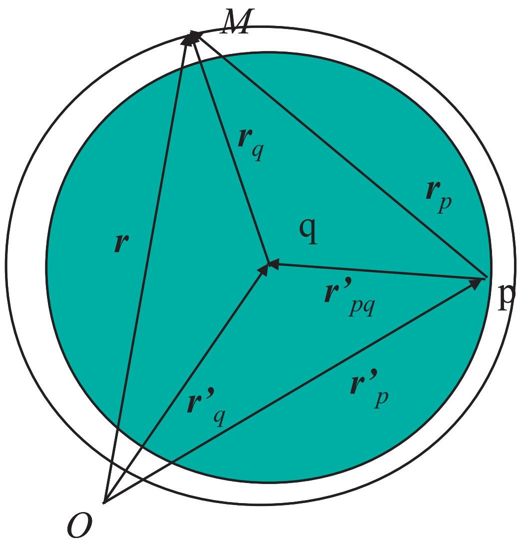

Fig. 3. *Illustration of the reexpansion of the singular to singular solution* (2.20)*. Such reexpansion can be performed outside the dark sphere. It can be used for a field point M, since the distance to this point from point q is larger than the radius of the dark sphere.*

function $\mathcal{F}(\mathbf{r}_p)$,

$$\psi(\mathbf{r}_p) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} A_n^m S_n^m(\mathbf{r}_p), \tag{2.22}$$

it can be converted to a local expansion near some point q with the aid of matrix $(R|R)_{ln}^{sm}$:

$$\psi(\mathbf{r}_p) = \sum_{l=0}^{\infty} \sum_{s=-l}^{l} C_l^s\left(\mathbf{r}'_{pq}\right) R_l^s(\mathbf{r}_q), \tag{2.23}$$

$$C_l^s\left(\mathbf{r}'_{pq}\right) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} (S|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) A_n^m, \quad |\mathbf{r}_q| < \left|\mathbf{r}'_{pq}\right|.$$

2.3. Rotations. We also consider transforms of multipole expansions due to rotation of one Cartesian system to another. Fast algorithms for computation of expansion coefficients of singular and regular solutions are needed for applications in quantum mechanics and, as will be seen, for fast computation of translation coefficients.

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 vector coordinates $\mathbf{a}$ in the first coordinate system to the vector coordinates $\hat{\mathbf{a}}$ in the second coordinate system, so that

$$\hat{\mathbf{a}} = Q\mathbf{a} \qquad \text{with} \qquad Q = \begin{bmatrix} \mathbf{i}_{\widehat{x}} \cdot \mathbf{i}_x & \mathbf{i}_{\widehat{x}} \cdot \mathbf{i}_y & \mathbf{i}_{\widehat{x}} \cdot \mathbf{i}_z \\ \mathbf{i}_{\widehat{y}} \cdot \mathbf{i}_x & \mathbf{i}_{\widehat{y}} \cdot \mathbf{i}_y & \mathbf{i}_{\widehat{y}} \cdot \mathbf{i}_z \\ \mathbf{i}_{\widehat{z}} \cdot \mathbf{i}_x & \mathbf{i}_{\widehat{z}} \cdot \mathbf{i}_y & \mathbf{i}_{\widehat{z}} \cdot \mathbf{i}_z \end{bmatrix}. \tag{2.24}$$

We have the following transform of the spherical harmonics due to rotation of coordinates (e.g., see Wigner [17]):

$$Y_n^m(\theta,\varphi) = \sum_{\nu=-n}^{n} T_n^{\nu m}(Q)\, Y_n^{\nu}\left(\widehat{\theta},\widehat{\varphi}\right), \tag{2.25}$$

where $T_n^{\nu m}(Q)$ are coefficients depending on the rotation matrix Q. Due to the definitions of the singular and regular solutions (2.14), and due to the fact that the magnitude of the vector does not change with rotation of coordinates, we can write the expansion for the multipole in the rotated coordinate system as

(2.26)

$$S_n^m(\mathbf{r}_p) = \sum_{\nu=-n}^{n} T_n^{\nu m}(Q)\, S_n^{\nu}(\widehat{\mathbf{r}}_p), \quad R_n^m(\mathbf{r}_p) = \sum_{\nu=-n}^{n} T_n^{\nu m}(Q)\, R_n^{\nu}(\widehat{\mathbf{r}}_p), \quad |\widehat{\mathbf{r}}_p| = |\mathbf{r}_p|,$$

where $\widehat{\mathbf{r}}_p$ denotes the point in the rotated coordinate system.

Using the reexpansions (e.g., (2.19)) the sum (2.22) can be represented in the form

$$\psi(\mathbf{r}_p) = \sum_{n=0}^{\infty}\sum_{\nu=-n}^{n} C_n^{\nu} S_n^{\nu}(\widehat{\mathbf{r}}_p), \qquad C_n^{\nu} = \sum_{m=-n}^{n} T_n^{\nu m}(Q)\, A_n^m. \tag{2.27}$$

2.4. Complexity of translations and rotations. Usually we deal with expansions of singular or regular solutions $\psi(\mathbf{r})$ (such as (2.22 or (2.16) with $B_n^m = 0$ or $A_n^m = 0$), where the outer sum is truncated at $n = N_t$. In this case the goal of the translation and rotation operations is to transform one set of N_t^2 coefficients representing $\psi(\mathbf{r})$ multiplying the regular or singular functions into another set of N_t^2 coefficients multiplying the regular or singular functions centered at another location, which represent the same function $\psi(\mathbf{r})$. A plausible way of doing this would be to look for relations between the N_t^2 coefficients. A general linear transform would employ a relation that involved the action of an $N_t^2 \times N_t^2$ matrix on the original coefficients to produce the new coefficients (see (2.23)). If the matrix were to be fully populated, it would contain $O(N_t^4)$ elements, and its evaluation would take $O(N_t^4 \times$ cost of evaluating an element) operations, while direct evaluation of the matrix-vector product for the coefficients would require $O(N_t^4)$ operations. In many application areas $N_t \simeq 10^2$ or larger, and this expense can be significant.

The first set of relations for obtaining the translation coefficients uses the so-called Wigner symbols and is well summarized in [8]. These expressions require $O(N_t^5)$ operations to evaluate the transformation matrix and $O(N_t^4)$ operations to perform the multiplication directly. Clearly, these are too expensive to evaluate for large N_t, especially when the computations must be done many times, as in the FMM, and where some error bounds suggest that the number of terms depends on the discretization. Since there are $O(N_t^2)$ coefficients, the minimum number of computations necessary to do the translations is $O(N_t^2)$.

To achieve faster methods for evaluation, research has progressed in two directions. A first approach, and that which is quite common in the FMM literature, avoids translation via matrix-vector products. In this approach, an analytical "Fourier" transform on the sphere is performed, and the transform integral is evaluated using numerical quadrature. Multilevel FMMs are implemented by referring to the transformed version of the multipole expansions. Details of this approach can be obtained from [9, 23, 21]. This approach, based on diagonal forms of translation operators, can achieve the translations necessary in a combination of several $O(N_t^2)$ operations with some $O(N_t^3)$ operations required for computation of surface integrals of the spherical transforms, which can be reduced to $O(N_t^2 \log^2 N_t)$ using fast spherical transforms.

However, we need to make some remarks about these translation methods used in the FMM. First, the numerical quadrature of oscillatory functions that must be performed on the sphere may introduce large multipliers to the order estimates. For a practical problem, the number of computations performed by an $O(N_t^3)$ method with a smaller asymptotic multiplier can be less than that performed by, say, an $O(N_t^2 \log^2 N_t)$ method with a larger asymptotic multiplier. These could be due to procedures such as global interpolation of band-limited functions on the sphere.

Second, estimates of the complexity of the FMM are usually presented as $O(PN)$, where P is the single translation cost and N is the number of points for which FMM is used. A recent detailed look at the FMM algorithm [25] shows that it can be optimized by using better data structures, particularly by selection of a so-called "clustering" parameter. In this case the complexity of the method is $O(P^{1/2}N + N_t^2 N)$. These estimates show that all translation algorithms with asymptotic complexity $P = O(N_t^4)$ or below result in an effective complexity of $O(N_t^2 N)$ or $O(N_t^2 N \log N)$ for the FMM. In this sense, $P = O(N_t^3)$ methods can be competitive with, say, $O(N_t^2 \log^2 N_t)$ methods (of course, any fast method providing the same accuracy is better than a slow method).

Finally, we note that at low frequencies the translation methods based on integral representations experience some problems, and there are publications dedicated to improvement of convergence of these methods [13]. The matrix-based method of translation is applicable at sufficiently low frequencies (e.g., we tested the accuracy of solutions for $k \simeq 10^{-3}$ and characteristic distances of order 1 and obtained good results [26]).

3. Differentiation of elementary solutions. To derive recurrence relations for computation of the reexpansion coefficients we first present some simple relations that arise from the differentiation of the elementary solutions. Let us define the following differential operators in spherical coordinates:

$$\partial_z \equiv \frac{\partial}{\partial z} = \mu \frac{\partial}{\partial r} + \frac{1-\mu^2}{r}\frac{\partial}{\partial \mu}, \quad \mu = \cos\theta. \tag{3.1}$$

$$\partial_{xy} \equiv \frac{\partial}{\partial x} + i\frac{\partial}{\partial y} = \frac{e^{i\varphi}}{r\sqrt{1-\mu^2}}\left[\left(1-\mu^2\right)\left(r\frac{\partial}{\partial r} - \mu\frac{\partial}{\partial \mu}\right) + i\frac{\partial}{\partial \varphi}\right],$$

$$\overline{\partial_{xy}} \equiv \frac{\partial}{\partial x} - i\frac{\partial}{\partial y} = \frac{e^{-i\varphi}}{r\sqrt{1-\mu^2}}\left[\left(1-\mu^2\right)\left(r\frac{\partial}{\partial r} - \mu\frac{\partial}{\partial \mu}\right) - i\frac{\partial}{\partial \varphi}\right],$$

$$\nabla \equiv \mathbf{i}_x\frac{\partial}{\partial x} + \mathbf{i}_y\frac{\partial}{\partial y} + \mathbf{i}_z\frac{\partial}{\partial z} = \mathbf{i}_x\frac{1}{2}\left(\partial_{xy} + \overline{\partial_{xy}}\right) - \mathbf{i}_y\frac{i}{2}\left(\partial_{xy} - \overline{\partial_{xy}}\right) + \mathbf{i}_z\partial_z$$
$$= \frac{1}{2}\left(\mathbf{i}_x - i\mathbf{i}_y\right)\partial_{xy} + \frac{1}{2}\left(\mathbf{i}_x + i\mathbf{i}_y\right)\overline{\partial_{xy}} + \mathbf{i}_z\partial_z.$$

Applying these operators we obtain the following theorems for the differentiation of the functions $S_n^m(\mathbf{r})$ and $R_n^m(\mathbf{r})$. The proofs of these theorems are based on the properties of the associated Legendre functions and spherical Hankel and Bessel functions and can be found in detail in [2], where numerical examples are provided as well. These theorems also can be found in [22].

THEOREM 3.1. *For $k \neq 0$ and integers n and m*

$$\frac{1}{k}\partial_z F_n^m(\mathbf{r}) = a_{n-1}^m F_{n-1}^m(\mathbf{r}) - a_n^m F_{n+1}^m(\mathbf{r}), \qquad F = S, R, \tag{3.2}$$

where

(3.3)

$$a_n^m = 0 \quad \text{for } n < |m|; \qquad a_n^m = a_n^{|m|} = \sqrt{\frac{(n+1+|m|)(n+1-|m|)}{(2n+1)(2n+3)}} \quad \text{for } n \geqslant |m|.$$

THEOREM 3.2. *For $k \neq 0$ and integers m and n*

$$\frac{1}{k}\partial_{xy} F_n^m(\mathbf{r}) = b_{n+1}^{-m-1} F_{n+1}^{m+1}(\mathbf{r}) - b_n^m F_{n-1}^{m+1}(\mathbf{r}), \qquad F = S, R, \tag{3.4}$$

where

$$b_n^m = \sqrt{\frac{(n-m-1)(n-m)}{(2n-1)(2n+1)}} \quad \text{for } 0 \leqslant m \leqslant n; \tag{3.5}$$

$$-\sqrt{\frac{(n-m-1)(n-m)}{(2n-1)(2n+1)}} \quad \text{for } -n \leqslant m < 0;$$

$$0 \quad \text{for } |m| > n.$$

THEOREM 3.3. *For $k \neq 0$ and integers n and m*

$$\frac{1}{k}\overline{\partial_{xy}} F_n^m(\mathbf{r}) = b_{n+1}^{m-1} F_{n+1}^{m-1}(\mathbf{r}) - b_n^{-m} F_{n-1}^{m-1}(\mathbf{r}), \qquad F = S, R, \tag{3.6}$$

where the coefficients b_n^m are as defined in (3.5).

THEOREM 3.4. *For $k \neq 0$ and integers n and m*

$$\begin{aligned} \frac{1}{k}\nabla F_n^m(\mathbf{r}) = {} & \frac{1}{2}(\mathbf{i}_x - i\mathbf{i}_y)\left[b_{n+1}^{-m-1} F_{n+1}^{m+1}(\mathbf{r}) - b_n^m F_{n-1}^{m+1}(\mathbf{r})\right] \\ & + \frac{1}{2}(\mathbf{i}_x + i\mathbf{i}_y)\left[b_{n+1}^{m-1} F_{n+1}^{m-1}(\mathbf{r}) - b_n^{-m} F_{n-1}^{m-1}(\mathbf{r})\right] \\ & + \mathbf{i}_z\left[a_{n-1}^m F_{n-1}^m(\mathbf{r}) - a_n^m F_{n+1}^m(\mathbf{r})\right], \qquad F = S, R, \end{aligned} \tag{3.7}$$

where the coefficients a_n^m and b_n^m are defined by (3.3) *and* (3.5).

4. Translation coefficients.

4.1. Integral representation of translation coefficients. Before considering the efficient evaluation of the translation coefficients $(S|R)_{ln}^{sm}(\mathbf{r}'_{pq})$, etc., we note their integral representations, which immediately follow from definitions (2.14), (2.19), and orthonormality of spherical harmonics (2.5):

(4.1)

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

Similarly, for the other reexpansion coefficients we have expressions

(4.2)
$$(R|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) = \frac{1}{j_l(kr_q)} \int_{-\pi}^{\pi} d\varphi_q \int_0^{\pi} j_n\left(kr_p\right) Y_n^m(\theta_p, \varphi_p) Y_l^{-s}(\theta_q, \varphi_q) \sin\theta_q d\theta_q,$$

(4.3)
$$(S|S)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) = \frac{1}{h_l(kr_q)} \int_{-\pi}^{\pi} d\varphi_q \int_0^{\pi} h_n\left(kr_p\right) Y_n^m(\theta_p, \varphi_p) Y_l^{-s}(\theta_q, \varphi_q) \sin\theta_q d\theta_q,$$
$$r_q > \left|\mathbf{r}'_{pq}\right|.$$

4.2. Structure of the translation coefficients. While the above 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, the representations (4.1), (4.2), and (4.3) use coordinates of *both* the source point $\mathbf{p}$ and the target point $\mathbf{q}$; the representations are not useful for FMMs. To be useful they would need to be rewritten in terms of the translation vector $\mathbf{r}'_{pq}$ alone.

According to (2.18) and (2.19) we have

$$S_n^m\left(\mathbf{r}_q + \mathbf{r}'_{pq}\right) = \sum_{l=0}^{\infty} \sum_{s=-l}^{l} (S|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) R_l^s\left(\mathbf{r}_q\right). \tag{4.4}$$

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

$$\left(\nabla^2 + k^2\right) S_n^m\left(\mathbf{r}_q + \mathbf{r}'_{pq}\right) = 0. \tag{4.5}$$

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

$$\left(\nabla^2 + k^2\right) R_l^s\left(\mathbf{r}_q\right) = 0, \tag{4.6}$$

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

$$\left(\nabla^2 + k^2\right) (S|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) = 0. \tag{4.7}$$

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

$$(S|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) = \sum_{\alpha=0}^{\infty} \sum_{\beta=-\alpha}^{\alpha} (s|r)_{\alpha ln}^{\beta sm} S_\alpha^\beta\left(\mathbf{r}'_{pq}\right). \tag{4.8}$$

Indeed, in the expansion we need 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 $\left|\mathbf{r}'_{pq}\right| \to \infty$, the solution should satisfy the Sommerfeld radiation conditions (see (4.4)). 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 [15], or to the Wigner 3-j

symbols [17], which are a more symmetrical form. The Clebsch–Gordan coefficients $(j_1 j_2 m_1 m_2 | j_1 j_2 j m)$ are given by [6]:

$$(j_1 j_2 m_1 m_2 | j_1 j_2 j m) = (-1)^{-j_1+j_2-m} (2j+1)^{1/2} \begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix}, \tag{4.9}$$

where the 2×3 matrix notation on the right-hand side is used for the Wigner 3-j symbols. In the paper of Epton and Dembart [8] the following expression (rewritten in the present notation) for the reexpansion coefficients is provided:

$$(S|R)_{ln}^{sm} \left(\mathbf{r}'_{pq}\right) = \sum_{\alpha=0}^{\infty} \sum_{\beta=-\alpha}^{\alpha} \left[\frac{(2n+1)(2l+1)\,(2\alpha+1)}{4\pi}\right]^{1/2} \cdot i^{l-n+\alpha} E \begin{pmatrix} m & -s & -\beta \\ n & l & \alpha \end{pmatrix} S_{\alpha}^{\beta} \left(\mathbf{r}'_{pq}\right), \tag{4.10}$$

where the symbol E is defined as

$$E \begin{pmatrix} m & -s & -\beta \\ n & l & \alpha \end{pmatrix} = 4\pi \left[\frac{4\pi}{(2n+1)(2l+1)\,(2\alpha+1)}\right]^{1/2} \int_{-\pi}^{\pi} d\varphi \cdot \int_0^{\pi} Y_n^m(\theta,\varphi) Y_l^{-s}(\theta,\varphi) Y_{\alpha}^{-\beta}(\theta,\varphi) \sin\theta d\theta, \tag{4.11}$$

and is related to the Wigner 3-j symbols:

$$E \begin{pmatrix} m & -s & -\beta \\ n & l & \alpha \end{pmatrix} = 4\pi \epsilon_m \epsilon_{-s} \epsilon_{-\beta} \begin{pmatrix} n & l & \alpha \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} n & l & \alpha \\ m & -s & -\beta \end{pmatrix}, \tag{4.12}$$
$$\epsilon_m = \begin{cases} (-1)^m, & m \geqslant 0, \\ 1, & m \leqslant 0. \end{cases}$$

Computation of the Wigner 3-j symbols or E symbols requires summations over several indices and is computationally inefficient. We will not consider this way of obtaining the reexpansion coefficients and refer the reader to [8] for details of their computation.

Comparing (4.10) with (4.8), we note that

$$(s|r)_{\alpha l n}^{\beta s m} = \left[\frac{(2n+1)(2l+1)\,(2\alpha+1)}{4\pi}\right]^{1/2} i^{l-n+\alpha} E \begin{pmatrix} m & -s & -\beta \\ n & l & \alpha \end{pmatrix}. \tag{4.13}$$

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

$$(s|r)_{\alpha l n}^{\beta s m} = 0 \text{ for } \beta \neq m-s. \tag{4.14}$$

It is also noteworthy that from the definition (4.11) and orthonormality of the spherical harmonics we have

$$E \begin{pmatrix} 0 & m & s \\ 0 & n & l \end{pmatrix} = E \begin{pmatrix} m & 0 & s \\ n & 0 & l \end{pmatrix} = E \begin{pmatrix} m & s & 0 \\ n & l & 0 \end{pmatrix} = 4\pi \left[\frac{1}{(2n+1)\,(2l+1)}\right]^{1/2} \delta_{m,-s}\delta_{nl}, \tag{4.15}$$

leading to

$$(s|r)_{\alpha l0}^{\beta s0} = \sqrt{(4\pi)}\,(-1)^l\,\delta_{\beta,-s}\delta_{\alpha l},$$
$$(s|r)_{\alpha 0n}^{\beta 0m} = \sqrt{(4\pi)}\delta_{\beta m}\delta_{\alpha n},$$
$$(s|r)_{0ln}^{0sm} = \sqrt{(4\pi)}\delta_{sm}\delta_{ln}, \tag{4.16}$$

Substituting (4.8) in (4.4) we have the expression

$$S_n^m\left(\mathbf{r}_q+\mathbf{r}'_{pq}\right) = \sum_{l=0}^{\infty}\sum_{s=-l}^{l}\sum_{\alpha=0}^{\infty}\sum_{\beta=-\alpha}^{\alpha}(s|r)_{\alpha ln}^{\beta sm}S_\alpha^\beta\left(\mathbf{r}'_{pq}\right)R_l^s\left(\mathbf{r}_q\right), \tag{4.17}$$

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

$$(R|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) = \sum_{\alpha=0}^{\infty}\sum_{\beta=-\alpha}^{\alpha}(r|r)_{\alpha ln}^{\beta sm}R_\alpha^\beta\left(\mathbf{r}'_{pq}\right),$$
$$(S|S)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) = \sum_{\alpha=0}^{\infty}\sum_{\beta=-\alpha}^{\alpha}(s|s)_{\alpha ln}^{\beta sm}R_\alpha^\beta\left(\mathbf{r}'_{pq}\right). \tag{4.18}$$

This leads to the addition theorems

$$R_n^m\left(\mathbf{r}_q+\mathbf{r}'_{pq}\right) = \sum_{l=0}^{\infty}\sum_{s=-l}^{l}\sum_{\alpha=0}^{\infty}\sum_{\beta=-\alpha}^{\alpha}(r|r)_{\alpha ln}^{\beta sm}R_\alpha^\beta\left(\mathbf{r}'_{pq}\right)R_l^s\left(\mathbf{r}_q\right), \tag{4.19}$$

$$S_n^m\left(\mathbf{r}_q+\mathbf{r}'_{pq}\right) = \sum_{l=0}^{\infty}\sum_{s=-l}^{l}\sum_{\alpha=0}^{\infty}\sum_{\beta=-\alpha}^{\alpha}(s|s)_{\alpha ln}^{\beta sm}R_\alpha^\beta\left(\mathbf{r}'_{pq}\right)S_l^s\left(\mathbf{r}_q\right). \tag{4.20}$$

Comparing (4.20) with (4.17), we see that these are indeed the same expansions of $S_n^m\left(\mathbf{r}_q+\mathbf{r}'_{pq}\right)$. We can simply transform one into the other by exchanging $\mathbf{r}'_{pq}$ with $\mathbf{r}_q$ and subscripts α and β with l and s, respectively. Therefore,

$$(s|s)_{\alpha ln}^{\beta sm} = (s|r)_{l\alpha n}^{s\beta m}. \tag{4.21}$$

The numerical coefficients $(r|r)_{\alpha ln}^{\beta sm}$ also can be related to the Wigner symbols in a manner similar to the expression for $(s|r)_{\alpha ln}^{\beta sm}$ (4.13). As will follow from our analysis below,

$$(S|S)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) = (R|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right), \tag{4.22}$$

and thus from (4.18) and (4.21) we have

$$(r|r)_{\alpha ln}^{\beta sm} = (s|s)_{\alpha ln}^{\beta sm} = (s|r)_{l\alpha n}^{s\beta m}. \tag{4.23}$$

However, even if the Wigner coefficients could be computed efficiently, calculation of the reexpansion coefficients $(S|R)_{ln}^{sm}$, $(R|R)_{ln}^{sm}$, and $(S|S)_{ln}^{sm}$ using them would require summation of series (4.8) and (4.18), which would be computationally expensive, since the reexpansion coefficients are 4-D (and numerical coefficients, such as $(s|r)_{\alpha ln}^{\beta sm}$ are 5-D (taking into account the relation (4.14)), leading to $O\left(N_t^5\right)$ operations. As an alternative method we develop a fast computational technique based on recurrent computation of the actual reexpansion coefficients.

4.3. Recurrence relations for translation 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 of regular and singular functions, 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:

$$E_n^m(\mathbf{r}_p) = E_n^m\left(\mathbf{r}_q + \mathbf{r}'_{pq}\right) = \sum_{l=0}^{\infty}\sum_{s=-l}^{l}(E|F)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)F_l^s(\mathbf{r}_q), \quad E,F = S,R. \tag{4.24}$$

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 (4.24) at fixed $\mathbf{r}'_{pq}$, we have

$$D_pE_n^m(\mathbf{r}_p) = D_qE_n^m\left(\mathbf{r}_q + \mathbf{r}'_{pq}\right) = \sum_{l=0}^{\infty}\sum_{s=-l}^{l}(E|F)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)D_qF_l^s(\mathbf{r}_q), \quad E,F = S,R. \tag{4.25}$$

The following theorems establish general recurrence relations. Their proofs are based on the theorems for differentiation of multipoles. We provide the proof only for the first theorem. The other theorems can be proved in a similar way or may be obtained from [2]. These relations, presumably, were first obtained by Chew [22].

THEOREM 4.1. *For $k \neq 0$ the following recurrence relation holds for $(E|F)_{ln}^{sm}(\mathbf{r}'_{pq})$:*

$$\begin{aligned} &a_{n-1}^m(E|F)_{l,n-1}^{sm}\left(\mathbf{r}'_{pq}\right) - a_n^m(E|F)_{l,n+1}^{sm}\left(\mathbf{r}'_{pq}\right)\\ &\quad = a_l^s(E|F)_{l+1,n}^{sm}\left(\mathbf{r}'_{pq}\right) - a_{l-1}^s(E|F)_{l-1,n}^{sm}\left(\mathbf{r}'_{pq}\right),\\ &E,F = S,R, \qquad l,n = 0,1,\ldots, \qquad s = -l,\ldots,l, \qquad m = -n,\ldots,n. \end{aligned} \tag{4.26}$$

Proof. Consider $D_p = k^{-1}\partial/\partial z_p = k^{-1}\partial/\partial z_q = D_q$. Using Theorem 3.1, (3.2), and (4.24) 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, again using Theorem 3.1, (3.2), and (4.24) we have

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

The last equality holds due to definition (3.3):

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

By comparing these two expressions and using the orthogonality and completeness of the surface harmonics we obtain the statement of the theorem. □

COROLLARY 4.2. *For* $n = |m|$

$$
\begin{aligned}
&a_{|m|}^m (E|F)_{l,|m|+1}^{sm}\left(\mathbf{r}'_{pq}\right) \\
&\quad = a_{l-1}^s (E|F)_{l-1,|m|}^{sm}\left(\mathbf{r}'_{pq}\right) - a_l^s (E|F)_{l+1,|m|}^{sm}\left(\mathbf{r}'_{pq}\right), \quad E,F = S,R, \\
&\quad l = 0,1,\ldots, \qquad s = -l,\ldots,l, \qquad m = 0,\pm1,\pm2,\ldots.
\end{aligned} \tag{4.27}
$$

For $l = |s|$

$$
\begin{aligned}
&a_{|s|}^s (E|F)_{|s|+1,n}^{sm}\left(\mathbf{r}'_{pq}\right) \\
&\quad = a_{n-1}^m (E|F)_{|s|,n-1}^{sm}\left(\mathbf{r}'_{pq}\right) - a_n^m (E|F)_{|s|,n+1}^{sm}\left(\mathbf{r}'_{pq}\right), \quad E,F = S,R, \\
&\quad n = 0,1,\ldots, \qquad m = -n,\ldots,n, \qquad s = 0,\pm1,\pm2,\ldots.
\end{aligned} \tag{4.28}
$$

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

$$
\begin{aligned}
&a_{|s|}^s (E|F)_{|s|+1,|m|}^{sm}\left(\mathbf{r}'_{pq}\right) = -a_{|m|}^m (E|F)_{|s|,|m|+1}^{sm}\left(\mathbf{r}'_{pq}\right), \quad E,F = S,R, \\
&\qquad m = 0,\pm1,\pm2,\ldots, \qquad s = 0,\pm1,\pm2,\ldots.
\end{aligned} \tag{4.29}
$$

THEOREM 4.3. *For* $k \neq 0$ *the following recurrence relation holds for* $(E|F)_{ln}^{sm}(\mathbf{r}'_{pq})$:

$$
\begin{aligned}
&b_n^m (E|F)_{l,n-1}^{s,m+1}\left(\mathbf{r}'_{pq}\right) - b_{n+1}^{-m-1} (E|F)_{l,n+1}^{s,m+1}\left(\mathbf{r}'_{pq}\right) \\
&\quad = b_{l+1}^{s-1} (E|F)_{l+1,n}^{s-1,m}\left(\mathbf{r}'_{pq}\right) - b_l^{-s} (E|F)_{l-1,n}^{s-1,m}\left(\mathbf{r}'_{pq}\right), \\
&E,F = S,R, \qquad l,n = 0,1,\ldots, \qquad s = -l,\ldots,l, \qquad m = -n,\ldots,n.
\end{aligned} \tag{4.30}
$$

COROLLARY 4.4. *For* $n = m$

$$
\begin{aligned}
&b_{m+1}^{-m-1} (E|F)_{l,m+1}^{s,m+1}\left(\mathbf{r}'_{pq}\right) = b_l^{-s} (E|F)_{l-1,m}^{s-1,m}\left(\mathbf{r}'_{pq}\right) - b_{l+1}^{s-1} (E|F)_{l+1,m}^{s-1,m}\left(\mathbf{r}'_{pq}\right), \\
&\qquad E,F = S,R, \qquad l = 0,1,\ldots, \qquad s = -l,\ldots,l, \qquad m = 0,1,2,\ldots.
\end{aligned} \tag{4.31}
$$

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

(4.32)
$$b_{|s|+1}^{-|s|-1} (E|F)_{|s|+1,n}^{-|s|-1,m} \left(\mathbf{r}'_{pq}\right) = b_n^m (E|F)_{|s|,n-1}^{-|s|,m+1} \left(\mathbf{r}'_{pq}\right) - b_{n+1}^{-m-1} (E|F)_{|s|,n+1}^{-|s|,m+1} \left(\mathbf{r}'_{pq}\right),$$
$$E,F = S,R, \qquad n = 0,1,\dots, \qquad m = -n,\dots,n, \qquad s = 0,-1,-2,\dots.$$

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

(4.33)
$$b_{m+1}^{-m-1} (E|F)_{|s|,m+1}^{-|s|,m+1} \left(\mathbf{r}'_{pq}\right) = -b_{|s|+1}^{-|s|-1} (E|F)_{|s|+1,m}^{-|s|-1,m} \left(\mathbf{r}'_{pq}\right),$$
$$E,F = S,R, \qquad m = 0,1,2,\dots, \qquad s = 0,-1,-2,\dots.$$

THEOREM 4.5. *For* $k \neq 0$ *the following recurrence relation holds for* $(E|F)_{ln}^{sm}(\mathbf{r}'_{pq})$:

(4.34)
$$b_{n+1}^{m-1} (E|F)_{l,n+1}^{s,m-1} \left(\mathbf{r}'_{pq}\right) - b_n^{-m} (E|F)_{l,n-1}^{s,m-1} \left(\mathbf{r}'_{pq}\right)$$
$$= b_l^s (E|F)_{l-1,n}^{s+1,m} \left(\mathbf{r}'_{pq}\right) - b_{l+1}^{-s-1} (E|F)_{l+1,n}^{s+1,m} \left(\mathbf{r}'_{pq}\right),$$
$$E,F = S,R, \qquad l,n = 0,1,\dots, \qquad s = -l,\dots,l, \qquad m = -n,\dots,n.$$

COROLLARY 4.6. *For* $n = |m|, m \leqslant 0$,

(4.35)
$$b_{|m|+1}^{-|m|-1} (E|F)_{l,|m|+1}^{s,-|m|-1} \left(\mathbf{r}'_{pq}\right) = b_l^s (E|F)_{l-1,|m|}^{s+1,-|m|} \left(\mathbf{r}'_{pq}\right) - b_{l+1}^{-s-1} (E|F)_{l+1,|m|}^{s+1,-|m|} \left(\mathbf{r}'_{pq}\right),$$
$$E,F = S,R, \qquad l = 0,1,\dots, \qquad s = -l,\dots,l, \qquad m = 0,-1,-2,\dots.$$

For $l = s$

(4.36)
$$b_{s+1}^{-s-1} (E|F)_{s+1,n}^{s+1,m} \left(\mathbf{r}'_{pq}\right) = b_n^{-m} (E|F)_{s,n-1}^{s,m-1} \left(\mathbf{r}'_{pq}\right) - b_{n+1}^{m-1} (E|F)_{s,n+1}^{s,m-1} \left(\mathbf{r}'_{pq}\right),$$
$$E,F = S,R, \qquad n = 0,1,\dots, \qquad m = -n,\dots,n, \qquad s = 0,1,2,\dots.$$

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

(4.37)
$$b_{|m|+1}^{-|m|-1} (E|F)_{s,|m|+1}^{s,-|m|-1} \left(\mathbf{r}'_{pq}\right) = -b_{s+1}^{-s-1} (E|F)_{s+1,|m|}^{s+1,-|m|} \left(\mathbf{r}'_{pq}\right), \quad E,F = S,R,$$
$$m = 0,-1,-2,\dots, \quad s = 0,1,2,\dots.$$

4.4. Particular values of translation coefficients. To use the recurrence relations we need some starting values. The following particular values provide these.

4.4.1. (S|R) coefficients. Expression (4.17) reveals a particular value of the reexpansion coefficients $(S|R)_{ln}^{sm}$. Setting $\mathbf{r}_q = \mathbf{0}$ we have

(4.38)
$$R_l^s(\mathbf{0}) = \sqrt{\frac{1}{4\pi}}\delta_{l0}\delta_{s0}, \qquad S_n^m\left(\mathbf{r}'_{pq}\right) = \sqrt{\frac{1}{4\pi}}\sum_{\alpha=0}^{\infty}\sum_{\beta=-\alpha}^{\alpha}(s|r)_{\alpha 0n}^{\beta 0m} S_\alpha^\beta\left(\mathbf{r}'_{pq}\right), \qquad p \neq q.$$

Due to the orthogonality of the surface harmonics,

(4.39)
$$(s|r)_{\alpha 0n}^{\beta 0m} = \sqrt{(4\pi)}\delta_{\alpha n}\delta_{\beta m}.$$

This value also can be obtained directly from (4.16). Substituting this expression in (4.8), we have

$$(S|R)_{0n}^{0m}\left(\mathbf{r}'_{pq}\right)=\sqrt{(4\pi)}S_n^m\left(\mathbf{r}'_{pq}\right), \qquad n=0,1,\ldots, \quad m=-n,\ldots,n. \tag{4.40}$$

Another particular value can be found from the well-known expansion of fundamental solution $G(\mathbf{r}_p)$ of the Helmholtz equation [5] in a series of spherical harmonics:

$$G(\mathbf{r}_p)=ik\sum_{l=0}^{\infty}\sum_{s=-l}^{s=l}S_l^{-s}\left(-\mathbf{r}'_{pq}\right)R_l^s(\mathbf{r}_q), \qquad |\mathbf{r}_q|\leqslant\left|\mathbf{r}'_{pq}\right|. \tag{4.41}$$

We recall that the fundamental solution is a monopole:

$$G(\mathbf{r}_p)=\frac{e^{ikr_p}}{4\pi r_p}=\frac{ik}{4\pi}h_0(kr_p)=\frac{ik}{\sqrt{(4\pi)}}S_0^0\left(\mathbf{r}_q+\mathbf{r}'_{pq}\right). \tag{4.42}$$

Thus, comparing (4.41) and (4.42) with (4.4), we obtain the following value for the reexpansion coefficients:

$$(S|R)_{l0}^{s0}\left(\mathbf{r}'_{pq}\right)=\sqrt{(4\pi)}S_l^{-s}\left(-\mathbf{r}'_{pq}\right)=\sqrt{(4\pi)}\,(-1)^l\,S_l^{-s}\left(\mathbf{r}'_{pq}\right), \quad l=0,1,\ldots, \quad s=-l,\ldots,l. \tag{4.43}$$

Comparing (4.43) with (4.8), we have

$$(s|r)_{\alpha l0}^{\beta s0}=\sqrt{(4\pi)}(-1)^l\delta_{\alpha l}\delta_{\beta,-s}, \tag{4.44}$$

which is consistent with (4.16).

Note that formulae (4.40) and (4.43) are consistent because they both provide the value of $(S|R)_{00}^{00}\left(\mathbf{r}'_{pq}\right)$ as

$$(S|R)_{00}^{00}\left(\mathbf{r}'_{pq}\right)=\sqrt{(4\pi)}S_0^0\left(\mathbf{r}'_{pq}\right)=h_0(kr'_{pq}). \tag{4.45}$$

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,

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

can be determined due to a symmetry relation. Indeed, changing the sign of the radius vector in (4.4) we have

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

Due to orthogonality of surface harmonics we obtain

$$(S|R)_{ln}^{sm}\left(\mathbf{r}'_{qp}\right)=(-1)^{n+l}(S|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right), \qquad p\neq q, \quad n,l=0,1,\ldots, \quad m=-n,\ldots,n, \quad l=-s,\ldots,s. \tag{4.46}$$

We also can find, using (4.4) and

$$S_n^m = 0, \quad R_n^m = 0 \quad \text{for } |m| > n, \tag{4.47}$$

that

$$(S|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) = 0 \quad \text{for } |m| > n \text{ or } |s| > l. \tag{4.48}$$

4.4.2. (R|R) coefficients. Setting $\mathbf{r}_q = \mathbf{0}$ in (4.19) and using (4.38) we have

$$R_n^m\left(\mathbf{r}'_{pq}\right) = \sqrt{\frac{1}{4\pi}} \sum_{\alpha=0}^{\infty} \sum_{\beta=-\alpha}^{\alpha} (r|r)_{\alpha 0 n}^{\beta 0 m} R_\alpha^\beta\left(\mathbf{r}'_{pq}\right). \tag{4.49}$$

Due to the orthogonality of the surface harmonics we obtain

$$(r|r)_{\alpha 0 n}^{\beta 0 m} = \sqrt{(4\pi)}\delta_{\alpha n}\delta_{\beta m}. \tag{4.50}$$

Substituting this expression in (4.49), we have

$$(R|R)_{0n}^{0m}\left(\mathbf{r}'_{pq}\right) = \sqrt{(4\pi)} R_n^m\left(\mathbf{r}'_{pq}\right), \qquad n = 0, 1, \dots, \quad m = -n, \dots, n. \tag{4.51}$$

In (4.19) we also can set $\mathbf{r}'_{pq} = \mathbf{0}$. In this case, from (4.38) we have

$$R_n^m\left(\mathbf{r}_q\right) = \sqrt{\frac{1}{4\pi}} \sum_{l=0}^{\infty} \sum_{s=-l}^{l} (r|r)_{0ln}^{0sm} R_l^s\left(\mathbf{r}_q\right). \tag{4.52}$$

This yields

$$(r|r)_{0ln}^{0sm} = \sqrt{(4\pi)}\delta_{ln}\delta_{sm}. \tag{4.53}$$

Both values (4.50) and (4.53) are consistent with those following from the particular values of the Wigner symbols (4.16). It may also be noted that (4.19) is symmetrical with respect to the exchange of $\mathbf{r}_q$ and $\mathbf{r}'_{pq}$. This leads to the symmetry relation

$$(r|r)_{\alpha l n}^{\beta s m} = (r|r)_{l \alpha n}^{s \beta m}. \tag{4.54}$$

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

$$j_n(kr) = \frac{1}{2}\left[h_n(kr) + \overline{h_n(kr)}\right]. \tag{4.55}$$

Particularly for $n = 0$ this results in

$$R_0^0(\mathbf{r}_q) = \frac{1}{2}\left[S_0^0(\mathbf{r}_q) + \overline{S_0^0(\mathbf{r}_q)}\right]. \tag{4.56}$$

Using this relation and the expansion of the fundamental solution (4.41), (4.42), and (4.55) we obtain

$$R_0^0(\mathbf{r}_q) = \sqrt{(4\pi)} \sum_{l=0}^{\infty} \sum_{s=-l}^{l} (-1)^l R_l^{-s}\left(\mathbf{r}'_{pq}\right) R_l^s\left(\mathbf{r}_q\right). \tag{4.57}$$

Comparing this expansion with (2.21) and using the orthogonality of the surface harmonics, we obtain

$$(R|R)_{l0}^{s0}\left(\mathbf{r}'_{pq}\right) = \sqrt{(4\pi)}\,(-1)^{l}\,R_{l}^{-s}\left(\mathbf{r}'_{pq}\right), \qquad l = 0,1,\ldots, \quad s = -l,\ldots,l. \tag{4.58}$$

In the same way as for $(S|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)$ (see (4.46) and (4.48)) we can show that

$$(R|R)_{ln}^{sm}\left(\mathbf{r}'_{qp}\right) = (-1)^{n+l}(R|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right), \tag{4.59}$$

$$n,l = 0,1,\ldots, \quad m = -n,\ldots,n, \quad l = -s,\ldots,s.$$

$$(R|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) = 0 \quad \text{for } |m| > n \text{ or } |s| > l. \tag{4.60}$$

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 the Wigner or Clebsch–Gordan coefficients.

4.5. Symmetry of translation coefficients. The reexpansion coefficients obey many symmetry properties, which can be a subject for a separate publication and study. These symmetry relations are very important for efficient computation as they enable evaluation of all coefficients by computing only a few of them and are important for developing fast numerical methods. Here we just mention the following symmetries (the proofs can be found in [2]).

THEOREM 4.7. *The following symmetry relation holds:*

$$(E|F)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) = (-1)^{n+l}\,(E|F)_{nl}^{-m,-s}\left(\mathbf{r}'_{pq}\right), \tag{4.61}$$

$$E,F = S,R, \quad l,n = 0,1,\ldots, \quad s = -l,\ldots,l, \quad m = -n,\ldots,n.$$

THEOREM 4.8. *The following symmetry relation holds:*

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

THEOREM 4.9. *The translation reexpansion coefficients* $(R|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)$ *and* $(S|S)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)$ *are the same:*

$$(S|S)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) = (R|R)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right), \qquad l,n = 0,1,\ldots, \quad s = -l,\ldots,l, \quad m = -n,\ldots,n. \tag{4.62}$$

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

$$(E|F)_{l}^{sm} = (E|F)_{l|m|}^{sm}, \quad (E|F)_{n}^{sm} = (E|F)_{|s|n}^{sm}, \quad E,F = S,R. \tag{4.63}$$

Particularly, we have from (4.40), (4.43) and (4.51), (4.58)

$$\begin{aligned} (S|R)_{l}^{s0}\left(\mathbf{r}'_{pq}\right) &= \sqrt{(4\pi)}\,(-1)^{l}\,S_{l}^{-s}\left(\mathbf{r}'_{pq}\right), \quad (S|R)_{n}^{0m}\left(\mathbf{r}'_{pq}\right) = \sqrt{(4\pi)}S_{n}^{m}\left(\mathbf{r}'_{pq}\right), \\ (R|R)_{l}^{s0}\left(\mathbf{r}'_{pq}\right) &= \sqrt{(4\pi)}\,(-1)^{l}\,R_{l}^{-s}\left(\mathbf{r}'_{pq}\right), \quad (R|R)_{n}^{0m}\left(\mathbf{r}'_{pq}\right) = \sqrt{(4\pi)}R_{n}^{m}\left(\mathbf{r}'_{pq}\right). \end{aligned} \tag{4.64}$$

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

$$(E|F)^{sm} = (E|F)_{|s||m|}^{sm}, \quad E,F = S,R. \tag{4.65}$$

Particularly, (4.64) provides

$$(4.66)\quad (S|R)^{s0}\left(\mathbf{r}'_{pq}\right) = \sqrt{(4\pi)}\,(-1)^s\, S_l^{-s}\left(\mathbf{r}'_{pq}\right), \quad (S|R)^{0m}\left(\mathbf{r}'_{pq}\right) = \sqrt{(4\pi)}S_n^m\left(\mathbf{r}'_{pq}\right),$$
$$(R|R)^{s0}\left(\mathbf{r}'_{pq}\right) = \sqrt{(4\pi)}\,(-1)^s\, R_l^{-s}\left(\mathbf{r}'_{pq}\right), \quad (R|R)^{0m}\left(\mathbf{r}'_{pq}\right) = \sqrt{(4\pi)}R_n^m\left(\mathbf{r}'_{pq}\right).$$

We pay special attention to the sectorial reexpansion coefficients because they either are known explicitly or can be computed via simple recurrence relations, and thus can be used as "boundary conditions" (i.e., initial values) for the recursive computation of the tesseral reexpansion coefficients $(E|F)_{ln}^{sm}$, $E, F = S, R$.

4.6.1. Computation of sectorial translation coefficients. The sectorial reexpansion coefficients can be computed independently from the other coefficients, since the initial values (4.64) and recurrence relations (4.31)–(4.32) and (4.35)–(4.36) include only sectorial coefficients and are sufficient for their computation. Note that only coefficients $(E|F)_l^{sm}$ can be computed while $(E|F)_l^{sm}$ can be determined using symmetry (4.61). These relations can be rewritten in the form

$$(4.67)\quad b_{m+1}^{-m-1}\,(E|F)_l^{s,m+1} = b_l^{-s}\,(E|F)_{l-1}^{s-1,m} - b_{l+1}^{s-1}\,(E|F)_{l+1}^{s-1,m},$$
$$l = 0, 1, \dots, \quad s = -l, \dots, l, \quad m = 0, 1, 2, \dots.$$

$$(4.68)\quad b_{m+1}^{-m-1}\,(E|F)_l^{s,-m-1} = b_l^{s}\,(E|F)_{l-1}^{s+1,-m} - b_{l+1}^{-s-1}\,(E|F)_{l+1}^{s+1,-m}, \quad E, F = S, R,$$
$$l = 0, 1, \dots, \qquad s = -l, \dots, l, \qquad m = 0, 1, 2, \dots.$$

Relations (4.67) and (4.68) provide values of coefficients $(E|F)_l^{sm}$ for layers with increasing $|m|$. This process starts with known values $(E|F)_l^{s0}$; see (4.64).

Note also the following relation for the sectorial reexpansion coefficients following from (4.29):

$$(4.69)\quad a_{|s|}^{s}\,(E|F)_{|s|+1}^{sm} = -a_{|m|}^{m}\,(E|F)_{|m|+1}^{sm}, \quad E, F = S, R,$$
$$m = 0, \pm 1, \pm 2, \dots, \qquad s = 0, \pm 1, \pm 2, \dots.$$

4.6.2. Particular values of double sectorial translation coefficients. Using the notation of (4.65) we can rewrite relation (4.33) in the form

$$(4.70)$$
$$b_{m+1}^{-m-1}\,(E|F)^{-s,m+1} = -b_{s+1}^{-s-1}\,(E|F)^{-s-1,m}, \quad E, F = S, R, \quad m, s = 0, 1, 2, \dots.$$

Recursive application of this formula and values of coefficients b_m^{-m} (3.5) enable expression of $(E|F)^{-s,m}$ coefficients $(m, s = 0, 1, 2, \dots)$ via $(E|F)^{-s-m,0}$:

$$(4.71)\quad (S|R)^{-s,m}\left(\mathbf{r}'_{pq}\right) = (-1)^s\,\frac{(s+m)!}{s!m!}\sqrt{\frac{4\pi(2m+1)!(2s+1)!}{(2s+2m+1)!}}S_{s+m}^{s+m}\left(\mathbf{r}'_{pq}\right),$$
$$(R|R)^{-s,m}\left(\mathbf{r}'_{pq}\right) = (S|S)^{-s,m}\left(\mathbf{r}'_{pq}\right)$$
$$= (-1)^s\,\frac{(s+m)!}{s!m!}\sqrt{\frac{4\pi(2m+1)!(2s+1)!}{(2s+2m+1)!}}R_{s+m}^{s+m}\left(\mathbf{r}'_{pq}\right),$$
$$m = 0, 1, 2, \dots, \qquad s = 0, 1, 2, \dots.$$

Using this and symmetry relation (4.61) we can also determine $(S|R)^{s,-m}\left(\mathbf{r}'_{pq}\right)$ and $(R|R)^{-s,m}\left(\mathbf{r}'_{pq}\right)$.

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

$$(E|F)_{ln}\left(\mathbf{r}'_{pq}\right) = (E|F)_{ln}^{00}\left(\mathbf{r}'_{pq}\right), \quad E,F = S,R, \quad l,n = 0,1,2,\ldots \tag{4.72}$$

"zonal" reexpansion coefficients.

Particularly, we have from (4.40), (4.43), (4.51), and (4.58)

$$\begin{aligned}(S|R)_{l0}\left(\mathbf{r}'_{pq}\right) &= \sqrt{(4\pi)}\,(-1)^l\, S_l^0\left(\mathbf{r}'_{pq}\right), \quad (S|R)_{0n}\left(\mathbf{r}'_{pq}\right) = \sqrt{(4\pi)}S_n^0\left(\mathbf{r}'_{pq}\right), \\ (R|R)_{l0}\left(\mathbf{r}'_{pq}\right) &= \sqrt{(4\pi)}\,(-1)^l\, R_l\left(\mathbf{r}'_{pq}\right), \quad (R|R)_{0n}\left(\mathbf{r}'_{pq}\right) = \sqrt{(4\pi)}R_n^m\left(\mathbf{r}'_{pq}\right).\end{aligned} \tag{4.73}$$

As sectorial coefficients, the zonal reexpansion coefficients can be computed independently from the other coefficients using (4.26), which can be rewritten as

$$a_{n-1}^0\,(E|F)_{l,n-1} - a_n^0\,(E|F)_{l,n+1} = a_l^0\,(E|F)_{l+1,n} - a_{l-1}^0\,(E|F)_{l-1,n}, \quad l,n = 0,1,\ldots. \tag{4.74}$$

4.8. Coaxial translation coefficients. The translation coefficients derived above correspond to the case where the fundamental solutions are translated from one 3-D reference frame to another arbitrary 3-D reference frame. In some situations the second reference frame may not be arbitrary, and in these cases there can be a substantial simplification in the expressions and a significant reduction in the computation necessary for the reexpansion coefficients. We consider the case where the translation direction has its axis z directed from point $\mathbf{r}'_p$ to the center of reexpansion $\mathbf{r}'_q$. Since, as discussed earlier, the reexpansion coefficients depend only on $\mathbf{r}'_{pq}$, in this case the reexpansion coefficients will be independent of the angular variables. In these particular cases the general reexpansion formulae (2.19)–(2.21) simplify considerably to

$$S_n^m\left(\mathbf{r}_p\right) = \sum_{l=|m|}^{\infty} (S|R)_{ln}^m\left(r'_{pq}\right) R_l^m\left(\mathbf{r}_q\right), \qquad \left|\mathbf{r}_q\right| < \left|\mathbf{r}'_{pq}\right|, \tag{4.75}$$

$$S_n^m\left(\mathbf{r}_p\right) = \sum_{l=|m|}^{\infty} (S|S)_{ln}^m\left(r'_{pq}\right) S_l^m\left(\mathbf{r}_q\right), \qquad \left|\mathbf{r}_q\right| > \left|\mathbf{r}'_{pq}\right|, \tag{4.76}$$

$$R_n^m\left(\mathbf{r}_p\right) = \sum_{l=|m|}^{\infty} (R|R)_{ln}^m\left(r'_{pq}\right) R_l^m\left(\mathbf{r}_q\right). \tag{4.77}$$

Since the coefficients are now only 3-D (three indices), we can say that they correspond to a "diagonalization" of the 4-D case. We call them "coaxial translation coefficients." These coefficients are related to the 4-index general translation coefficients. The equation

$$\begin{aligned}(E|F)_{ln}^m\left(r'_{pq}\right) &= (E|F)_{ln}^{mm}\left(\mathbf{r}'_{pq}\right)\Big|_{\theta'_{pq}=0}, \\ E,F = S,R, \quad l,n &= 0,1,\ldots, \quad m = -n,\ldots,n,\end{aligned} \tag{4.78}$$

also satisfies the general recurrence relations derived earlier and can be computed using the algorithm for their computation. However, it is possible to derive simpler relations that allow for their fast computation.

The recurrence formula (4.26) does not act on the orders of the reexpansion coefficients, so setting $s = m$ there, we have

$$a_{n-1}^{m}(E|F)_{l,n-1}^{m} - a_{n}^{m}(E|F)_{l,n+1}^{m} = a_{l}^{m}(E|F)_{l+1,n}^{m} - a_{l-1}^{m}(E|F)_{l-1,n}^{m}, \quad l,n = 0,1,\dots, \quad m = -n,\dots,n. \tag{4.79}$$

In relation (4.30) we set $s = m+1$ to obtain

$$b_{n}^{m}(E|F)_{l,n-1}^{m+1} - b_{n+1}^{-m-1}(E|F)_{l,n+1}^{m+1} = b_{l+1}^{m}(E|F)_{l+1,n}^{m} - b_{l}^{-m-1}(E|F)_{l-1,n}^{m}, \quad l,n = 0,1,\dots, \quad m = -n,\dots,n. \tag{4.80}$$

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 $m = 1,2,\dots$ by using (4.80) and obtain all the coefficients. Since the recurrence coefficients in (4.80) for propagation in positive and negative directions of m are the same, we come to the conclusion that

$$(E|F)_{ln}^{m} = (E|F)_{ln}^{-m} = (E|F)_{ln}^{|m|}, \quad l,n = 0,1,\dots, \qquad m = -n,\dots,n. \tag{4.81}$$

Therefore computation of $(E|F)_{ln}^{m}$ is required only for nonnegative m, and formulae (4.79) and (4.80) are sufficient for this purpose. Due to (4.61) we also have the following symmetry property, enabling further efficiencies:

$$(E|F)_{ln}^{m} = (-1)^{n+l}(E|F)_{nl}^{m}, \quad l,n = 0,1,\dots, \qquad m = -n,\dots,n. \tag{4.82}$$

4.8.1. Computation of the coaxial translation coefficients. Due to the symmetry $(E|F)_{ln}^{m}$ can be computed only for $l \geqslant n \geqslant m \geqslant 0$. The process of recurrent computation of the coefficients $\{(E|F)_{ln}^{m}\}$ can be performed by computing the entries corresponding to the degrees l and n followed by advancement with respect to the order m. We need to initialize the procedure by providing values for $m = 0$. According to (4.78) and (4.64) we have

$$(S|R)_{l0}^{0}(r'_{pq}) = \sqrt{(4\pi)}(-1)^{l}S_{l}^{0}(\mathbf{r}'_{pq})\big|_{\theta'_{pq}=0} = (-1)^{l}\sqrt{(2l+1)}h_{l}(kr'_{pq}), \quad (R|R)_{l0}^{0}(r'_{pq}) = (-1)^{l}\sqrt{(2l+1)}j_{l}(kr'_{pq}). \tag{4.83}$$

For advancement with respect to m it is convenient to use (4.80) for $n = m$:

$$b_{m+1}^{-m-1}(E|F)_{l,m+1}^{m+1} = b_{l}^{-m-1}(E|F)_{l-1,m}^{m} - b_{l+1}^{m}(E|F)_{l+1,m}^{m}, \quad l = m+1,\ m+2,\dots, \tag{4.84}$$

and obtain other $(E|F)_{ln}^{m+1}$ using (4.79) and (4.82) in the same way as $(E|F)_{ln}^{0}$ are computed.

Formulae (4.84) and (4.83) employ sectorial coefficients of type $(E|F)_{lm}^{m}$, which can conveniently be denoted as

$$(E|F)_{l}^{m} = (E|F)_{lm}^{m}, \quad l = m, m+1,\dots, \tag{4.85}$$

which satisfy the relations

$$\begin{aligned} &(S|R)_{l}^{0} = (-1)^{l}\sqrt{(2l+1)}h_{l}(kr'_{pq}),\\ &(R|R)_{l}^{0}(r'_{pq}) = (S|S)_{l}^{0}(r'_{pq}) = (-1)^{l}\sqrt{(2l+1)}j_{l}(kr'_{pq}),\\ &b_{m+1}^{-m-1}(E|F)_{l}^{m+1} = b_{l}^{-m-1}(E|F)_{l-1}^{m} - b_{l+1}^{m}(E|F)_{l+1}^{m},\\ &E,F = S,R, \quad l = m+1, m+2,\dots. \end{aligned} \tag{4.86}$$

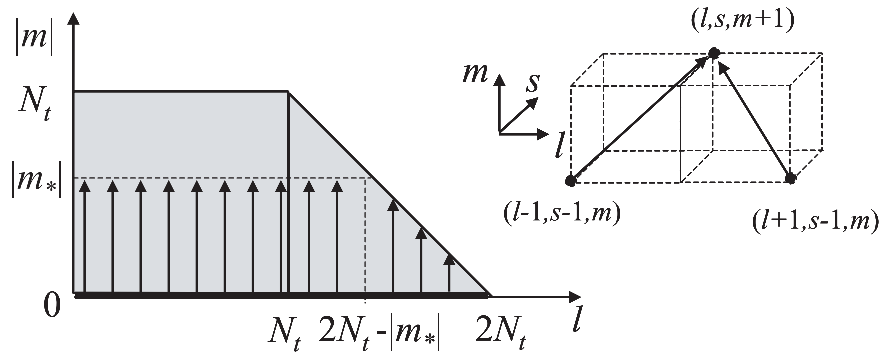

FIG. 4. *A scheme for computation of the sectorial coefficients. Schematic of relation* (4.67)*, which enables propagation in (l, s, m)-space for increasing m, is shown on the right. Schematic of filling a block of coefficients in this space from initial values specified at $m = 0$ is shown on the left (upon projection into the (l, m)-plane).*

Note that for computation of the reexpansion coefficients inside an (l, n, m) cube of size (N_t, N_t, N_t), the coefficients $(E|F)_{l0}^{0}$ must be computed for $l = 0, \ldots, 2N_t$. This is because the recurrence relations for increase of n (see (4.79)) and for increase of l (see (4.86)) require knowledge of $(E|F)_{l+1,n}^{m}$ to compute $(E|F)_{l,n+1}^{m}$ and $(E|F)_{ln}^{m+1}$.

4.9. Computation of translation coefficients. A variety of recurrence relations provide various strategies for computation of translation coefficients $(E|F)_{ln}^{sm}(\mathbf{r}'_{pq})$ in a specified range of indices n, l, m, and s. Below we represent one of the possible algorithms, which we used for computation of the $S|R$-translation matrix in multiple scattering problems [24]. In this problem we needed a truncated matrix, where the indices lie in the range $-N_t \leqslant m, s \leqslant N_t$, $0 \leqslant n, l \leqslant N_t$, where N_t is the truncation number. First, we note that the range of nonzero coefficients is bounded by $m \leqslant n$ and $|s| \leqslant l$.

The process starts with specification of initial values $(E|F)_{l0}^{s0}$ using (4.43) or (4.58) for $l = 0, \ldots, 2N_t$ and $s = -l, \ldots, l$. Equation (4.67) shows that these data provide computation of the sectorial coefficients $(E|F)_{l}^{sm}$ at $m = 1$ for $l = 0, \ldots, 2N_t - 1$ and $s = -l, \ldots, l$ and further until $m = N_t$, where the range $l = 0, \ldots, N_t$, $s = -l, \ldots, l$ is covered. Similarly, (4.68) enables computation of the sectorial coefficients $(E|F)_{l}^{sm}$ for $m = -1, \ldots, -N_t$ and the same range of l and s. Symmetry (4.61) is used to find sectorial coefficients $(E|F)_{n}^{sm}$ for $s = -N_t, \ldots, N_t$ and $n = 0, \ldots, 2N_t - |s|$, $m = -n, \ldots, n$. A scheme for computation of the sectorial translation coefficients is shown in Figure 4.

Consider now computation of other coefficients. For this purpose we use (4.26) at the layer $m =$ const, $s =$ const. Assume that $|s| \leqslant |m|$. For such a layer we have coefficients known at $n = |m|$ and $l = |s|, \ldots, 2N_t - |m|$. At $n = |m| + 1$ (4.26) yields values of the translation coefficients for $l = |s|, \ldots, 2N_t - |m| - 1$ and further until $n = N_t$ and $l = |s|, \ldots, N_t$. This fills some trapezoidal domain in the (n, l)-plane from left to right (see Figure 5). The rest of the domain required for filling is performed by applying the same recurrence relation, but with filling from the bottom to the top by propagation with respect to l. So we use known values of the sectorial coefficients at $l = |s|$ and $n = |m|, \ldots, 2N_t - |s|$ and use recursion (4.26) resolved with respect to coefficients for $l + 1$. A similar procedure holds for $|m| \leqslant |s|$ (see Figure 5). So

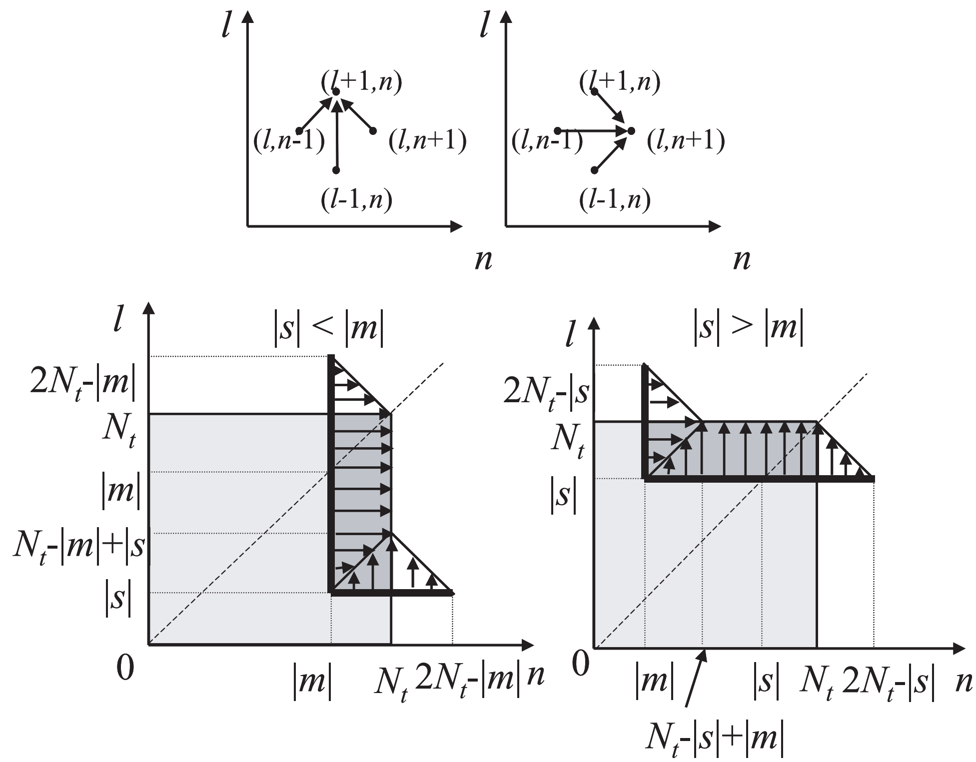

FIG. 5. *A scheme for recursive computation of the translation coefficients at layer* $m = \mathrm{const}$, $s = \mathrm{const}$. *Propagation according to* (4.26) *can be performed with respect to* l *or to* n *as shown in the top graphs. Using precomputed sectorial coefficients at* $l = |s|$ *and* $n = |m|$ *and these propagation schemes one can compute all translation coefficients in the specified range,* $|s| \leqslant l \leqslant N_t$, $|m| \leqslant n \leqslant N_t$. *To reduce the amount of unnecessary computations, two cases,* $|s| \leqslant |m|$ *and* $|m| < |s|$, *can be considered as shown on the bottom right and left.*

this algorithm enables computation of all translation coefficients inside the specified domain.

4.9.1. Number of operations.

THEOREM 4.10. *Computation of multipole reexpansion, or translation, coefficients* $(E|F)^{sm}_{ln}(\mathbf{r}_{pq})$ *for all values of* $l = 0, \ldots, N_t$, $s = -l, \ldots, l$, $n = 0, \ldots, N_t$, $m = -n, \ldots, n$, *can be performed within* $O(N_t^4)$ *operations.*

Proof. The total number of coefficients $(E|F)^{sm}_{ln}$, $l = 0, \ldots, N_t$, $s = -l, \ldots, l$, $n = 0, \ldots, N_t$, $m = -n, \ldots, n$, is $(N_t + 1)^4 = O(N_t^4)$. So, even if each coefficient can be computed in constant time, the number of operations will be bounded from below by $O(N_t^4)$. Computation of the initial values $(E|F)^{s0}_{l0}$ and $(E|F)^{0m}_{0n}$ requires $O(N_t)$ operations. Computation of the sectorial coefficients $(E|F)^{sm}_{l|m|}$ and $(E|F)^{sm}_{|s|n}$ using the initial values and recurrence relations, which include not more than two 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 $(E|F)^{sm}_{ln}$ using the values of the sectorial coefficients recurrence relations which include not more than three multiplications and two additions requires $O(N_t^4)$ operations. In the recurrence process additional values of $(E|F)^{sm}_{ln}$ for $l > N_t$

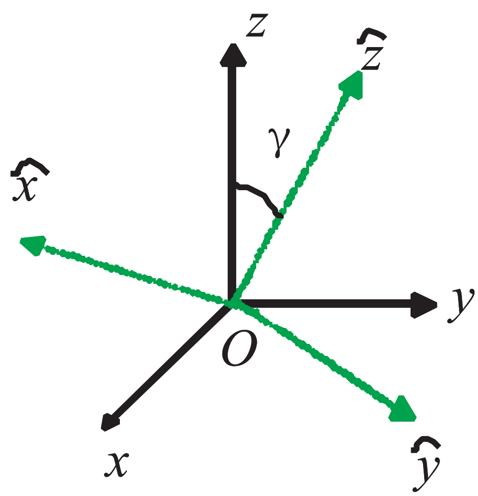

Fig. 6. *Rotation of axes.*

and $n > N_t$ may be required. However, the maximum size of l and n is limited by $2N_t$. Thus the number of operations is $O(N_t^4)$. □

Theorem 4.11. *Computation of coaxial multipole reexpansion, or translation, coefficients* $(E|F)_{ln}^{m}(r_{pq})$ *for all values of* $l = 0, \ldots, N_t$, $n = 0, \ldots, N_t$, $m = -n, \ldots, n$, *can be performed in* $O(N_t^3)$ *operations.*

Proof. The proof follows similarly to the proof of Theorem 4.10. □

5. Rotation coefficients.

5.1. Rotation matrix. It is often convenient (and physically meaningful) to link the entries of the matrix Q (see (2.24)) 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 in 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 [20] 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 6, 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, and 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

$$\cos\gamma = e_z.$$

The direction of the axis of rotation can be specified as

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

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

$$\mathbf{i}_{\widehat{x}} = \frac{-e_y \mathbf{i}_x + e_x \mathbf{i}_y}{\sqrt{\left(e_x^2 + e_y^2\right)}}. \tag{5.1}$$

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

$$\mathbf{i}_{\widehat{y}} = \mathbf{i}_{\widehat{z}} \times \mathbf{i}_{\widehat{x}} = \frac{1}{\sqrt{\left(e_x^2 + e_y^2\right)}} \begin{vmatrix} \mathbf{i}_x & \mathbf{i}_y & \mathbf{i}_z \\ e_x & e_y & e_z \\ -e_y & e_x & 0 \end{vmatrix} = \frac{-e_z e_x \mathbf{i}_x - e_z e_y \mathbf{i}_y}{\sqrt{\left(e_x^2 + e_y^2\right)}} + \sqrt{\left(e_x^2 + e_y^2\right)}\mathbf{i}_z. \tag{5.2}$$

We can now evaluate the matrix Q using (2.24) as

$$Q = \begin{bmatrix} \mathbf{i}_{\widehat{x}} \cdot \mathbf{i}_x & \mathbf{i}_{\widehat{x}} \cdot \mathbf{i}_y & \mathbf{i}_{\widehat{x}} \cdot \mathbf{i}_z \\ \mathbf{i}_{\widehat{y}} \cdot \mathbf{i}_x & \mathbf{i}_{\widehat{y}} \cdot \mathbf{i}_y & \mathbf{i}_{\widehat{y}} \cdot \mathbf{i}_z \\ \mathbf{i}_{\widehat{z}} \cdot \mathbf{i}_x & \mathbf{i}_{\widehat{z}} \cdot \mathbf{i}_y & \mathbf{i}_{\widehat{z}} \cdot \mathbf{i}_z \end{bmatrix} = \begin{bmatrix} -\frac{e_y}{\sqrt{\left(e_x^2+e_y^2\right)}} & \frac{e_x}{\sqrt{\left(e_x^2+e_y^2\right)}} & 0 \\ -\frac{e_z e_x}{\sqrt{\left(e_x^2+e_y^2\right)}} & -\frac{e_z e_y}{\sqrt{\left(e_x^2+e_y^2\right)}} & \sqrt{\left(e_x^2 + e_y^2\right)} \\ e_x & e_y & e_z \end{bmatrix}. \tag{5.3}$$

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

$$Q = \begin{bmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} -\frac{e_y}{\sqrt{\left(e_x^2+e_y^2\right)}} & \frac{e_x}{\sqrt{\left(e_x^2+e_y^2\right)}} & 0 \\ -\frac{e_z e_x}{\sqrt{\left(e_x^2+e_y^2\right)}} & -\frac{e_z e_y}{\sqrt{\left(e_x^2+e_y^2\right)}} & \sqrt{\left(e_x^2 + e_y^2\right)} \\ e_x & e_y & e_z \end{bmatrix}, \tag{5.4}$$

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

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 $(\mathbf{i}_x, \mathbf{i}_y, \mathbf{i}_z)$ (see Figure 7). 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.

The relation between the components of the rotation matrix (5.4) and angles θ' and φ' is provided by the following:

$$\begin{aligned} \cos\theta' &= \mathbf{i}_z \cdot \mathbf{i}_{\widehat{z}} = Q_{33} = e_z, \qquad \theta' = \gamma, \\ \cos\varphi' \sin\theta' &= \mathbf{i}_z \cdot \mathbf{i}_{\widehat{x}} = Q_{13} = -\sqrt{\left(e_x^2 + e_y^2\right)}\sin\phi, \\ \sin\varphi' \sin\theta' &= \mathbf{i}_z \cdot \mathbf{i}_{\widehat{y}} = Q_{23} = \sqrt{\left(e_x^2 + e_y^2\right)}\cos\phi. \end{aligned} \tag{5.5}$$

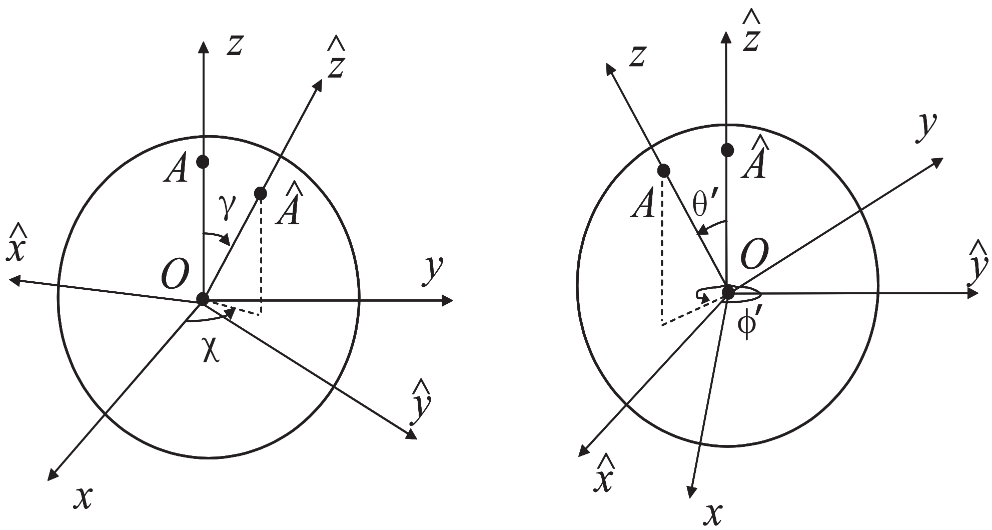

FIG. 7. *The figure on the left shows the transformed axes $(\hat{x}, \hat{y}, \hat{z})$ in the original reference frame (x, y, z). The spherical polar coordinates of the point $\hat{A}$ lying on the $\hat{z}$ axis on the unit sphere are (γ, χ). The figure on the right shows the original axes (x, y, 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.*

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

$$\phi = \varphi' - \frac{\pi}{2}. \tag{5.6}$$

At the same time we have

$$\begin{aligned} e_x &= \mathbf{i}_{\hat{z}} \cdot \mathbf{i}_x = \sin\gamma\cos\chi = \sin\theta'\cos\chi, \\ e_y &= \mathbf{i}_{\hat{z}} \cdot \mathbf{i}_y = \sin\gamma\sin\chi = \sin\theta'\sin\chi. \end{aligned} \tag{5.7}$$

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

(5.8)

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

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

Since Q is an orthogonal rotation matrix, it satisfies

$$\left[Q(\theta', \varphi', \chi)\right]^{-1} = \left[Q(\theta', \varphi', \chi)\right]^{T} = Q(\theta', \chi, \varphi'). \tag{5.9}$$

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

(5.10)
$$Q\left(\theta', \varphi', \chi\right) = \begin{bmatrix} \sin\varphi' & \cos\varphi' & 0 \\ -\cos\varphi' & \sin\varphi' & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} -1 & 0 & 0 \\ 0 & -\cos\theta' & \sin\theta' \\ 0 & \sin\theta' & \cos\theta' \end{bmatrix} \begin{bmatrix} \sin\chi & -\cos\chi & 0 \\ \cos\chi & \sin\chi & 0 \\ 0 & 0 & 1 \end{bmatrix}$$
$$= A(\varphi')B\left(\theta'\right)A^T(\chi).$$

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

(5.11)
$$\left[Q\left(\theta', \varphi', \chi\right)\right]^{-1} = \left[A(\varphi')B\left(\theta'\right)A^T(\chi)\right]^{-1} = \left[A^T(\chi)\right]^{-1}\left[B\left(\theta'\right)\right]^{-1}\left[A(\varphi')\right]^{-1}$$
$$= A(\chi)B\left(\theta'\right)A^T(\varphi') = Q\left(\theta', \chi, \varphi'\right).$$

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

Note that the angles $(\varphi', \theta', \chi)$ are simply related to the standard Euler rotation angles (denote them $\alpha_E, \beta_E, \gamma_E$ to avoid confusion with previously defined angles):

$$\alpha_E = \pi - \chi, \quad \beta_E = \theta', \quad \gamma_E = \varphi'. \tag{5.12}$$

This can be checked in a straightforward way by comparing the representations of the rotation matrix Q in the form (5.8) and via the Euler angles which can be found elsewhere (e.g., [20]).

5.2. Integral representation of rotation coefficients. Before considering the efficient evaluation of the rotation coefficients $T_n^{\nu m}(Q)$, we consider their evaluation using their definition (2.25) and the fact that spherical harmonics (2.5) form a complete orthonormal system. Using the definition of the scalar product (2.2) we obtain

(5.13)
$$T_n^{\nu m}(Q) = \left(Y_n^m(\theta,\varphi), Y_n^\nu\left(\widehat{\theta},\widehat{\varphi}\right)\right) = \int_{-\pi}^{\pi} d\widehat{\varphi}\int_0^{\pi} Y_n^m(\theta,\varphi)Y_n^{-\nu}\left(\widehat{\theta},\widehat{\varphi}\right)\sin\widehat{\theta}d\widehat{\theta}.$$

5.3. Structure of the rotation coefficients. The structure of the rotation coefficients can be found from the properties of the rotation matrix. Since the rotation matrix can be decomposed to three rotations about the axes with angles χ, θ', and φ' we can see how spherical harmonics change with such a transform. First we note that rotation of coordinates with the angles χ and φ' does not change quantities that depend on θ' or γ. For example, the χ-rotation conserves the original z axis and, by denoting the angle φ in the original coordinates as φ_1 in the rotated coordinates, we have

$$\varphi = \varphi_1 + \chi.$$

The spherical harmonics then change as

$$Y_n^m(\theta,\varphi) = Y_n^m(\theta,\varphi_1+\chi) = e^{im\chi}Y_n^m(\theta,\varphi_1). \tag{5.14}$$

The transform of the spherical harmonics from the χ-rotated coordinates to the final coordinates can be described by

$$Y_n^m(\theta,\varphi_1) = \sum_{\nu=-n}^{n} T_n^{(1)\nu m}\left(\theta',\varphi'\right)Y_n^\nu\left(\widehat{\theta},\widehat{\varphi}\right). \tag{5.15}$$

When we perform the last rotation of coordinates to arrive at the angle $\phi = \varphi' - \frac{\pi}{2}$, we have the same situation, and so

$$\widehat{\varphi} = \varphi_2 + \phi = \varphi_2 + \varphi' - \frac{\pi}{2},$$

where φ_2 is the angle corresponding to the given point in coordinates where the last rotation was not performed. So

$$Y_n^\nu\left(\widehat{\theta}, \widehat{\varphi}\right) = Y_n^\nu\left(\widehat{\theta}, \varphi_2 + \varphi' - \frac{\pi}{2}\right) = (-i)^\nu e^{i\nu\varphi'} Y_n^\nu\left(\widehat{\theta}, \varphi_2\right). \tag{5.16}$$

The transform from $Y_n^m(\theta, \varphi_1)$ to $Y_n^m(\widehat{\theta}, \varphi_2)$ occurs only because of the rotation related to angle θ', and so

$$Y_n^m(\theta, \varphi_1) = \sum_{\nu=-n}^{n} T_n^{(12)\nu m}(\theta') Y_n^\nu\left(\widehat{\theta}, \varphi_2\right). \tag{5.17}$$

Combining these results we find that

$$Y_n^m(\theta, \varphi) = e^{im\chi} \sum_{\nu=-n}^{n} i^\nu e^{-i\nu\varphi'} T_n^{(12)\nu m}(\theta') Y_n^\nu\left(\widehat{\theta}, \widehat{\varphi}\right). \tag{5.18}$$

This shows that

$$T_n^{\nu m}(\theta', \varphi', \chi) = e^{im\chi} e^{-i\nu\varphi'} H_n^{\nu m}(\theta'), \quad H_n^{\nu m}(\theta') = i^\nu T_n^{(12)\nu m}(\theta'). \tag{5.19}$$

An explicit expression for $H_n^{\nu m}(\theta')$ can be found in the paper of Stein [15] and in the notation of this paper[1] can be represented in the form

$$\begin{aligned} H_n^{\nu m}(\theta') = {} & \epsilon_m \epsilon_\nu \left[(n+\nu)!(n-\nu)!(n+m)!(n-m)!\right]^{1/2} \\ & \cdot \sum_{\sigma=\max(0,-(m+\nu))}^{\min(n-m,n-\nu)} \frac{(-1)^{n-\sigma} \cos^{2\sigma+\nu+m} \frac{1}{2}\theta' \sin^{2n-2\sigma-\nu-m} \frac{1}{2}\theta'}{\sigma!\,(n-m-\sigma)!\,(n-\nu-\sigma)!\,(m+\nu+\sigma)!}. \end{aligned} \tag{5.20}$$

5.4. Recurrence relations for rotation coefficients.

THEOREM 5.1. *The following recurrence relations hold for* $T_n^{\nu m}(Q)$:

$$\begin{aligned} & \frac{1}{2}(\mathbf{i}_x - i\mathbf{i}_y) b_{n+1}^{-m-1} T_{n+1}^{\nu,m+1} + \frac{1}{2}(\mathbf{i}_x + i\mathbf{i}_y) b_{n+1}^{m-1} T_{n+1}^{\nu,m-1} - \mathbf{i}_z a_n^m T_{n+1}^{\nu m} \\ & \quad = \frac{1}{2}(\mathbf{i}_{\hat{x}} - i\mathbf{i}_{\hat{y}}) b_{n+1}^{-\nu} T_n^{\nu-1,m} \\ & \qquad + \frac{1}{2}(\mathbf{i}_{\hat{x}} + i\mathbf{i}_{\hat{y}}) b_{n+1}^{\nu} T_n^{\nu+1,m} - \mathbf{i}_{\hat{z}} a_n^\nu T_n^{\nu m}, \end{aligned} \tag{5.21}$$

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

$$\begin{aligned} & \frac{1}{2}(\mathbf{i}_x - i\mathbf{i}_y) b_n^{m} T_{n-1}^{\nu,m+1} + \frac{1}{2}(\mathbf{i}_x + i\mathbf{i}_y) b_n^{-m} T_{n-1}^{\nu,m-1} - \mathbf{i}_z a_{n-1}^m T_{n-1}^{\nu m} \\ & \quad = \frac{1}{2}(\mathbf{i}_{\hat{x}} - i\mathbf{i}_{\hat{y}}) b_n^{\nu-1} T_n^{\nu-1,m} \\ & \qquad + \frac{1}{2}(\mathbf{i}_{\hat{x}} + i\mathbf{i}_{\hat{y}}) b_n^{-\nu-1} T_n^{\nu+1,m} - \mathbf{i}_{\hat{z}} a_{n-1}^\nu T_n^{\nu m}, \end{aligned} \tag{5.22}$$

[1]Note that in [15] the Euler angles are defined with sign opposite to our definitions of α_E, β_E, and γ_E.

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

Proof. Applying the operator $k^{-1}\nabla$ to any of the relations (2.26), we obtain

$$k^{-1}\nabla F_n^m(\mathbf{r}_p) = \sum_{\nu=-n}^{n} T_n^{\nu m}(Q)\, k^{-1}\nabla F_n^{\nu}(\widehat{\mathbf{r}}_p), \qquad |\widehat{\mathbf{r}}_p| = |\mathbf{r}_p|, \qquad F = S, R. \tag{5.23}$$

The operator ∇ is independent of the reference frame in which it is represented. This applies to rotations as well, and so $\nabla = \widehat{\nabla}$. We can use (3.7) to represent the left- and right-hand sides of (5.23). By grouping terms corresponding to the same basis functions $F_n^{\nu}(\widehat{\mathbf{r}}_p)$, we obtain the statement of the theorem. A more detailed proof is provided in Gumerov and Duraiswami [2]. ◻

THEOREM 5.2. *The following recurrence relations hold for* $T_n^{\nu m}(Q)$:

$$b_{n+1}^{-m-1}T_{n+1}^{\nu,m+1} + b_{n+1}^{m-1}T_{n+1}^{\nu,m-1} = W_{11}b_{n+1}^{-\nu}T_n^{\nu-1,m} + W_{12}b_{n+1}^{\nu}T_n^{\nu+1,m} + W_{13}a_n^{\nu}T_n^{\nu m}, \tag{5.24}$$

$$b_{n+1}^{-m-1}T_{n+1}^{\nu,m+1} - b_{n+1}^{m-1}T_{n+1}^{\nu,m-1} = W_{21}b_{n+1}^{-\nu}T_n^{\nu-1,m} + W_{22}b_{n+1}^{\nu}T_n^{\nu+1,m} + W_{23}a_n^{\nu}T_n^{\nu m}, \tag{5.25}$$

$$a_n^m T_{n+1}^{\nu m} = W_{31}b_{n+1}^{-\nu}T_n^{\nu-1,m} + W_{32}b_{n+1}^{\nu}T_n^{\nu+1,m} + W_{33}a_n^{\nu}T_n^{\nu m}, \tag{5.26}$$

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

$$\mathbf{W} = \begin{pmatrix} \mathbf{i}_x \cdot (\mathbf{i}_{\hat{x}} - i\mathbf{i}_{\hat{y}}) & \mathbf{i}_x \cdot (\mathbf{i}_{\hat{x}} + i\mathbf{i}_{\hat{y}}) & -2\mathbf{i}_x \cdot \mathbf{i}_{\hat{z}} \\ i\mathbf{i}_y \cdot (\mathbf{i}_{\hat{x}} - i\mathbf{i}_{\hat{y}}) & i\mathbf{i}_y \cdot (\mathbf{i}_{\hat{x}} + i\mathbf{i}_{\hat{y}}) & -2i\mathbf{i}_y \cdot \mathbf{i}_{\hat{z}} \\ -\frac{1}{2}\mathbf{i}_z \cdot (\mathbf{i}_{\hat{x}} - i\mathbf{i}_{\hat{y}}) & -\frac{1}{2}\mathbf{i}_z \cdot (\mathbf{i}_{\hat{x}} + i\mathbf{i}_{\hat{y}}) & \mathbf{i}_z \cdot \mathbf{i}_{\hat{z}} \end{pmatrix}. \tag{5.27}$$

Proof. Taking the scalar product with $\mathbf{i}_x, i\mathbf{i}_y$, and $\mathbf{i}_z$ of both sides of (5.21), we obtain the theorem. ◻

COROLLARY 5.3. *Summing and subtracting relations* (5.24) *and* (5.25) *we have*

$$\begin{aligned} 2b_{n+1}^{-m-1}T_{n+1}^{\nu,m+1} = (W_{11}+W_{21})\, b_{n+1}^{-\nu}T_n^{\nu-1,m} &+ (W_{12}+W_{22})\, b_{n+1}^{\nu}T_n^{\nu+1,m} \\ &+ (W_{13}+W_{23})\, a_n^{\nu}T_n^{\nu m}, \end{aligned} \tag{5.28}$$

$$\begin{aligned} 2b_{n+1}^{m-1}T_{n+1}^{\nu,m-1} = (W_{11}-W_{21})\, b_{n+1}^{-\nu}T_n^{\nu-1,m} &+ (W_{12}-W_{22})\, b_{n+1}^{\nu}T_n^{\nu+1,m} \\ &+ (W_{13}-W_{23})\, a_n^{\nu}T_n^{\nu m}. \end{aligned} \tag{5.29}$$

For $\nu = n+1$ *we have*

$$2b_{n+1}^{-m-1}T_{n+1}^{n+1,m+1} = (W_{11}+W_{21})\, b_{n+1}^{-n-1}T_n^{nm}, \tag{5.30}$$

$$2b_{n+1}^{m-1}T_{n+1}^{n+1,m-1} = (W_{11}-W_{21})\, b_{n+1}^{-n-1}T_n^{nm}, \tag{5.31}$$

$$a_n^m T_{n+1}^{n+1,m} = W_{31}b_{n+1}^{-n-1}T_n^{nm}. \tag{5.32}$$

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

$$2b_{n+1}^{-m-1}T_{n+1}^{-n-1,m+1} = (W_{12}+W_{22})\, b_{n+1}^{-n-1}T_n^{-n,m}, \tag{5.33}$$

$$2b_{n+1}^{m-1}T_{n+1}^{-n-1,m-1} = (W_{12}-W_{22})\, b_{n+1}^{-n-1}T_n^{-n,m}, \tag{5.34}$$

$$a_n^m T_{n+1}^{-n-1,m} = W_{32}b_{n+1}^{-n-1}T_n^{-n,m}. \tag{5.35}$$

THEOREM 5.4. *The following recurrence relations holds for* $T_n^{\nu m}(Q)$:

$$b_n^m T_{n-1}^{\nu,m+1} + b_n^{-m} T_{n-1}^{\nu,m-1} = W_{11} b_n^{\nu-1} T_n^{\nu-1,m} + W_{12} b_n^{-\nu-1} T_n^{\nu+1,m} + W_{13} a_{n-1}^{\nu} T_n^{\nu m}, \tag{5.36}$$

$$b_n^m T_{n-1}^{\nu,m+1} - b_n^{-m} T_{n-1}^{\nu,m-1} = W_{21} b_n^{\nu-1} T_n^{\nu-1,m} + W_{22} b_n^{-\nu-1} T_n^{\nu+1,m} + W_{23} a_{n-1}^{\nu} T_n^{\nu m}, \tag{5.37}$$

$$a_{n-1}^m T_{n-1}^{\nu m} = W_{31} b_n^{\nu-1} T_n^{\nu-1,m} + W_{32} b_n^{-\nu-1} T_n^{\nu+1,m} + W_{33} a_{n-1}^{\nu} T_n^{\nu m}. \tag{5.38}$$

where $n = 0, 1, 2, \ldots, m = -n, \ldots, n, \nu = -n+1, \ldots, n-1$*, and* $W_{\alpha\beta}$ *are components of complex rotation matrix* (5.27).

Proof. Taking the scalar product of both sides of (5.21) with $\mathbf{i}_x, i\mathbf{i}_y$, and $\mathbf{i}_z$, we obtain the theorem. ∎

COROLLARY 5.5. *Summing and subtracting relations* (5.36) *and* (5.37) *we have*

$$2b_n^m T_{n-1}^{\nu,m+1} = (W_{11} + W_{21}) b_n^{\nu-1} T_n^{\nu-1,m} + (W_{12} + W_{22}) b_n^{-\nu-1} T_n^{\nu+1,m} + (W_{13} + W_{23}) a_{n-1}^{\nu} T_n^{\nu m}, \tag{5.39}$$

$$2b_n^{-m} T_{n-1}^{\nu,m-1} = (W_{11} - W_{21}) b_n^{\nu-1} T_n^{\nu-1,m} + (W_{12} - W_{22}) b_n^{-\nu-1} T_n^{\nu+1,m} + (W_{13} - W_{23}) a_{n-1}^{\nu} T_n^{\nu m}. \tag{5.40}$$

For $m = n$ *we have*

$$(W_{11} + W_{21}) b_n^{\nu-1} T_n^{\nu-1,n} + (W_{12} + W_{22}) b_n^{-\nu-1} T_n^{\nu+1,n} + (W_{13} + W_{23}) a_{n-1}^{\nu} T_n^{\nu n} = 0, \tag{5.41}$$

$$W_{31} b_n^{\nu-1} T_n^{\nu-1,n} + W_{32} b_n^{-\nu-1} T_n^{\nu+1,n} + W_{33} a_{n-1}^{\nu} T_n^{\nu n} = 0. \tag{5.42}$$

For $m = -n$ *we have*

$$(W_{11} - W_{21}) b_n^{\nu-1} T_n^{\nu-1,-n} + (W_{12} - W_{22}) b_n^{-\nu-1} T_n^{\nu+1,-n} + (W_{13} - W_{23}) a_{n-1}^{\nu} T_n^{\nu,-n} = 0, \tag{5.43}$$

$$W_{31} b_n^{\nu-1} T_n^{\nu-1,-n} + W_{32} b_n^{-\nu-1} T_n^{\nu+1,-n} + W_{33} a_{n-1}^{\nu} T_n^{\nu,-n} = 0. \tag{5.44}$$

5.5. Computational procedure. We describe briefly a computational procedure to obtain the coefficients $T_n^{\nu m}\left(Q'_{pq}\right)$ via recurrence relations. It is noteworthy to remark that these coefficients are not a property of the Helmholtz equation but purely a property of spherical harmonics. Due to their dependence only on the angular part, these results should be the same for the Laplace, Schrödinger, heat, etc. equations. The spherical harmonics have been studied in greater depth than the translation coefficients for the Helmholtz equation (see, e.g., Stein [15] for addition theorems and explicit relations to Wigner's symbols). However, this classical problem is still of interest, and research is still ongoing in the stable and rapid computation of the rotation coefficients based on the recurrence relations for real spherical harmonics [18] and the general complex case [19]. Our derivation of the recurrence relations differs from these cited papers and has comparable or superior complexity.[2]

5.5.1. Initial values. Consider (2.25) for $m = 0$:

$$Y_n^0(\theta, \varphi) = \sqrt{\frac{2n+1}{4\pi}} P_n(\cos\theta) = \sum_{\nu=-n}^{n} T_n^{\nu 0}(Q) Y_n^{\nu}\left(\widehat{\theta}, \widehat{\varphi}\right). \tag{5.45}$$

[2] Care should be taken when comparing our results with those of these papers, as we use different definitions of the spherical harmonics.

A well-known addition theorem for spherical harmonics (it is reproduced, e.g., in [4]) yields:

$$P_n(\cos\theta) = \frac{4\pi}{2n+1} \sum_{\nu=-n}^{n} Y_n^{-\nu}(\theta', \varphi') \, Y_n^{\nu}\left(\widehat{\theta}, \widehat{\varphi}\right), \tag{5.46}$$

where θ is the angle between points with spherical coordinates (θ', φ') and $(\widehat{\theta}, \widehat{\varphi})$ on the unit sphere. Comparing (5.45) and (5.46) we obtain

$$T_n^{\nu 0}(Q) = \sqrt{\frac{4\pi}{2n+1}} Y_n^{-\nu}(\theta', \varphi'), \quad n = 0, 1, \dots, \quad \nu = -n, \dots, n. \tag{5.47}$$

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 (5.8) and (5.10) provide explicit expressions for components of Q through these angles. Relations (2.5) and (5.47) also provide the following expression for functions $H_n^{\nu m}(\theta')$ defined by (5.19):

$$H_n^{\nu 0}(\theta') = (-1)^{\nu} \sqrt{\frac{(n-|\nu|)!}{(n+|\nu|)!}} P_n^{|\nu|}(\cos\theta'), \quad n = 0, 1, \dots, \quad \nu = -n, \dots, n. \tag{5.48}$$

5.5.2. Symmetry of rotation coefficients.

THEOREM 5.6. *The following symmetry holds*:

$$T_n^{-\nu,-m}(Q) = \overline{T_n^{\nu m}(Q)}, \qquad n = 0, 1, \dots, \quad \nu, m = -n, \dots, n. \tag{5.49}$$

Proof. Since $Y_n^{-\nu} = \overline{Y_n^{\nu}}$ for any $n = 0, 1, \dots$, $\nu = -n, \dots, n$, we have from (2.25):

(5.50)

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

Comparing this result with expansion of $Y_n^m(\theta, \varphi)$ (see (2.25)) we obtain the statement of the theorem, since $Y_n^{\nu}(\widehat{\theta}, \widehat{\varphi})$ is orthonormal and representation (2.25) is unique. □

COROLLARY 5.7. *Substituting* (5.19) *in* (2.24) *and taking into account that* $H_n^{\nu m}(\theta')$ *is real, we have*

$$H_n^{\nu m}(\theta') = H_n^{-\nu,-m}(\theta'), \quad n = 0, 1, \dots, \qquad \nu, m = -n, \dots, n. \tag{5.51}$$

Note also that

$$H_n^{\nu m}(\theta') = H_n^{m \nu}(\theta'), \quad n = 0, 1, \dots, \qquad \nu, m = -n, \dots, n. \tag{5.52}$$

This follows from (5.20).

5.5.3. Recursive computation. Since $T_n^{\nu 0}(Q)$ are known explicitly for arbitrary $n = 0, 1, 2, \ldots$ and $v = -n, \ldots, n$, we need only perform 1-D 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 $T_n^{\nu m}$ because such m can be simply found using symmetry relation (5.49). For nonnegative m we can use any of the relations (5.28) or (5.39).

For example, using the following relation between the elements of matrices W (5.27) and Q (see (2.24)):

$$W_{11} + W_{21} = Q_{11} + Q_{22} + i(Q_{12} - Q_{21}), \quad W_{12} + W_{22} = Q_{11} - Q_{22} + i(Q_{12} + Q_{21}), \quad W_{13} + W_{23} = -2(Q_{31} + iQ_{32}), \tag{5.53}$$

and expressions for elements of Q through the polar angles (5.8), we obtain from (5.39) the following explicit relation for the rotation coefficients through the reference frame rotation angles θ', φ', and χ:

$$T_{n-1}^{\nu,m+1} = \frac{e^{i\chi}}{b_n^m}\left\{\frac{1}{2}\left[b_n^{-\nu-1}e^{i\varphi'}(1-\cos\theta')\,T_n^{\nu+1,m} - b_n^{\nu-1}(1+\cos\theta')\,e^{-i\varphi'}\,T_n^{\nu-1,m}\right] - a_{n-1}^{\nu}\,\sin\theta' T_n^{\nu m}\right\}, \tag{5.54}$$

$$n = 2, 3, \ldots, \quad \nu = -n+1, \ldots, n-1, \quad m = 0, \ldots, n-2,$$

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).

Note also that recurrence relation (5.54) enables computation of the complex-valued functions $T_n^{\nu m}$. The computational procedure can be simplified if we use the factorization (5.19) and then rewrite (5.54) for the real-valued functions $H_n^{\nu m}(\theta')$:

$$H_{n-1}^{\nu,m+1} = \frac{1}{b_n^m}\left\{\frac{1}{2}\left[b_n^{-\nu-1}(1-\cos\theta')\ H_n^{\nu+1,m} - b_n^{\nu-1}(1+\cos\theta')\ H_n^{\nu-1,m}\right] - a_{n-1}^{\nu}\sin\theta'\ H_n^{\nu m}\right\}, \tag{5.55}$$

$$n = 2, 3, \ldots, \quad \nu = -n+1, \ldots, n-1, \quad m = 0, \ldots, n-2.$$

This process starts with initial value (5.48).

6. 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 with rotation angles $(\Theta_{pq}, \Phi_{pq}, \chi_{pq})$ to make the axis $\mathbf{i}_{\widehat{z}}$ directed from point p to point q and then apply the theory for coaxial coefficients. Such a rotation occurs in the plane determined by vectors $\mathbf{i}_z$ and $\mathbf{i}_{\widehat{z}} = \mathbf{r}'_{pq}/\left|\mathbf{r}'_{pq}\right|$, and therefore

$$\cos\theta_{pq} = \mathbf{i}_z \cdot \mathbf{i}_{\widehat{z}} = \frac{\mathbf{i}_z \cdot \mathbf{r}'_{pq}}{\left|\mathbf{r}'_{pq}\right|} = \frac{z'_q - z'_p}{r'_{pq}}, \tag{6.1}$$

where z'_q and z'_p are z-coordinates of points q and p in the original coordinate system.

Equations (2.26) can be rewritten as

$$E_n^m(\mathbf{r}_p) = \sum_{\nu=-n}^{n} T_n^{\nu m}\left(Q'_{pq}\right) E_n^{\nu}(\widehat{\mathbf{r}}_p), \qquad |\widehat{\mathbf{r}}_p| = |\mathbf{r}_p|, \qquad E = S, R, \tag{6.2}$$

where $\widehat{\mathbf{r}}_p$ is the radius-vector of the point in the rotated coordinate system, and the rotation matrix $Q'_{pq}(\Theta_{pq}, \Phi_{pq}, \chi_{pq})$ is provided by (5.10).

The functions $E_n^{\nu}(\widehat{\mathbf{r}}_p)$ then can be translated/reexpanded near the reexpansion point q according to (4.75)–(4.77):

$$E_n^{\nu}(\widehat{\mathbf{r}}_p) = \sum_{l=|\nu|}^{\infty} (E|F)_{ln}^{\nu}\left(r'_{pq}\right) F_l^{\nu}(\widehat{\mathbf{r}}_q), \qquad F, E = S, R, \tag{6.3}$$

where $\widehat{\mathbf{r}}_q$ is the radius vector centered at point q in the rotated coordinate system. To return to the initial coordinates we rotate the coordinates back, so we perform rotation of the coordinate system, specified by the rotation matrix $\left[Q'_{pq}\right]^T = Q'^{-1}_{pq}$:

$$F_l^{\nu}(\widehat{\mathbf{r}}_q) = \sum_{s=-l}^{l} T_l^{s\nu}\left(Q'^{-1}_{pq}\right) F_l^{s}(\mathbf{r}_q), \qquad |\widehat{\mathbf{r}}_q| = |\mathbf{r}_q|, \qquad E = S, R. \tag{6.4}$$

Combining (6.2) and (6.4) we obtain

$$E_n^m(\mathbf{r}_p) = \sum_{\nu=-n}^{n} \sum_{l=|\nu|}^{\infty} \sum_{s=-l}^{l} T_l^{s\nu}\left(Q'^{-1}_{pq}\right) T_n^{\nu m}\left(Q'_{pq}\right) (E|F)_{ln}^{\nu}\left(r'_{pq}\right) F_l^{s}(\mathbf{r}_q), \qquad E = S, R. \tag{6.5}$$

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

$$E_n^m(\mathbf{r}_p) = \sum_{l=0}^{\infty} \sum_{s=-l}^{l} \sum_{\nu=-\min(l,n)}^{\min(l,n)} T_l^{s\nu}\left(Q'^{-1}_{pq}\right) T_n^{\nu m}\left(Q'_{pq}\right) (E|F)_{ln}^{\nu}\left(r'_{pq}\right) F_l^{s}(\mathbf{r}_q), \quad E = S, R. \tag{6.6}$$

On the other hand we have the representation (4.24). Comparing it with (6.6) and taking into account that the elementary solutions $F_l^s(\mathbf{r}_q)$ are independent and orthogonal on a sphere with the center at the point q, we obtain

$$(E|F)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right) = \sum_{\nu=-\min(l,n)}^{\min(l,n)} (E|F)_{ln}^{\nu}\left(r'_{pq}\right) T_l^{s\nu}\left(Q'^{-1}_{pq}\right) T_n^{\nu m}\left(Q'_{pq}\right), \qquad E = S, R. \tag{6.7}$$

Note that according to (5.9) and (5.19) we have

$$\begin{aligned} T_n^{\nu m}\left(Q'_{pq}\right) &= T_n^{\nu m}(\Theta_{pq}, \Phi_{pq}, \chi_{pq}) = e^{im\chi_{pq}} e^{-i\nu\Phi_{pq}} H_n^{\nu m}(\Theta_{pq}), \\ T_l^{s\nu}\left(Q'^{-1}_{pq}\right) &= T_l^{s\nu}(\Theta_{pq}, \Phi_{pq}, \chi_{pq}) = e^{-is\chi_{pq}} e^{i\nu\Phi_{pq}} H_l^{s\nu}(\Theta_{pq}). \end{aligned} \tag{6.8}$$

We also note that angles of rotation Θ_{pq} and χ_{pq}, as defined in (5.7), are nothing but the spherical polar angles θ'_{pq} and φ'_{pq} of the vector $\mathbf{r}'_{pq} = (r'_{pq}\cos\varphi'_{pq}\sin\theta'_{pq},$

$r'_{pq}\sin\varphi'_{pq}\sin\theta'_{pq}$, $r'_{pq}\cos\theta'_{pq}$) in the original reference frame (in the rotated reference frame they are $\widehat{\mathbf{r}}'_{pq} = (0,0,r'_{pq})$). Thus, the product of the two functions (6.8) depends only on these angles and can be expressed as

$$\mathbb{T}^{s\nu m}_{ln}(\theta'_{pq},\varphi'_{pq}) = T^{s\nu}_{l}\left(Q'^{-1}_{pq}\right)T^{\nu m}_{n}\left(Q'_{pq}\right) = e^{i(m-s)\varphi'_{pq}}H^{s\nu}_{l}\left(\theta'_{pq}\right)H^{\nu m}_{n}\left(\theta'_{pq}\right) \tag{6.9}$$

and form (6.7) is a *separation* of the angular and distance variables for the translation reexpansion coefficients. Note that since rotation and inverse rotation preserve the vector, we have

$$\sum_{\nu=-\min(l,n)}^{\min(l,n)} \mathbb{T}^{s\nu m}_{ln} = \delta_{ln}\delta_{sm}. \tag{6.10}$$

6.1. Relation between rotation and translation reexpansion coefficients. The structure of the coefficients $\mathbb{T}^{s\nu m}_{ln}(\theta'_{pq},\varphi'_{pq})$ can be found using (4.8) for the $(S|R)$-coefficients, or (4.18) for the $(R|R)$-coefficients. Substituting (4.8) for $(S|R)^{sm}_{ln}\left(\mathbf{r}'_{pq}\right)$ and $(S|R)^{\nu}_{ln}\left(r'_{pq}\right) = (S|R)^{\nu\nu}_{ln}\left(\widehat{\mathbf{r}}'_{pq}\right)\big|_{\widehat{\theta}'_{pq}=0}$ in (6.7) we obtain, using the definition of the multipoles (2.14),

$$\sum_{\alpha=0}^{\infty} h_{\alpha}\left(kr'_{pq}\right)\sum_{\beta=-\alpha}^{\alpha}(s|r)^{\beta sm}_{\alpha ln}Y^{\beta}_{\alpha}(\theta'_{pq},\varphi'_{pq}) = \sum_{\alpha=0}^{\infty} h_{\alpha}\left(kr'_{pq}\right)\sum_{\beta=-\alpha}^{\alpha}\sum_{\nu=-\min(l,n)}^{\min(l,n)}(s|r)^{\beta\nu\nu}_{\alpha ln}\mathbb{T}^{s\nu m}_{ln}(\theta'_{pq},\varphi'_{pq})Y^{\beta}_{\alpha}(0,0). \tag{6.11}$$

Since the functions $h_{\alpha}\left(kr'_{pq}\right)$ at $\alpha = 0,1,\ldots$ are linearly independent, each term in the sum over α in the left-hand side of this equation must be equal to the corresponding term on the right-hand side. We also notice that due to (4.14) only one term on each side of (6.11) represents the sum over β. So, dropping the prime and the subscript near the spherical angles we have

$$(s|r)^{m-s,sm}_{\alpha ln}Y^{m-s}_{\alpha}(\theta,\varphi) = \sqrt{\frac{2\alpha+1}{4\pi}}\sum_{\nu=-\min(l,n)}^{\min(l,n)}(s|r)^{0\nu\nu}_{\alpha ln}\mathbb{T}^{s\nu m}_{ln}(\theta,\varphi), \quad \alpha,l,n = 0,1,\ldots. \tag{6.12}$$

This relation is very general since it holds at arbitrary α, l, n, m, and s. In the particular case $s = 0$, substituting (6.9) and (5.55) here, we obtain

$$(s|r)^{m0m}_{\alpha ln}Y^{m}_{\alpha}(\theta,\varphi) = \sqrt{\frac{2\alpha+1}{2l+1}}\sum_{\nu=-\min(l,n)}^{\min(l,n)}(s|r)^{0\nu\nu}_{\alpha ln}e^{i(m-\nu)\varphi}H^{\nu m}_{n}(\theta)\,Y^{\nu}_{l}(\theta,\varphi). \tag{6.13}$$

For $m = 0$ this yields

$$(s|r)^{000}_{\alpha ln}Y^{0}_{\alpha}(\theta,\varphi) = \sqrt{\frac{4\pi\,(2\alpha+1)}{(2l+1)\,(2n+1)}}\sum_{\nu=-\min(l,n)}^{\min(l,n)}(s|r)^{0\nu\nu}_{\alpha ln}Y^{-\nu}_{n}(\theta,\varphi)Y^{\nu}_{l}(\theta,\varphi), \tag{6.14}$$

while for $n = m$ using the expression for $H_m^{\nu m}(\theta)$ following from (5.20) we obtain

$$(6.15)\quad (s|r)_{\alpha lm}^{m0m} Y_\alpha^m(\theta,\varphi) = \sum_{\nu=-\min(l,m)}^{\min(l,m)} \epsilon_m \epsilon_\nu \left[\frac{(2\alpha+1)(2m)!}{(2l+1)(m+\nu)!(m-\nu)!}\right]^{1/2} \cdot (s|r)_{\alpha lm}^{0\nu\nu} \cos^{m+\nu}\frac{\theta}{2}\left[e^{i\varphi}\sin\frac{\theta}{2}\right]^{m-\nu} Y_l^\nu(\theta,\varphi).$$

These formulae provide relations between spherical harmonics of different order and degree. We also note that $\mathbb{T}_{ln}^{s\nu m}(\theta,\varphi)$ are surface functions that can be expanded in terms of spherical harmonics:

$$(6.16)\qquad \mathbb{T}_{ln}^{s\nu m}(\theta,\varphi) = \sum_{\gamma=|m-s|}^{\infty} t_{l\gamma n}^{s\nu m} Y_\gamma^{m-s}(\theta,\varphi),$$

where the numerical rotation coefficients $t_{\gamma ln}^{s\nu m}$ can be related to the translation re-expansion coefficients $(s|r)_{\gamma lm}^{s\nu m}$ (or to Wigner 3-j and other symbols; see (4.13) and above).

6.2. Complexity of rotation-coaxial translation decomposition. It must be noted that the representation (6.6) and the above expressions for $\mathbb{T}_{ln}^{s\nu m}(\theta,\varphi)$ in the form of series are conceptual. In practice computation of the translation reexpansion coefficients $(E|F)_{ln}^{sm}\left(\mathbf{r}'_{pq}\right)$ would be performed by a composition of successive products (thereby avoiding expensive matrix-matrix products). The computational advantage of translation decomposition 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.

7. Summary and conclusions.

7.1. Summary of basic recursions. As the paper dealt with many recurrence relations, the tables below provide a summary of the main results. In columns n, l, m, s, we list the indices of the translation and rotation coefficients, or their shifts, that are involved in the recursions listed in the Formula column.

Translation coefficients:

Formula	n	l	m	s
(4.26)	$-1,0,1$	$-1,0,1$	0	0
(4.30)	$-1,0,1$	$-1,0,1$	$0,1$	$-1,0$
(4.34)	$-1,0,1$	$-1,0,1$	$-1,0$	$0,1$
(4.27)	$=\lvert m\rvert$	$-1,0,1$	$0,\pm1$	0
(4.28)	$-1,0,1$	$=\lvert s\rvert$	0	$0,\pm1$
(4.29)	$=\lvert m\rvert$	$=\lvert s\rvert$	$0,\pm1$	$0,\pm1$
(4.31)	$=m$	$-1,0,1$	$0,1\,(\geqslant 0)$	$-1,0$
(4.32)	$-1,0,1$	$=-s$	$0,1$	$-1,0\,(\leqslant 0)$
(4.33)	$=m$	$=-s$	$0,1\,(\geqslant 0)$	$-1,0\,(\leqslant 0)$
(4.35)	$=-m$	$-1,0,1$	$-1,0\,(\leqslant 0)$	$0,1$
(4.36)	$-1,0,1$	$=s$	$-1,0$	$0,1\,(\geqslant 0)$
(4.37)	$=-m$	$=s$	$-1,0\,(\leqslant 0)$	$0,1\,(\geqslant 0)$
(4.80)	$-1,0,1$	$-1,0,1$	$0,1$	$=m$
(4.84)	$=m$	$-1,0,1$	$0,1\,(\geqslant 0)$	$=m$

Rotation coefficients:

Formula	n	m	ν
(5.24)	0,1	$-1, 0, 1$	$-1, 0, 1$
(5.25)	0,1	$-1, 0, 1$	$-1, 0, 1$
(5.26)	0,1	0	$-1, 0, 1$
(5.36)	$-1, 0$	$-1, 0, 1$	$-1, 0, 1$
(5.37)	$-1, 0$	$-1, 0, 1$	$-1, 0, 1$
(5.38)	$-1, 0$	0	$-1, 0, 1$
(5.55)	$-1, 0$	0,1	$-1, 0, 1$

7.2. Conclusions. We have presented a method for fast computation of the multipole translation and rotation coefficients for the 3-D Helmholtz equation using recurrence relations, which are derived. This method enables computation of the full matrix of translation coefficients for a multipole expansion truncated at N_t terms in degree (the total number of expansion coefficients is $O(N_t^2)$) using $O(N_t^4)$ operations, as opposed to $O(N_t^5)$ operations required for computations using the Wigner or Clebsch–Gordan summations. We provided an $O(N_t^4)$ algorithm for translation of multipole expansions and proved recurrence theorems for translation coefficients. These theorems also were checked numerically by comparing the exact values of multipoles and the values computed using multipole reexpansions. Using rotation-coaxial translation decomposition of the translation operators, the set of N_t^2 expansion coefficients for a solution of the Helmholtz equation can be computed in $O(N_t^3)$ operations, if coaxial coefficients are used. Since we provide explicit relations requiring two or three multiplications/additions, the constants multiplying the order symbols for all our algorithms are small.

Acknowledgments. We thank the reviewers whose comments improved the initial version of this manuscript.

REFERENCES

[1] J.J. Dongarra and F. Sullivan, *The top* 10 *algorithms*, Comput. Sci. Engrg., 2 (2000), pp. 22–23.
[2] N.A. Gumerov and R. Duraiswami, *Fast, Exact, and Stable Computation of Multipole Translation and Rotation Coefficients for the* 3*-D Helmholtz Equation*, UMIACS Technical Report TR 2001-44, University of Maryland, Institute for Advanced Computer Studies, College Park, MD, 2001. Available online at http://www.umiacs.edu/%7Egumerov/
[3] P. Moon and D.E. Spencer, *Field Theory Handbook*, 2nd ed., Springer-Verlag, Berlin, 1988.
[4] L. Greengard, *The Rapid Evaluation of Potential Fields in Particle Systems*, MIT Press, Cambridge, MA, 1988.
[5] P.M. Morse and H. Feshbach, *Methods of Theoretical Physics* Vol. I, McGraw-Hill, New York, 1953.
[6] M. Abramowitz and I.A. Stegun, *Handbook of Mathematical Functions*, National Bureau of Standards, Washington, DC, 1964.
[7] R. Coifman, V. Rokhlin, and S. Wandzura, *The fast multipole method: A pedestrian prescription*, IEEE Trans. Antennas and Propagation, 35 (1993), pp. 7–12.
[8] M.A. Epton and B. Dembart, *Multipole translation theory for the three-dimensional Laplace and Helmholtz equations*, SIAM J. Sci. Comput., 16 (1995), pp. 865–897.
[9] V. Rokhlin, *Diagonal form of translation operators for the Helmholtz equation in three dimensions*, Appl. Comput. Harmon. Anal., 1 (1993), pp. 82–93.
[10] J.M. Song and W.C. Chew, *Multilevel fast-multipole algorithm for solving combined field integral equations of electromagnetic scattering*, Microwave Opt. Technol. Lett., 10 (1995), pp. 14–19.

[11] J. Rahola, *Experiments on Iterative Methods and the Fast Multipole Method in Electromagnetic Scattering*, CERFACS Technical Report TR/PA/98/49, CERFACS, Toulous, 1998.
[12] L. Greengard and V. Rokhlin, *A fast algorithm for particle simulations*, J. Comput. Phys., 73 (1987), pp. 325–348.
[13] L. Greengard, J. Huang, V. Rokhlin, and S. Wandzura, *Accelerating fast multipole methods for the Helmholtz equation at low frequencies*, IEEE Comput. Sci. Engrg., 5 (1998), pp. 32–38.
[14] S. Koc and W.C. Chew, *Calculation of acoustical scattering from a cluster of scatterers,* J. Acoust. Soc. Amer., 103 (1998), pp. 721–734.
[15] S. Stein, *Addition theorems for spherical wave functions*, Quart. Appl. Math., 19 (1961), pp. 15–24.
[16] X. Sun and N.P. Pitsianis, *A matrix version of the fast multipole method*, SIAM Rev., 43 (2001), pp. 289–300.
[17] E. Wigner, *Gruppentheorie und ihre Anwendung auf die Quanten-mechanik der Atomspektren*, Vieweg, Wiesbaden, Germany, 1931.
[18] J. Ivanic and K. Ruedenberg, *Rotation matrices for real spherical harmonics. Direct determination by recursion*, J. Chem. Phys., 100 (1996), pp. 6342–6347. *Errata*, 102 (1998), pp. 9099–9100.
[19] C.H. Choi, J. Ivanic, M. S. Gordon, and K. Ruedenberg, *Rapid and stable determination of rotation matrices between spherical harmonics by direct recursion*, J. Chem. Phys., 111 (1999), pp. 8825–8831.
[20] H. Goldstein, *Classical Mechanics*, 2nd ed., Addison-wesley, Reading, MA, 1980.
[21] E. Darve, *The fast multipole method: Numerical implementation*, J. Comput. Phys., 160 (2000), pp. 195–240.
[22] W.C. Chew, *Recurrence relations for three-dimensional scalar and addition theorem*, J. Electromagn. Waves Appl., 6 (1992), pp. 133–142.
[23] W.C. Chew, J.M. Jin, E. Michielssen, and J. Song, *Fast and Efficient Algorithms in Computational Electromagnetics*, Artech House, Norwood, MA, 2001.
[24] N.A. Gumerov and R. Duraiswami, *Computation of scattering from N spheres using multipole reexpansion*, J. Acoust. Soc. Amer., 112 (2002), pp. 2688–2701.
[25] N.A. Gumerov, R. Duraiswami, and E.A. Borovikov, *Data Structures, Optimal Choice of Parameters, and Complexity Results for Generalized Multilevel Fast Multipole Methods in d Dimensions*, UMIACS Technical Report TR 2003-28, University of Maryland, Institute for Advanced Computer Studies, College Park, MD, 2003. Available online at http://www.umiacs.umd.edu/%7Egumerov/
[26] N.A. Gumerov and R. Duraiswami, *Acoustical scattering from N spheres using a multilevel fast multipole method*, J. Acoust. Soc. Amer., 113 (2003), p. 2334.
[27] M.F. Gyure and M.A. Stalzer, *A prescription for the multilevel Helmholtz FMM*, IEEE Comput. Sci. Engrg., 5 (1998), pp. 39–47.