PROCEEDINGS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

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Proc. R. Soc. Lond. A 1991 **433**, 599-614
doi: 10.1098/rspa.1991.0066

Analysis of radiative scattering for multiple sphere configurations

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An analysis of radiative scattering for an arbitrary configuration of neighbouring spheres is presented. The analysis builds upon the previously developed superposition solution, in which the scattered field is expressed as a superposition of vector spherical harmonic expansions written about each sphere in the ensemble. The addition theorems for vector spherical harmonics, which transform harmonics from one coordinate system into another, are rederived, and simple recurrence relations for the addition coefficients are developed. The relations allow for a very efficient implementation of the 'order of scattering' solution technique for determining the scattered field coefficients for each sphere.

1. Introduction

Prediction of the radiative absorption and scattering characteristics of small particles is important to researchers in a number of fields, e.g. atmospheric modelling, analysis of radiative transfer from flames, and development of non-intrusive laser-based optical diagnostic methods. Computation of the radiative characteristics of spherical particles from Lorenz–Mie theory is practically a trivial matter due to the existence of efficient computer codes (Bohren & Huffman 1983). However, it is not unusual to encounter situations in which the individual particles, while spherical in shape, are so close together that the 'isolated sphere' assumption inherent in Lorenz–Mie theory is questionable. A common example is soot formed in combustion processes. Electron micrographs of the individual soot particles reveal them to be agglomerates of a large number of primary, spherical particles (Dobbins & Megaridis 1987).

Several investigations have been conducted into the radiative scattering behaviour of such 'neighbouring sphere' particles. Liang & Lo (1967) and Brunning & Lo (1971) were the first to formulate the general solution to Maxwell's wave equations for neighbouring spheres. Their analysis basically involves a superposition technique, in that the total solution for the field external to the particle is constructed from a superposition of individual solutions, in the form of vector spherical harmonic expansions, written about each sphere. To satisfy the boundary conditions on each sphere, addition theorems are used to transform a spherical harmonic from one coordinate origin to another. Ultimately, their formulation leads to a set of linear equations for the expansion coefficients of the individual solutions. Fuller & Kattawar (1988*a*, *b*) refined the superposition formulation, and investigated an 'order of scattering' technique for solving the system of equations. A superposition solution to the neighbouring sphere scattering problem has also been independently formulated by Borghese *et al.* (1979, 1984).

Proc. R. Soc. Lond. A (1991) **433**, 599–614
Printed in Great Britain

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A different approach to the problem was presented by Jones (1979*a*, *b*), who started with the integral formulation of the wave equations (Saxon 1955). By assuming the electric field to be uniform within each of the primary spheres (i.e. the Rayleigh approximation), his analysis also leads to a system of linear equations for the cartesian components of the field within each sphere. His solution, however, is completely equivalent to that obtained from the superposition technique for similar Rayleigh-limit conditions, since it begins with the same governing equations and boundary conditions.

Presented here is a further refinement of the superposition solution method. The contribution of this work to the multiple sphere scattering problem is that the formulation and computational aspects of the addition theorems have been greatly simplified, and enables an efficient implementation of the order-of-scattering solution technique.

2. Formulation

2.1. *The superposition solution*

The basic framework for the multiple sphere scattering problem follows directly from Lorenz–Mie theory for an isolated sphere (Stratton 1941; Bohren & Huffman 1983), and this theory is outlined here. Assuming time-harmonic dependence with factor $\exp(-\mathrm{i}\omega t)$, expressions for the incident, scattered, and internal electric fields, denoted $\boldsymbol{E}_0, \boldsymbol{E}_\mathrm{s}$, and $\boldsymbol{E}_1$, respectively, satisfying Maxwell's wave equations are given as

$$\boldsymbol{E}_0 = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} [p_{mn} \boldsymbol{N}_{mn}^{(1)}(r,\theta,\phi) + q_{mn} \boldsymbol{M}_{mn}^{(1)}(r,\theta,\phi)], \tag{1}$$

$$\boldsymbol{E}_s = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} [a_{mn} \boldsymbol{N}_{mn}^{(3)}(r,\theta,\phi) + b_{mn} \boldsymbol{M}_{mn}^{(3)}(r,\theta,\phi)], \tag{2}$$

$$\boldsymbol{E}_1 = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} [d_{mn} \boldsymbol{N}_{mn}^{(1)}(mr,\theta,\phi) + c_{mn} \boldsymbol{M}_{mn}^{(1)}(mr,\theta,\phi)]. \tag{3}$$

In the above, (p_{mn}, q_{mn}), (a_{mn}, b_{mn}) and (c_{mn}, d_{mn}) are the expansion coefficients for the incident, scattered and internal fields, respectively, and $m = n + \mathrm{i}k$ is the complex index of refraction of the sphere. The vector spherical harmonics $\boldsymbol{M}_{mn}$ and $\boldsymbol{N}_{mn}$ are defined by

$$\boldsymbol{M}_{mn}^{(j)} = \nabla \times \boldsymbol{r} u_{mn}^{(j)}, \quad \boldsymbol{N}_{mn}^{(j)} = (1/\mathrm{k}) \nabla \times \boldsymbol{M}_{mn}^{(j)}, \tag{4}$$

where $u_{mn}^{(j)}$ is the scalar spherical harmonic given by

$$u_{mn}^{(1)} = j_n(r) P_n^m(\cos\theta)\, \mathrm{e}^{\mathrm{i}m\phi}, \quad u_{mn}^{(3)} = h_n(r) P_n^m(\cos\theta)\, \mathrm{e}^{\mathrm{i}m\phi}. \tag{5}$$

In the above, j_n and $h_n = j_n + \mathrm{i}y_n$ are spherical Bessel functions, and P_n^m is the associated Legendre function (Abramowitz & Stegun 1964). In the above and following equations, it is to be understood that the radial position γ has been non-dimensionalized by the factor $\mathrm{k} = 2\pi/\lambda$, where λ is the wavelength of the incident radiation. Expressions for the incident, scattered, and internal magnetic field are obtained from (1)–(3) via the relation $\boldsymbol{H} = (\nabla \times \boldsymbol{E})/\mathrm{i}\omega\mu$, where ω and μ are the circular frequency and magnetic permeability, respectively.

Across the surface of the sphere, the tangential components of the electric and magnetic fields are continuous:

$$(\boldsymbol{E}_0 + \boldsymbol{E}_\mathrm{s} - \boldsymbol{E}_1) \times \hat{\boldsymbol{e}}_r = 0, \quad (\boldsymbol{H}_0 + \boldsymbol{H}_\mathrm{s} - \boldsymbol{H}_1) \times \hat{\boldsymbol{e}}_r = 0. \tag{6}$$

By applying the above boundary conditions and utilizing the orthogonality properties of the spherical harmonics, the scattered field coefficients a_{mn} and b_{mn} can be expressed in terms of the incident field coefficients p_{mn} and q_{mn}, the sphere size parameter k, where a is the sphere radius, and the index of refraction m.

The only modification to the formulation for multiple-sphere scattering is that the scattered field is now taken to be the superposition of scattered waves originating from each sphere in the configuration. Referring to figure 1, each of the N_s spheres in the configuration is located at a point X^i, Y^i, Z^i, and is characterized by a size parameter x^i and refractive index m^i. The scattered field $\boldsymbol{E}_s$ is thus expressed as

$$\boldsymbol{E}_s = \sum_{i=1}^{N_s} \boldsymbol{E}_s^i. \tag{7}$$

The ith component of the scattered field is written using equation (2), with the spherical harmonics evaluated in a spherical coordinate system referenced to sphere i:

$$\boldsymbol{E}_s^i = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} [a_{mn}^i \boldsymbol{N}_{mn}^{(3)}(r^i, \theta^i, \phi^i) + b_{mn}^i \boldsymbol{M}_{mn}^{(3)}(r^i, \theta^i, \phi^i)]. \tag{8}$$

To apply the boundary conditions, and ultimately obtain the field coefficients a_{mn}^i, b_{mn}^i about each sphere, it is necessary to transform the harmonics written about sphere j into harmonics about sphere i. This transformation is accomplished through an addition theorem. For the condition $r^{ji} > r^i$, where r^{ji} represents the distance from origin j to i, the addition theorem for vector spherical harmonics can be written

$$\boldsymbol{M}_{mn}^{(3)}(r^j, \theta^j, \phi^j) = \sum_{l=1}^{\infty} \sum_{k=-l}^{l} [A_{kl}^{mn} \boldsymbol{M}_{kl}^{(1)}(r^i, \theta^i, \phi^i) + B_{kl}^{mn} \boldsymbol{N}_{kl}^{(1)}(r^i, \theta^i, \phi^i)], \tag{9}$$

$$\boldsymbol{N}_{mn}^{(3)}(r^j, \theta^j, \phi^j) = \sum_{l=1}^{\infty} \sum_{k=-l}^{l} [A_{kl}^{mn} \boldsymbol{N}_{kl}^{(1)}(r^i, \theta^i, \phi^i) + B_{kl}^{mn} \boldsymbol{M}_{kl}^{(1)}(r^i, \theta^i, \phi^i)]. \tag{10}$$

The coefficients A_{kl}^{mn} and B_{kl}^{mn} depend upon r^{ji} and the direction of translation, θ^{ji}, ϕ^{ji}, of origin j to i. The formulation and computation of these coefficients, which is the focus of this paper, will be discussed in the following section.

Using the addition theorem, a linear relationship can be obtained between the scattering coefficients corresponding to sphere i and those for all the other spheres. This is given as

$$a_{mn}^i = -\alpha_n^i \left(p_{mn}^i + \sum_{\substack{j=1 \\ j\neq i}}^{N_s} \sum_{l=1}^{\infty} \sum_{k=-l}^{l} [A_{mn}^{kl}(r^{ji}, \theta^{ji}, \phi^{ji})\, a_{kl}^j + B_{mn}^{kl}(r^{ji}, \theta^{ji}, \phi^{ji})\, b_{kl}^j] \right), \tag{11}$$

$$b_{mn}^i = -\beta_n^i \left(q_{mn}^i + \sum_{\substack{j=1 \\ j\neq i}}^{N_s} \sum_{l=1}^{\infty} \sum_{k=-l}^{l} [A_{mn}^{kl}(r^{ji}, \theta^{ji}, \phi^{ji})\, b_{kl}^j + B_{mn}^{kl}(r^{ji}, \theta^{ji}, \phi^{ji})\, a_{kl}^j] \right). \tag{12}$$

Here, α_n^i and β_n^i are the familiar Lorenz–Mie single sphere coefficients defined by

$$\alpha_n^i = \frac{m^i \psi_n'(x^i)\, \psi_n(m^i x^i) - \psi_n(x^i)\, \psi_n'(m^i x^i)}{m^i \xi_n'(x^i)\, \psi_n(m^i x^i) - \xi_n(x^i)\, \psi_n'(m^i x^i)}, \tag{13}$$

$$\beta_n^i = \frac{\psi_n'(x^i)\, \psi_n(m^i x^i) - m^i \psi_n(x^i)\, \psi_n'(m^i x^i)}{\xi_n'(x^i)\, \psi_n(m^i x^i) - m^i \xi_n(x^i)\, \psi_n'(m^i x^i)}, \tag{14}$$

where ψ_n and ξ_n are Ricatti–Bessel functions, and the prime denotes differentiation with respect to argument.

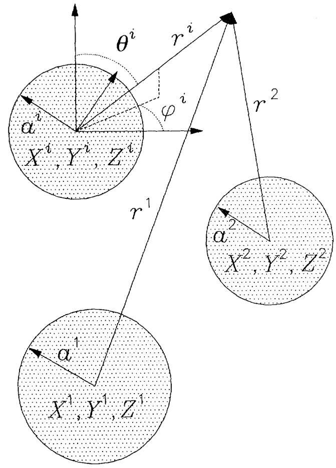

Figure 1. Sphere configuration.

By truncating the series representation for the scattered field, equation (8), at $n = N_t$, equations (11) and (12) are reduced to a system of linear equations for the coefficients. In matrix form, this system is expressed

$$\boldsymbol{a}^i + \sum_{\substack{j=1\\ j\neq i}}^{N_s} \boldsymbol{T}^{ji}\boldsymbol{a}^j = \boldsymbol{p}^i, \tag{15}$$

where $\boldsymbol{a}^i = (a^i_{mn}, b^i_{mn})$, $\boldsymbol{p}^i = -(\alpha^i_n p^i_{mn}, \beta^i_n q^i_{mn})$, $n = 1, 2, \ldots, N_t$; $m = 0, \pm 1, \pm 2, \ldots \pm n$, and $\boldsymbol{T}^{ji}$ represents the 'translation' matrix from sphere j to sphere i. The elements of $\boldsymbol{T}^{ji}$ are given by

$$T^{ji}_{mnkl} = \begin{pmatrix} \alpha^i_n A^{kl}_{mn}(r^{ji}, \theta^{ji}, \phi^{ji}) & \alpha^i_n B^{kl}_{mn}(r^{ji}, \theta^{ji}, \phi^{ji}) \\ \beta^i_n B^{kl}_{mn}(r^{ji}, \theta^{ji}, \phi^{ji}) & \beta^i_n A^{kl}_{mn}(r^{ji}, \theta^{ji}, \phi^{ji}) \end{pmatrix}. \tag{16}$$

The coefficients p^i_{mn}, q^i_{mn} are specified by the nature of the incident field. A convenient choice is to assume the incident field propagates in the z-direction and is polarized in the x-direction. For this situation (Saxon 1955),

$$p^i_{1n} = -\tfrac{1}{2}\mathrm{i}^{n+1}\frac{2n+1}{n(n+1)}\exp(\mathrm{i}Z^i), \quad p^i_{-1n} = \tfrac{1}{2}\mathrm{i}^{n+1}(2n+1)\exp(\mathrm{i}Z^i), \tag{17}$$

$$q^i_{1n} = p^i_{1n}, \quad q^i_{-1n} = -p^i_{-1n}, \tag{18}$$

$$p^i_{mn} = q^i_{mn} = 0, \quad |m| \neq 1. \tag{19}$$

2.2. *Far-field scattering and cross sections*

At distances $r \gg r_{\max}$, where $r_{\max}$ is the largest distance between the spheres, the scattered field from the ensemble can be represented as a spherical, transverse wave. Using the asymptotic limit of the Hankel function $h_n(r)$, the θ and ϕ components of this wave can be expressed in terms of a single coordinate system by the form

$$E_{s\theta} = \mathrm{i}/r\,\mathrm{e}^{\mathrm{i}r}\sum_{n=1}^{\infty}\sum_{m=-n}^{n}(-\mathrm{i})^{n+1}[a^{\mathrm{T}}_{mn}\tau_{mn}(\theta) + b^{\mathrm{T}}_{mn}\pi_{mn}(\theta)]\,\mathrm{e}^{\mathrm{i}m\phi}, \tag{20}$$

$$E_{s\phi} = -1/r\,\mathrm{e}^{\mathrm{i}r}\sum_{n=1}^{\infty}\sum_{m=-n}^{n}(-\mathrm{i})^{n+1}[a^{\mathrm{T}}_{mn}\pi_{mn}(\theta) + b^{\mathrm{T}}_{mn}\tau_{mn}(\theta)]\,\mathrm{e}^{\mathrm{i}m\phi}, \tag{21}$$

where the functions π_{mn} and τ_{mn} are defined by

$$\pi_{mn}(\theta) = (m)/(\sin\theta)P_n^m(\cos\theta), \quad \tau_{mn}(\theta) = \mathrm{d}/\mathrm{d}\theta\, P_n^m(\cos\theta). \tag{22}$$

The total scattering coefficients $a_{mn}^{\mathrm{T}}, b_{mn}^{\mathrm{T}}$ are obtained by transforming the scattered field expansions for the individual spheres to an expression based on a single origin. For simplicity, this origin will be taken to correspond to sphere 1. For the condition $r^1 > r^{j1}$, the addition theorem for vector harmonics has the form

$$\boldsymbol{M}_{mn}^{(3)}(r^j,\theta^j,\phi^j) = \sum_{l=1}^{\infty}\sum_{k=-1}^{l}[A_{kl}^{\prime mn}\boldsymbol{M}_{kl}^{(3)}(r^1,\theta^1,\phi^1)+B_{kl}^{\prime mn}\boldsymbol{N}_{kl}^{(3)}(r^1,\theta^1,\phi^1)], \tag{23}$$

$$\boldsymbol{N}_{mn}^{(3)}(r^j,\theta^j,\phi^j) = \sum_{l=1}^{\infty}\sum_{k=-1}^{l}[A_{kl}^{\prime mn}\boldsymbol{N}_{kl}^{(3)}(r^1,\theta^1,\phi^1)+B_{kl}^{\prime mn}\boldsymbol{M}_{kl}^{(3)}(r_1,\theta^1,\phi^1)]. \tag{24}$$

The addition coefficients $A_{kl}^{\prime mn}, B_{kl}^{\prime mn}$ are similar to A_{kl}^{mn}, B_{kl}^{mn} defined by equations (9) and (10), but have a different dependence on r^{j1}. Applying the above two equations to each sphere (except sphere 1), the total scattering coefficients defined about origin 1 can be written

$$a_{mn}^{\mathrm{T}} = a_{mn}^1 + \sum_{\substack{j=1\\ j\neq i}}^{N_{\mathrm{S}}}\sum_{l=1}^{\infty}\sum_{k=-l}^{l}[A_{mn}^{\prime kl}(r^{j1},\theta^{j1},\phi^{j1})\,a_{kl}^j + B_{mn}^{\prime kl}(r^{j1},\theta^{j1},\phi^{j1})\,b_{kl}^j], \tag{25}$$

$$b_{mn}^{\mathrm{T}} = b_{mn}^1 + \sum_{\substack{j=1\\ j\neq i}}^{N_{\mathrm{S}}}\sum_{l=1}^{\infty}\sum_{k=-l}^{l}[A_{mn}^{\prime kl}(r^{j1},\theta^{j1},\phi^{j1})\,b_{kl}^j + B_{mn}^{\prime kl}(r^{j1},\theta^{j1},\phi^{j1})\,a_{kl}^j]. \tag{26}$$

The scattering cross section of the sphere ensemble is obtained by integrating the scattered radiant intensity over a spherical surface enclosing the ensemble, i.e.

$$\begin{aligned} C_{\mathrm{sca}} &= \frac{r^2}{I_0}\int_0^{2\pi}\int_0^{\pi} I_{\mathrm{s}}\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi \\ &= \frac{r^2}{2I_0}\,\mathrm{Re}\int_0^{2\pi}\int_0^{\pi}(E_{\mathrm{s}\theta}H_{\mathrm{s}\phi}^* - E_{\mathrm{s}\phi}H_{\mathrm{s}\theta}^*)\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi, \end{aligned} \tag{27}$$

where the asterisk denotes complex conjugate. Using the expressions for the scattered field, and the relations

$$\int_0^{2\pi}\int_0^{\pi}(\pi_{mn}\pi_{kl}+\tau_{mn}\tau_{kl})\,\mathrm{e}^{\mathrm{i}(m-k)\phi}\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi = 4\pi\frac{n(n+1)}{2n+1}\frac{(n+m)!}{(n-m)!}\delta_{ln}\delta_{km}, \tag{28}$$

$$\int_0^{2\pi}\int_0^{\pi}(\pi_{mn}\tau_{kl}+\tau_{mn}\pi_{kl})\,\mathrm{e}^{\mathrm{i}(m-k)\phi}\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi = 0, \tag{29}$$

the scattering cross section can be written

$$C_{\mathrm{sca}} = \frac{2\pi}{\mathrm{k}^2}\sum_{n=1}^{\infty}\sum_{m=-n}^{n}\frac{n(n+1)}{2n+1}\frac{(n+m)!}{(n-m)!}(|a_{mn}^{\mathrm{T}}|^2+|b_{mn}^{\mathrm{T}}|^2). \tag{30}$$

The extinction cross section of the ensemble is obtained simply from the sum of the extinction cross sections of the individual spheres. From the optical theorem (Bohren & Huffman 1983), the latter, for sphere i, is given by

$$C_{\mathrm{ext}}^i = \frac{2\pi}{\mathrm{k}^2}\,\mathrm{Re}\sum_{n=1}^{\infty}\sum_{m=-n}^{n}\frac{n(n+1)}{2n+1}\frac{(n+m)!}{(n-m)!}(a_{mn}^i\,p_{mn}^{*i}+b_{mn}^i\,q_{mn}^{*i}). \tag{31}$$

For the z-propagating, x-polarized incident field assumed here, the above equation becomes

$$C^i_{\text{ext}} = \frac{2\pi}{k^2} \operatorname{Re}\left\{\exp(-iZ^i) \sum_{n=1}^{\infty} (-i)^{n+1}[n(n+1)(a^i_{1n}+b^i_{1n}) - a^i_{-1n} + b^i_{-1n}]\right\} \tag{32}$$

and, for the entire ensemble,

$$C_{\text{ext}} = \sum_{i=1}^{N_s} C^i_{\text{ext}}. \tag{33}$$

The total absorption cross section for the ensemble can be obtained from $C_{\text{abs}} = C_{\text{ext}} - C_{\text{sca}}$. Alternatively, the absorption cross section can be obtained by calculating the radiant energy absorbed by each sphere, via

$$\begin{aligned} C^i_{\text{abs}} &= \frac{a^{i2}}{I_0} \int_0^{2\pi} \int_0^{\pi} I_1(r = a^i) \sin\theta \, d\theta \, d\phi \\ &= \frac{a^{i2}}{2I_0} \operatorname{Re} \int_0^{2\pi} \int_0^{\pi} (E_{1\theta} H^*_{1\phi} - E_{1\phi} H^*_{1\theta})|_{r=a^i} \sin\theta \, d\theta \, d\phi. \end{aligned} \tag{34}$$

Substituting the expression for the internal field $\boldsymbol{E}_1$, equation (3), into the above and integrating, one obtains

$$C^i_{\text{abs}} = \frac{2\pi}{|m^i|^2 k^2} \operatorname{Re} \sum_{n=1}^{\infty} \sum_{m=-n}^{n} i \frac{n(n+1)}{2n+1} \frac{(n+m)!}{(n-m)!} \psi'_n(m^i x^i)\, \psi^*_n(m^i x^i) \times (m^{i*} |d^i_{mn}|^2 + m^i |c^i_{mn}|^2), \tag{35}$$

where the internal field coefficients c^i_{mn} and d^i_{mn} are related to the scattering coefficients by

$$c^i_{mn} = \frac{i m^i}{\psi_n(m^i x^i)\, \psi'_n(x^i) - m^i \psi_n(x^i)\, \psi'_n(m^i x^i)} b^i_{mn}, \tag{36}$$

$$d^i_{mn} = \frac{i m^i}{m^i \psi_n(m^i x^i)\, \psi'_n(x^i) - \psi_n(x^i)\, \psi'_n(m^i x^i)} a^i_{mn}. \tag{37}$$

As was the case with extinction, the ensemble absorption cross section is the sum of the individual sphere absorption cross sections, i.e.

$$C_{\text{abs}} = \sum_{i=1}^{N_s} C^i_{\text{abs}}. \tag{38}$$

3. Addition theorems

3.1. *Solid translation of coordinates*

The formulation of the multiple-sphere scattering problem is, up to this point, relatively straightforward. The analysis, however, becomes significantly more complicated once the details of the addition coefficients A^{mn}_{kl} and B^{mn}_{kl} are addressed. Explicit expressions exist for the scalar (Friedman & Russek 1954) and vector (Stein 1961; Cruzan 1962) spherical harmonic addition theorems. The derivations are

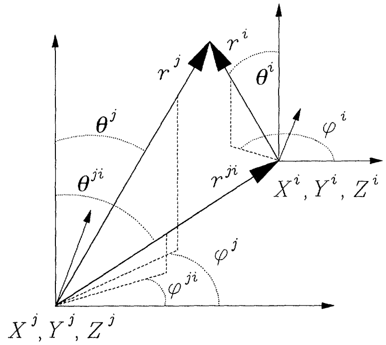

Figure 2. Translation of coordinates from origin j to origin i.

lengthy, and the results are simply listed here. From Cruzan (1962), the vector addition coefficients for the solid translation from origin X^j, Y^j, Z^j to X^i, Y^i, Z^i illustrated in figure 2 is given as

$$A_{kl}^{mn}(r^{ji}, \theta^{ji}, \phi^{ji}) = (-1)^k \, \mathrm{i}^{(l-n)} \frac{2l+1}{2l(l+1)} \sum_p \mathrm{i}^p [n(n+1)+l(l+1)-p(p+1)] \times a(m,n;-k,l;p)\, h_p(r^{ji})\, P_p^{m-k}(\cos\theta^{ji}) \exp[\mathrm{i}(m-k)\phi^{ji}], \quad (39)$$

$$B_{kl}^{mn}(r^{ji}, \theta^{ji}, \phi^{ji}) = -(-1)^k \, \mathrm{i}^{(l-n)} \frac{2l+1}{2l(l+1)} \sum_p \mathrm{i}^{p+1} \frac{2p+3}{2p+1} \times \{(l-k)(l+k+1)\, a(m,n;-k-1,l;p) + 2k(p-m+k+1)\, a(m,n;-k,l;p) - (p-m+k+1)(p-m+k)\, a(m,n;-k+1,l;p)\} \times h_{p+1}(r^{ji})\, P_{p+1}^{m-k}(\cos\theta^{ji}) \exp[\mathrm{i}(m-k)\phi^{ji}]. \quad (40)$$

The quantity $a(m,n;k,l;p)$ is defined by the linearization expansion for Legendre functions:

$$P_n^m(\cos\theta)\, P_l^k(\cos\theta) = \sum_p a(m,n;k,l;p)\, P_p^{m+k}(\cos\theta). \quad (41)$$

The summation over p in equations (39)–(41) runs over the values $p = |n-l|$, $|n-l|+2, \ldots, n+l$. Expressions for the addition coefficients $A_{kl}^{\prime mn}$ and $B_{kl}^{\prime mn}$ defined in equations (23) and (24) are obtained by replacing $h_p(r^{ji})$ with $j_p(r^{ji})$ in equations (39) and (40).

Explicit relations for $a(m,n;k,l;p)$ exist (Stein 1961), but they envolve additional summations and are not easily implemented. Alternatively, recurrence relations for these quantities can be obtained (Cruzan 1962). These relations, however, are rather complicated. They also cannot be put in the form where the index p is the only independent variable, which would be the ideal form from inspection of equations (39) and (40).

An alternate formulation of the addition coefficients can be derived, which bypasses the computation of the $a(m,n;k,l;p)$ functions and the evaluation of the series in equations (39) and (40). It yields relatively simple recurrence relations from which A_{kl}^{mn} and B_{kl}^{mn} can be obtained directly, and considerably speeds up the computation of these quantities.

The derivation begins with consideration of the addition theorem for scalar spherical harmonics. This theorem, for the problem at hand, can be written

$$u_{mn}^{(3)}(r^j,\theta^j,\phi^j) = \sum_{l=1}^{\infty}\sum_{k=-l}^{l} C_{kl}^{mn}(r^{ji},\theta^{ji},\phi^{ji})\, u_{kl}^{(1)}(r^i,\theta^i,\phi^i), \quad r^{ji} > r^i. \tag{42}$$

The explicit expression for the scalar addition coefficient C_{kl}^{mn} is given as (Friedman & Russek 1954; Stein 1961)

$$C_{kl}^{mn}(r^{ji},\theta^{ji},\phi^{ji}) = (-1)^k\, \mathrm{i}^{(l-n)}\,(2l+1)\sum_p \mathrm{i}^p\, a(m,n;-k,l;p) \times h_p(r^{ji})\, P_p^{m-k}(\cos\theta^{ji}) \exp[\mathrm{i}(m-k)\,\phi^{ji}]. \tag{43}$$

Recurrence relations will now be developed for the C_{kl}^{mn} coefficients. By taking the gradient of u_{mn}, resolving into cartesian components, and utilizing the recurrence relations for Bessel and Legendre functions, the following equations are obtained:

$$(\hat{\boldsymbol{e}}_x+\mathrm{i}\hat{\boldsymbol{e}}_y)\cdot\nabla u_{mn} = (2n+1)^{-1}[u_{m+1\,n-1}+u_{m+1\,n+1}], \tag{44}$$

$$(\hat{\boldsymbol{e}}_x-\mathrm{i}\hat{\boldsymbol{e}}_y)\cdot\nabla u_{mn} = (2n+1)^{-1}[(n+m)(n+m-1)\,u_{m-1\,n-1} + (n-m+1)(n-m+2)\,u_{m-1\,n+1}], \tag{45}$$

$$\hat{\boldsymbol{e}}_z\cdot\nabla u_{mn} = (2n+1)^{-1}[(n+m)\,u_{m-1\,n-1}-(n-m+1)\,u_{m-1\,n+1}]. \tag{46}$$

One sees from the above that the cartesian components of the gradient of a scalar harmonic can be expressed in terms of harmonics of neighbouring degree and order. The gradient operator is invariant with coordinate system, and the cartesian components of a vector are unaltered by a solid translation of coordinates. Thus, by taking the gradient of both sides of equation (42), matching components, and rearranging, the following equations are obtained

$$(2n+1)^{-1}[u_{mn-1}^{(3)}+u_{mn+1}^{(3)}] = \sum_{l=1}^{\infty}\sum_{k=-l}^{l}\left[\frac{1}{2l+3}C_{k-1\,l+1}^{m-1\,n}+\frac{1}{2l-1}C_{k-1\,l-1}^{m-1\,n}\right]u_{kl}^{(1)}, \tag{47}$$

$$(2n+1)^{-1}[(n+m)(n+m+1)\,u_{mn-1}^{(3)}+(n-m)(n-m+1)\,u_{mn+1}^{(3)}] = \sum_{l=1}^{\infty}\sum_{k=-l}^{l}\left[\frac{(l+k+1)(l+k+2)}{2l+3}C_{k+1\,l+1}^{m+1\,n}+\frac{(l-k)(l-k-1)}{2l-1}C_{k+1\,l-1}^{m+1\,n}\right]u_{kl}^{(1)}, \tag{48}$$

$$(2n+1)^{-1}[(n+m)\,u_{mn-1}^{(3)}-(n-m+1)\,u_{mn+1}^{(3)}] = \sum_{l=1}^{\infty}\sum_{k=-l}^{l}\left[\frac{l+k+1}{2l+3}C_{kl+1}^{mn}-\frac{l-k}{2l-1}C_{kl-1}^{mn}\right]u_{kl}^{(1)}, \tag{49}$$

where the harmonics $u_{mn}^{(3)}$ and $u_{kl}^{(1)}$ are expressed in terms of r^j, θ^j, ϕ^j and r^i, θ^i, ϕ^i, respectively. The addition theorem, equation (42), is now applied to the left-hand side of the above three equations. Using the orthogonality of the harmonics yields

$$(2n+1)^{-1}[C_{kl}^{mn-1}+C_{kl}^{mn+1}] = (2l-1)^{-1}C_{k-1\,l-1}^{m-1\,n}+(2l+3)^{-1}C_{k-1\,l+1}^{m-1\,n}, \tag{50}$$

$$(2n+1)^{-1}[(n+m)(n+m+1)\,C_{kl}^{mn-1}+(n-m)(n-m+1)\,C_{kl}^{mn+1}] = \frac{(l-k)(l-k-1)}{2l-1}C_{k+1\,l-1}^{m+1\,n}+\frac{(l+k+1)(l+k+2)}{2l+3}C_{k+1\,l+1}^{m+1\,n}, \tag{51}$$

$$(2n+1)^{-1}[(n+m)\,C_{kl}^{mn-1}-(n-m+1)\,C_{kl}^{mn+1}] = -\frac{l-k}{2l-1}C_{kl-1}^{mn}+\frac{l+k+1}{2l+3}C_{kl+1}^{mn}. \tag{52}$$

The above three equations are recurrence relations for the C_{kl}^{mn} functions. They are noteworthy in that r^{ji}, θ^{ji}, and ϕ^{ji} do not explicitly appear in the relations, indicating a geometrical relationship among the different degrees and orders. Of course, for the recurrence relationships to be of practical use starting values are needed. This is accomplished by combining addition theorems for spherical Bessel functions and Legendre polynomials (Abramowitz & Stegun 1964; Hobson 1931) to yield:

$$\begin{aligned}\exp(\mathrm{i}r^j)/\mathrm{i}r^j &= u_{00}^{(3)}(r^j,\theta^j,\phi^j)\\ &= \sum_{l=1}^{\infty}\sum_{k=-l}^{l}(-1)^{k+1}(2l+1)\,h_l(r^{ji})\,P_l^{-k}(\cos\theta^{ji})\exp(-\mathrm{i}k\phi^{ji})\\ &\quad\times j_l(r^i)\,P_l^k(\cos\theta^i)\exp(\mathrm{i}k\phi^i),\quad r^i<r^{ji},\end{aligned} \tag{53}$$

or

$$C_{kl}^{00}=(-1)^{k+l}(2l+1)\,h_l(r^{ji})\,P_l^{-k}(\cos\theta^{ji})\exp(-\mathrm{i}k\phi^{ji}). \tag{54}$$

Using the starting expression, the recurrence relations can be used to calculate C_{kl}^{mn} for arbitrary k, l, m and n. A practical method of doing so uses the fact that $C_{kl}^{mn}=0$ if $|m|>n$ or $|k|>l$. Equations (50) and (51) can thus be written for the specific case of $|m|=n$ as

$$C_{kl}^{n+1\,n+1}=(2n+1)\,[(2l-1)^{-1}\,C_{k-1\,l-1}^{nn}+(2l+3)^{-1}\,C_{k-1\,l+1}^{nn}], \tag{55}$$

$$C_{kl}^{-n-1\,n+1}=\frac{1}{2(n+1)}\left[\frac{(l-k)(l-k-1)}{2l-1}C_{k+1\,l-1}^{-nn}+\frac{(l+k+1)(l+k+2)}{2l+3}C_{k+1\,l+1}^{-nn}\right]. \tag{56}$$

Starting with the above two equations, $C_{kl}^{m|m|}$ can be obtained from C_{kl}^{00} for all values of k, l. Equation (52) can then be used to compute C_{kl}^{mn} for $n=|m|+1,\ |m|+2,\ldots,N$. Note that, because of the relationship between l and n in the recurrence relations, calculation of C_{kl}^{mn} up to $l=n=N$ requires that one start with C_{kl}^{00} calculated up to $l=2N$. Extensive numerical tests of the recurrence relations confirmed their stability.

Additional recurrence formulas for the C_{kl}^{mn} can be obtained through analysis of the vector spherical harmonic $\boldsymbol{M}_{mn}=\nabla u_{mn}\times\boldsymbol{r}$. It can be shown that

$$(\hat{\boldsymbol{e}}_x+\mathrm{i}\hat{\boldsymbol{e}}_y)\cdot\boldsymbol{M}_{mn}=\mathrm{i}u_{m+1n}, \tag{57}$$

$$(\hat{\boldsymbol{e}}_x-\mathrm{i}\hat{\boldsymbol{e}}_y)\cdot\boldsymbol{M}_{mn}=\mathrm{i}(n+m)(n-m+1)\,u_{m-1n}, \tag{58}$$

$$\hat{\boldsymbol{e}}_z\cdot\boldsymbol{M}_{mn}=-\mathrm{i}mu_{mn}. \tag{59}$$

Consider the translation from coordinates j to i as illustrated in figure 2. Then

$$\begin{aligned}\nabla u_{mn}^{(3)}(r^j,\theta^j,\phi^j)\times\boldsymbol{r}^j &= \boldsymbol{M}_{mn}^{(3)}(r^j,\theta^j,\phi^j)\\ &= \sum_{l=1}^{\infty}\sum_{k=-l}^{l}C_{kl}^{mn}\,\nabla u_{kl}^{(1)}(r^i,\theta^i,\phi^i)\times\boldsymbol{r}^j\\ &= \sum_{l=1}^{\infty}\sum_{k=-l}^{l}C_{kl}^{mn}\,\nabla u_{kl}^{(1)}(r^i,\theta^i,\phi^i)\times(\boldsymbol{r}^{ji}+\boldsymbol{r}^i)\\ &= \sum_{l=1}^{\infty}\sum_{k=-l}^{l}C_{kl}^{mn}[\nabla u_{kl}^{(1)}(r^i,\theta^i,\phi^i)\times\boldsymbol{r}^{ji}+\boldsymbol{M}_{kl}^{(1)}(r^i,\theta^i,\phi^i)].\end{aligned} \tag{60}$$

By taking $\boldsymbol{r}^{ji}=\hat{\boldsymbol{e}}_xX+\hat{\boldsymbol{e}}_yY+\hat{\boldsymbol{e}}_zZ$, and using equations (44)–(46) and (57)–(59), both sides of equation (60) can be resolved into cartesian components. By equating the components, and then applying the scalar addition theorem to the left-hand side (as was done in equations (50) and (51)), the following relations can be derived:

$$C^{m+1n}_{k+1l} = (2l+3)^{-1}[ZC^{mn}_{kl+1}+(l+k+2)\,\xi C^{mn}_{k+1l+1}] + (2l-1)^{-1}[ZC^{mn}_{kl-1}-(l-k-1)\,\xi C^{mn}_{k+1l-1}]+C^{mn}_{kl}, \quad (61)$$

$$(n-m+1)(n+m)\,C^{m-1n}_{k-1l} = (l+k)(2l+3)^{-1}[(l+k+1)\,ZC^{mn}_{kl+1}-\eta C^{mn}_{k-1l+1}] + (l-k+1)(2l-1)^{-1}[(l-k)\,ZC^{mn}_{k-1l}+\eta C^{mn}_{k-1l-1}]+(l+k)(l-k+1)\,C^{mn}_{kl}, \quad (62)$$

$$2(k-m)\,C^{mn}_{kl} = (2l+3)^{-1}[\eta C^{mn}_{k-1l+1}+(l+k+1)(l+k+2)\,\xi C^{mn}_{k+1l+1}] + (2l-1)^{-1}[\eta C^{mn}_{k-1l-1}+(l-k)(l-k-1)\,\xi C^{mn}_{k+1l-1}], \quad (63)$$

where $\eta = X+\mathrm{i}Y$, $\xi = X-\mathrm{i}Y$.

An additional symmetry relation for C^{mn}_{kl} can be obtained from the explicit expression, equation (43):

$$C^{-kl}_{-mn} = (-1)^{k+l+n+m}\,(2n+1)(2l+1)^{-1}\,C^{mn}_{kl}. \quad (64)$$

The next step is to relate the vector addition coefficients A^{mn}_{kl} and B^{mn}_{kl} to the scalar addition coefficient C^{mn}_{kl}. The vector harmonic $\boldsymbol{N}_{mn}$ is first resolved into cartesian components, yielding

$$(\hat{\boldsymbol{e}}_x+\mathrm{i}\hat{\boldsymbol{e}}_y)\cdot\boldsymbol{N}_{mn} = (2n+1)^{-1}[nu_{m+1n+1}-(n+1)\,u_{m+1n-1}], \quad (65)$$

$$(\hat{\boldsymbol{e}}_x-\mathrm{i}\hat{\boldsymbol{e}}_y)\cdot\boldsymbol{N}_{mn} = (2n+1)^{-1}[n(n-m+1)(n-m+2)\,u_{m-1n+1} - (n+1)(n+m)(n+m-1)\,u_{m-1n-1}], \quad (66)$$

$$\hat{\boldsymbol{e}}_z\cdot\boldsymbol{N}_{mn} = (2n+1)^{-1}[n(n-m+1)\,u_{mn+1}+(n+1)(n+m)\,u_{mn-1}]. \quad (67)$$

By expanding the vector addition theorem, equations (9) and (10), into components and following the procedure used in the previous derivations, C^{mn}_{kl} can be related to A^{mn}_{kl} and B^{mn}_{kl}. After some algebraic manipulations, one obtains

$$A^{mn}_{kl} = [2l(l+1)]^{-1}[(l-k)(l+k+1)\,C^{m+1n}_{k+1l}+2mkC^{mn}_{kl}+(n+m)(n-m+1)\,C^{m-1n}_{k-1l}], \quad (68)$$

$$B^{mn}_{kl} = -\mathrm{i}(2l+1)\,[2l(l+1)(2l-1)]^{-1}[(l-k)(l-k-1)\,C^{m+1n}_{k+1l-1} + 2m(l-k)\,C^{mn}_{kl-1}-(n+m)(n-m+1)\,C^{m-1n}_{k-1l-1}]$$
$$= \mathrm{i}(2l+1)\,[2l(l+1)(2l+3)]^{-1}[(l+k+1)(l+k+2)\,C^{m+1n}_{k+1l+1} - 2m(l+k+1)\,C^{mn}_{kl+1}-(n+m)(n-m+1)\,C^{m-1n}_{k-1l+1}]. \quad (69)$$

Substitution of equations (61)–(63) into the above yield the additional relations:

$$A^{mn}_{kl} = [(l+1)^{-1}(2l+3)]^{-1}\{(l+k+1)\,ZC^{mn}_{kl+1} + \tfrac{1}{2}[(l+k+1)(l+k+2)\,\xi C^{mn}_{k+1l+1}-\eta C^{mn}_{k-1l+1}]\} + [l(2l-1)]^{-1}\{(l-k)\,ZC^{mn}_{kl-1} - \tfrac{1}{2}[(l-k)(l-k-1)\,\xi C^{mn}_{k+1l-1}-\eta C^{mn}_{k-1l-1}]\}+C^{mn}_{kl}, \quad (70)$$

$$B^{mn}_{kl} = \mathrm{i}\,[2l(l+1)]^{-1}[2ZC^{mn}_{kl}-(l-k)(l+k+1)\,\xi C^{mn}_{k+1l}-\eta C^{mn}_{k-1l}]. \quad (71)$$

The above equations are identical to those derived (in a completely different manner) by Stein (1961).

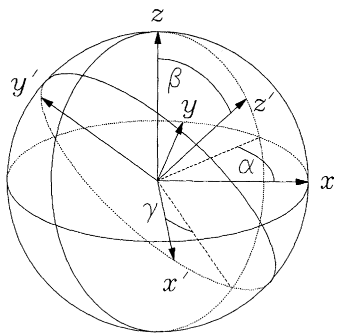

Figure 3. Euler angles of rotation α, β, and γ.

Using the explicit expressions for A_{kl}^{mn} and B_{kl}^{mn}, (39) and (40), symmetry relations analogous to equation (64) can be obtained:

$$A_{-mn}^{-kl} = (-1)^{k+l+m+n} \frac{2n+1}{2l+1} \frac{l(l+1)}{n(n+1)} A_{kl}^{mn}, \tag{72}$$

$$B_{-mn}^{-kl} = -(-1)^{k+l+m+n} \frac{2n+1}{2l+1} \frac{l(l+1)}{n(n+1)} B_{kl}^{mn}. \tag{73}$$

The specific case of axial translation from origin j to i results in a simplification of the addition theorem. In this situation, the two coordinate systems share a common azimuth angle ϕ, and the addition theorem becomes orthogonal in order m. Equations (54), (70) and (71) reduce is this case to

$$C_{0l}^{00} = (-t)^l (2l+1)\, h_l(r^{ji}), \tag{74}$$

$$A_{ml}^{mn} = t^{l+n} \left\{ r^{ji} \left[\frac{l+m+1}{(l+1)(2l+3)} C_{ml+1}^{mn} + \frac{l-m}{l(2l-1)} C_{ml-1}^{mn} \right] + C_{ml}^{mn} \right\}, \tag{75}$$

$$B_{ml}^{mn} = \mathrm{i} t^{l+n+1} r^{ji}\, m\, C_{ml}^{mn} / l(l+1) \tag{76}$$

$$A_{kl}^{mn} = B_{kl}^{mn} = C_{kl}^{mn} = 0, \quad m \neq k, \tag{77}$$

where $t = 1$ and -1 for $\theta^{ij} = 0$ and π, respectively.

3.2. *Rotation of coordinates*

In this section, the transformation of the vector spherical harmonics occurring due to a rotation of the coordinate system will be addressed. The techniques developed here will later be useful in numerical computation of the multiple-sphere scattering problem.

From Edmonds (1960), surface spherical harmonics are transformed by the rotation of a coordinate system through the Euler angles α, β, γ (figure 3) according to the relation

$$P_n^m(\cos\theta)\, \mathrm{e}^{\mathrm{i}m\phi} = \mathrm{e}^{\mathrm{i}m\gamma} \sum_{k=-n}^{n} D_{kn}^m(\beta)\, \mathrm{e}^{\mathrm{i}k\alpha} P_n^k(\cos\theta')\, \mathrm{e}^{\mathrm{i}k\phi'}. \tag{78}$$

It can be readily shown that the rotation transformation for scalar or vector spherical harmonics is identical (Stein 1961), i.e.

$$\boldsymbol{M}_{mn}^{(1)}(r,\theta,\phi) = \mathrm{e}^{\mathrm{i}m\gamma} \sum_{k=-n}^{n} D_{kn}^m(\beta)\, \mathrm{e}^{\mathrm{i}k\alpha} \boldsymbol{M}_{kn}^{(1)}(r,\theta',\phi'). \tag{79}$$

The techniques developed in the previous section can be applied here to obtain simple recurrence relations for the D^m_{kn} functions. Without loss of generality, assume that a rotation is characterized by $\alpha = \gamma = 0$. The relationship between the unit vectors in the initial and rotated coordinate systems is

$$\hat{e}_\xi = \cos^2(\tfrac{1}{2}\beta)\,\hat{e}'_\xi - \sin^2(\tfrac{1}{2}\beta)\,\hat{e}'_\eta + \sin\beta\hat{e}'_z, \tag{80}$$

$$\hat{e}_\eta = -\sin^2(\tfrac{1}{2}\beta)\,\hat{e}'_\xi + \cos^2(\tfrac{1}{2}\beta)\,\hat{e}'_\eta + \sin\beta\hat{e}'_z, \tag{81}$$

$$\hat{e}_z = -\tfrac{1}{2}(\sin\beta\hat{e}'_\xi + \sin\beta\hat{e}'_\eta) + \cos\beta\hat{e}'_x, \tag{82}$$

where $\hat{e}_\xi = \hat{e}_x + \mathrm{i}\hat{e}_y$ and $\hat{e}_\eta = \hat{e}_x - \mathrm{i}\hat{e}_y$. By matching the cartesian components of equation (79) (using the above and equations (57)–(59)) and rearranging, the following recurrence relationships can be obtained:

$$D^{m+1}_{kn} = \cos^2(\tfrac{1}{2}\beta)\,D^m_{k-1n} - (n-k)(n+k+1)\sin^2(\tfrac{1}{2}\beta)\,D^m_{k+1n} - k\sin\beta D^m_{kn}, \tag{83}$$

$$(n+m)(n-m+1)\,D^{m-1}_{kn} = -\sin^2(\tfrac{1}{2}\beta)\,D^m_{k-1n} + (n-k)(n+k+1)\cos^2(\tfrac{1}{2}\beta)\,D^m_{k+1n} - k\sin\beta D^m_{kn}, \tag{84}$$

$$(k\cos\beta - m)\,D^m_{kn} = -\tfrac{1}{2}(\sin\beta D^m_{k-1n} + (n-k)(n+k+1)\sin\beta D^m_{k+1n}). \tag{85}$$

The coefficients D^m_{kn} also have the symmetry relations:

$$D^{-m}_{-kn} = (-1)^{k+m}\frac{(n+k)!\,(n-m)!}{(n-k)!\,(n+m)!}D^m_{kn}, \tag{86}$$

$$D^{-k}_{-mn} = D^m_{kn}. \tag{87}$$

Starting values for the recurrence relations are obtained from the addition theorem for Legendre functions (Hobson 1931). Applied to this situation, it can be written

$$P_n(\cos\theta) = \sum_{k=-n}^{n} P^{-k}_n(\cos\beta)\,P^k_n(\cos\theta')\,\mathrm{e}^{\mathrm{i}k\phi'}, \tag{88}$$

or

$$D^0_{kn}(\beta) = P^{-k}_n(\cos\beta). \tag{89}$$

Numerical tests of the recurrence relations were performed by direct computation of the rotation transformation, equation (78). Results indicated that equations (83) and (84) were unconditionally stable. Equation (85), on the other hand, is stable only in increasing k.

4. Numerical computation

Armed with the recurrence relations developed above, it is a relatively simple task to compute the elements in the translation matrix $\boldsymbol{T}^{ji}$. The scattering coefficients a_{mn} and b_{mn} for each sphere in the problem can then be calculated from equation (15) using an appropriate linear equation solution technique.

An efficient solution technique is the 'order of scattering' method developed by Fuller & Kattawar (1988*a*, *b*). This method, which is essentially an iterative scheme, is based upon the physical concept of multiple reflections. The external field about a given sphere can always be decomposed into the incident field plus the field arising from first, second, third, and higher reflections off of neighbouring spheres. The scattering coefficients for this sphere can thus be expressed as a series of 'partial' scattering coefficients, each corresponding to the particular reflection order of the external field. Using this approach, the system of equations for the scattering coefficients, equation (15), can be written

$$\boldsymbol{a}^{i} = \sum_{p=0}^{\infty} \boldsymbol{a}^{i,p}, \tag{90}$$

$$\boldsymbol{a}^{i,p} = -\sum_{\substack{j=1\\ j\neq i}}^{N_s} \boldsymbol{T}^{ji}\, \boldsymbol{a}^{j,p-1}, \tag{91}$$

$$\boldsymbol{a}^{i,0} = \boldsymbol{p}^{i}, \tag{92}$$

where the index p refers to the scattering order. Note that the zero-order contribution corresponds to the isolated-sphere Lorenz–Mie solution.

The recurrence relations developed here allow for a very efficient implementation of this method, particularly in situations where there is insufficient computer memory to store the complete translation matrix $\boldsymbol{T}^{ji}$ for each pair of spheres j, i. Indeed, the memory requirements for the multiple-sphere scattering problem easily become excessive. In general, the number of scattering coefficients needed to characterize the scattered field will be on the order of N_t^2, and the translation matrix $\boldsymbol{T}^{ji}$ will thus be $O(N_t^4)$ in size. For an ensemble of N_s spheres, there will be $N_s(N_s-1)$ pairs of interactions between the spheres. Thus, the overall memory requirements of the problem are $O(N_s^2 N_t^4)$. Considering that the number of expansion terms N_t is generally larger than the size parameter at which the field is referenced (Bohren & Huffman 1983), memory requirements will quickly exceed capacity as the size and number of spheres in the ensemble are increased.

Under such conditions, it becomes necessary to compute the matrix elements sequentially during the calculation of a 'translated' scattering coefficient vector $\boldsymbol{a}^{ji} \equiv [\boldsymbol{T}^{ji}]\,\boldsymbol{a}^{j}$. Considering a solid translation of coordinates, this transformation could be accomplished through the equations

$$a_{mn}^{ji} = \alpha_n^i \sum_{l=1}^{N_t} \sum_{k=-l}^{l} [A_{mn}^{kl}(r^{ji}, \theta^{ji}, \phi^{ji})\, a_{kl}^{j} + B_{mn}^{kl}(r^{ji}, \theta^{ji}, \phi^{ji})\, b_{kl}^{j}], \tag{93}$$

$$b_{mn}^{ji} = \beta_n^i \sum_{l=1}^{N_t} \sum_{k=-l}^{l} [A_{mn}^{kl}(r^{ji}, \theta^{ji}, \phi^{ji})\, b_{kl}^{j} + B_{mn}^{kl}(r^{ji}, \theta^{ji}, \phi^{ji})\, a_{kl}^{j}]. \tag{94}$$

Computation of the above equations for all m and n will generally involve $O(N_t^4)$ steps. For the particular case of spheres i and j aligned on a common z-axis, the transformation is accomplished in $O(N_t^3)$ steps. In general, the spheres will not be aligned on a common z-axis. However, through rotation of coordinates, the numerical advantages to a common axis can be exploited. A transformation from j to i could thus be accomplished through the three steps.

1. The coordinate system of j is rotated so that the z-axis of j points towards the origin of i. The Euler angles for this rotation are $\alpha = \phi^{ji}, \beta = \theta^{ji}$ and $\gamma = 0$, and the transformation yields

$$a_{mn}'^{j} = \sum_{k=-n}^{n} D_{mn}^{k}(\theta^{ji}) \exp(\mathrm{i}k\phi^{ji})\, a_{kn}^{j}, \tag{95}$$

$$b_{mn}'^{j} = \sum_{k=-n}^{n} D_{mn}^{k}(\theta^{ji}) \exp(\mathrm{i}k\phi^{ji})\, b_{kn}^{j}. \tag{96}$$

2. The rotated coefficients at j are axially translated to the origin of i:

$$a'^{ji}_{mn} = \alpha^i_n \sum_{l=1}^{N_t} [A^{ml}_{mn}(r^{ji})\, a'^j_{ml} + B^{ml}_{mn}(r^{ji})\, b'^j_{kl}], \tag{97}$$

$$b'^{ji}_{mn} = \beta^i_n \sum_{l=1}^{N_t} [A^{ml}_{mn}(r^{ji})\, b'^j_{ml} + B^{ml}_{mn}(r^{ji})\, a'^j_{kl}]. \tag{98}$$

Step 3. The coefficients are rotated back to the original orientation. For this, $\alpha = \pi$, $\beta = \theta^{ji}$, and $\gamma = \pi - \phi^{ji}$. This completes the translation transformation:

$$a^{ji}_{mn} = (-1)^m \exp(-\mathrm{i}m\phi^{ji}) \sum_{k=-n}^{n} (-1)^k D^k_{mn}(\theta^{ji})\, a'^{ji}_{kn}, \tag{99}$$

$$b^{ji}_{mn} = (-1)^m \exp(-\mathrm{i}m\phi^{ji}) \sum_{k=-n}^{n} (-1)^k D^k_{mn}(\theta^{ji})\, b'^{ji}_{kn}. \tag{100}$$

Note that each of the three steps of the transformation involve $O(N_t^3)$ steps. Therefore, the translation transformation accomplished using this rotation-axial translation–rotation scheme will generally be $\frac{1}{3}N_t$ times faster than that accomplished through a pure solid translation, equation (94).

A completely different approach to obtaining the scattering coefficients has been developed by Borghese *et al.* (1984). Their formulation uses the powerful techniques of group theory to make use of the symmetry properties of a particular sphere configuration. Depending upon the configuration, the analysis can lead to a considerable reduction in order of the system of equations for the scattering coefficients. The recurrence relations developed herein could possibly speed up the computation of the symmetrized coefficient matrices, but this has not been explored in detail.

5. Discussion and conclusions

The veracity of the multiple-sphere scattering formulation and computational scheme presented herein was established through comparison of extinction and scattering computational results with previously published values (Kattawar & Dean 1983; Fuller & Kattawar 1988*a*, *b*). An example of the calculation results appear in figures 4 and 5, in which the extinction and absorption efficiencies and scattered intensities for a close-packed tetrahedral cluster of four identical spheres of size parameter $x = 3.114$ and refractive index $m = 1.366 + 0.005\mathrm{i}$ are presented. Calculations were performed on a 386-based PC, and required about 20 s to compute the scattering coefficients of the cluster for a particular orientation. In figure 4, the extinction and absorption efficiencies are given as a function of cluster orientation to the incident radiation. The efficiencies are around 10–20% greater than those obtained for non-interacting spheres, and display the orientation symmetry expected for the tetrahedral configuration. The scattered intensity in the direction $\theta = 30°$, $\phi = 90°$, normalized with the total scattered intensity, is given in figure 5 against the orientation angle. The purpose of this plot is mainly to illustrate the agreement of the present method with previously published results for the same configuration (Fuller & Kattawar 1988*b*).

The intention of this work has been to present a relatively simple and numerically efficient formulation of the neighbouring sphere scattering problem. Future investigations will concentrate on physical situations where the method would be

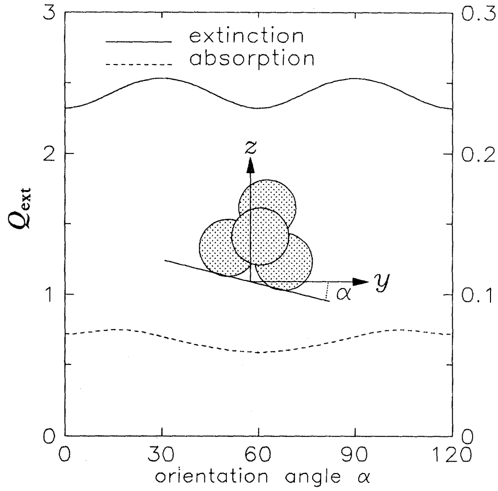

Figure 4. Extinction and absorption efficiencies Q_{ext} and Q_{abs} for a close-packed tetrahedral cluster of four identical spheres against cluster orientation angle α. Sphere size parameter $x = 3.114$ and refractive index $m = 1.366+0.005i$. Incident radiation is z-propagating and x-polarized.

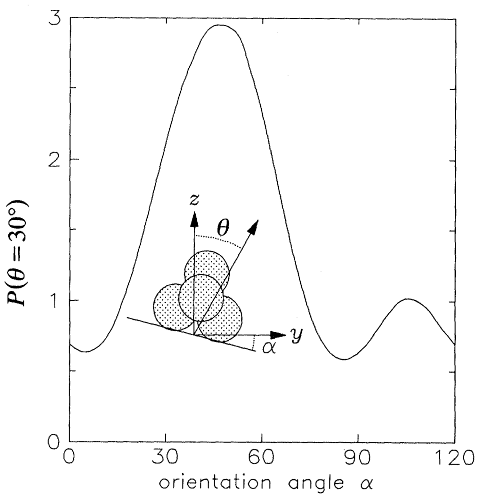

Figure 5. Scattered intensity phase function at the scattering angle $\theta = 30°$, $\phi = 90°$ against cluster orientation angle α. Conditions are the same as in figure 4.

useful, such as prediction of the radiative behaviour of agglomerated aerosol particles. Finally, it should be added that the convergence properties of the order-of-scattering method need to be addressed. It is not at all certain whether this solution method will converge for arbitrary numbers and sizes of spheres. Indeed, actual computations indicate that convergence of equations (90)–(92) is not guaranteed once the number and/or sizes of the spheres exceed a certain limit. Additional work is needed to quantify the convergence limits, and apply alternative methods (Borghese 1984) for solving the system of equations.

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Received 12 November 1990; accepted 12 December 1990