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An alternative expression for the addition theorems of spherical wave solutions of the Helmholtz equation

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An alternative formulation of the addition theorem for spherical wave solutions of the Helmholtz equation is presented. The 3-j symbols of Wigner, or more precisely the Gaunt coefficient (complete solid angle integral of a triple product of spherical harmonics), which appear in the formerly introduced expressions of these addition theorems are replaced by an explicit matrix expression relating the spherical wave solutions defined with respect to the different origins. The generalized Gaunt coefficients, which are complete solid angle integrals of a multiple product of spherical harmonics, can then be written in terms of a matrix product of basic matrices representing the Gaunt coefficient.

I. INTRODUCTION

In many fields of physics it is necessary to introduce methods to expand multipole waves, defined with respect to a specific origin, into multipole waves defined with respect to a shifted origin. These expansions are generally referred to as addition theorems. We can think of interaction problems in atomic physics, nuclear physics, solid state physics, and also some scattering problems in classical physics. Some interesting examples of problems in (quantum) physics are described in an article by Danos and Maximon. In a recent article by the authors, concerning retarded hydrodynamic interactions among spherical particles suspended in a viscous unbounded fluid, an alternative expansion has been introduced. However, a proof of a more general form of this expansion was not presented in that article. Our expression is based on a matrix relation which expresses a differential operation on spherical wave solutions of the wave equation in terms of a linear relation of all the members of the complete set of spherical wave solutions. The numerical implementation of our expansion is very efficient because it is explicitly written down in terms of a matrix formulation and does not contain the so-called 3-j symbols of Wigner. These Wigner symbols appear in the formerly introduced addition theorems (see, e.g., Refs. 1,4) because of the appearance of the integral of the triple product of spherical harmonics (Gaunt’s integral)

\[ \langle \ell m \mid Y_{nl} \mid pq \rangle = \int Y_{im}(\theta, \phi) Y_{n'l'}(\theta, \phi) Y_{pq}(\theta, \phi) d\Omega, \quad (1.1) \]

with \( Y_{nl}(\theta, \phi) \) the usual spherical harmonics and \( d\Omega \) the element of solid angle. Consequently an explicit matrix formulation for \( \langle \ell m \mid Y_{nl} \mid pq \rangle \) can be presented which might be generalized for the case of solid angle integrals of products of \( n+2 \) spherical harmonics, i.e., an explicit matrix formulation for the generalized form of Gaunt’s integral \( \langle \ell m \mid Y_{n1} \cdots Y_{n'p} \mid pq \rangle \).

In the literature several methods have been presented to obtain addition theorems for (vector) spherical wave solutions of the scalar (or vector) wave equation (or the Helmholtz wave equation)

\[ \nabla^2 \psi_{\ell m}(\mathbf{r}) + k^2 \psi_{\ell m}(\mathbf{r}) = 0. \quad (1.2) \]

The spherical wave solutions are
with $f_i(kr)$ any of the spherical Bessel functions $j_i(kr)$, $y_i(kr)$, $h^{(1)}_i(kr)$, or $h^{(2)}_i(kr)$. In this introductory section we restrict ourselves to the regular wave solution of the Helmholtz equation, $f_i(kr) = j_i(kr)$. The most commonly used method to obtain the addition theorem starts with the expansion of the plane-wave identity into spherical waves $\psi^{(r)}_{lm}(r)$

$$\exp(ik \cdot r) = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i^l \psi^{(r)}_{lm}(r) Y^{*}_{lm}(\theta, \phi),$$  

(1.4)

where the sum over the azimuthal index $m$ is restricted to $|m| < l$. $\psi_{lm}$ is given by Eq. (1.3) with $j_l$ substituted for $f_l$, and $(\theta_k, \phi_k)$ represent the polar and azimuthal angles of the wave vector $k$ with respect to $r$. Consider now three vectors, $r$, $r'$, and $R$, with $r + R = r'$ and the relation $\exp(ik \cdot r') = \exp(ik \cdot r)\exp(ik \cdot K)$. Expansion of both sides according to Eq. (1.4), multiplication by $Y_{lm}(\theta_k, \phi_k)$, and integration of the resulting triple product of spherical harmonics over the directions of the wave vector $k$ leads to the final result

$$\psi_{lm}(r) = \sum_{p > 0} \sum_{q > 0} C(l, m | p, q | s, t) \psi_{st}(R) \psi_{pq}(r'),$$  

(1.5)

with

$$C(l, m | p, q | s, t) = \delta^{p+s-l}(-1)^m \sqrt{4\pi(2l+1)(2s+1)(2p+1)} \begin{pmatrix} l & p & s \\ 0 & 0 & 0 \\ -m & q & t \end{pmatrix}.$$  

(1.6)

The $(l, m | p, q | s, t)$ are the 3-j symbols of Wigner. For a brief overview of some recent developments (including some results concerning vector addition theorems) we refer to an article by Felderhof and Jones.

II. SPHERICAL WAVE SOLUTIONS AND THEIR GENERATING DIFFERENTIAL OPERATORS

The spherical wave solutions $\psi_{lm}(r)$ of the Helmholtz wave equation (1.2) are of the form $f_i(kr)Y_{lm}(\theta, \phi)$, with $f_i(kr)$ any of the spherical Bessel functions $j_i(kr)$, $y_i(kr)$, $h^{(1)}_i(kr)$, or $h^{(2)}_i(kr)$. However, the spherical wave solutions used in the study of retarded hydrodynamic interactions among spherical particles, obtained by considering the following wave equation:

$$\nabla^2 \psi_{lm}(r) = \alpha^2 \psi_{lm}(r) = 0,$$  

(2.1)

have the following form:

$$\psi^{(r)}_{lm}(r) = g_i(\alpha r) Y_{lm}(\theta, \phi),$$  

(2.2)

$$\psi^{(s)}_{lm}(r) = k_i(\alpha r) Y_{lm}(\theta, \phi).$$  

(2.3)

The functions $g_i(\alpha r)$ and $k_i(\alpha r)$ are the regular and singular modified spherical Bessel functions, respectively, which are related to the modified Bessel functions of order equal to half an odd integer

$$g_i(\alpha r) = \sqrt{\pi/(2\alpha r)} I_{l+1/2}(\alpha r),$$  

(2.4)
It is obvious that this formulation is not really different if compared with the regular and singular spherical Bessel functions. The relations connecting the spherical Bessel functions with the modified spherical Bessel functions can be found in Abramowitz and Stegun (see also Sec. III for some more details). However, the method introduced in Ref. 2 is concerned with addition theorems of modified spherical Bessel functions. We restrict ourselves to these addition theorems, but it is obvious that with some minor adjustments the results presented below may also be expressed in terms of the spherical Bessel functions. As an illustration we also present a few results concerning these spherical Bessel functions.

We are now interested in a relation which expresses the spherical wave solution \( \psi_{l,m}(r) \), defined with respect to origin \( O \), in terms of \( \psi_{l,m}(r') \), defined with respect to a shifted origin \( O' \). In order to obtain an alternative expression for the addition theorem we have to prove two differential operator relations, acting upon the basic modified spherical Bessel functions \( k_0(\alpha r) \) and \( g_0(\alpha r) \), which generate the spherical wave solutions \( \psi_{l,m}(r) \) and \( \psi_{l,m}(r) \), respectively. First we introduce the spherical harmonics \( Y_{l,m}(\theta,\varphi) \). Although we assume that the reader is familiar with these functions we think it is advisable to consider these functions more carefully. We use a notation as in Messiah

\[
Y_{l,m}(\theta,\varphi) = \frac{(-1)^m}{n_{lm}} \frac{\sin \theta \phi^m}{\alpha^m} \frac{d^m P_l(u)}{du^m},
\]

with \( u = \cos \theta \). The indices \( l \) and \( m \) are assumed to be larger or equal to zero, and \( m \leq l \). The function \( P_l(u) \) is a Legendre polynomial. Furthermore we have introduced the shorthand notation \( n_{lm} \)

\[
n_{lm} = \left( \frac{4\pi}{2l+1} \frac{(l+m)!}{(l-m)!} \right)^{1/2}.
\]

The spherical harmonics for negative values of the azimuthal index are related with those presented above by \( Y_{l,-m}(\theta,\varphi) = (-1)^m Y_{l,m}^{*}(\theta,\varphi) \). The asterisk denotes complex conjugation. It is obvious from Eq. (2.6) that the \( Y_{l,m}(\theta,\varphi) \) may be written in the following form:

\[
Y_{l,m}(\theta,\varphi) = (\sin \theta \phi^m) \sum_{n=0}^{l-m} C_{n,lm} \cos^n \theta,
\]

where the normalization constant \( n_{lm} \) is incorporated in the coefficients \( C_{n,lm} \). With this relation of the \( Y_{l,m}(\theta,\varphi) \) as a function of \( \sin \theta \phi^m \) and \( \cos \theta \) in mind we define the operator \( Y_{l,m}(1/\alpha)\mathbf{\nabla} \). This operator is related with the spherical harmonics through the following replacements:

\[
\cos \theta \rightarrow \frac{1}{\alpha} \frac{\partial}{\partial z} \equiv M^0,
\]

\[
\sin \theta \phi \rightarrow \frac{1}{\alpha} \left( \frac{\partial}{\partial x} + i \frac{\partial}{\partial y} \right) \equiv M^+,
\]

\[
\sin \theta \phi \rightarrow \frac{1}{\alpha} \left( \frac{\partial}{\partial x} - i \frac{\partial}{\partial y} \right) \equiv M^-,
\]

with \( \alpha \) an arbitrary (complex) constant. It is obvious that \( M^+ \) appears if the azimuthal index \( m > 0 \), and \( M^- \) if \( m < 0 \). The shorthand notations \( M^\alpha \), with \( \alpha = \{0,+,-\} \), are introduced for later use.

We want to prove the following two relations:

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We shall only prove relation (2.10). The following steps are necessary [and an analogous set to prove Eq. (2.11)]:

(i) show $Y_{00}((1/\alpha)\nabla)g_0(r) = \psi_0^+(r)$;
(ii) prove by induction $Y_{l,l}((1/\alpha)\nabla)g_0(r) = \psi_{l,l}^+(r)$, \(\forall l \geq 1\);
(iii) prove by induction $Y_{l,1}((1/\alpha)\nabla)g_0(r) = \psi_{l,1}^+(r)$, \(\forall l \geq 1\);
(iv) show $Y_{l+1,l}((1/\alpha)\nabla)g_0(r) = \psi_{l+1,l}^+(r)$, \(\forall l \geq 0\);
(v) show $Y_{l+1,1}((1/\alpha)\nabla)g_0(r) = \psi_{l+1,1}^+(r)$, \(\forall l \geq 0\);
(vi) prove by induction $Y_{l,m}((1/\alpha)\nabla)g_0(r) = \psi_{l,m}^+(r)$, \(\forall l \geq 0\), \(|m| < l\).

To prove some of these steps one needs recursion relations for the modified spherical Bessel functions $g_l(r)$ (Ref. 8) and the associated Legendre polynomials $P_l^m(\cos \theta)$ (Ref. 9) which are summarized below. The proof of Eq. (2.11) is completely analogous but now one needs the recursion relations for the modified spherical Bessel functions $k_l(r)$. We do not prove Eq. (2.11), thus it is not necessary to present these latter recursion relations.

\[
\frac{d}{d\rho} g_l(\rho) = \frac{l}{\rho} g_l(\rho) + g_{l+1}(\rho),
\]

\[
(2l+1) \frac{g_l(\rho)}{\rho} = g_{l-1}(\rho) - g_{l+1}(\rho),
\]

\[
(2l+1) uP_l^m(u) = (l+1-m)P_{l+1}^m(u) + (l+m)P_{l-1}^m(u),
\]

\[
(1-u^2) \frac{d}{du} P_l^m(u) = (l+1)uP_l^m(u) - (l+1-m)P_{l+1}^m(u),
\]

with, for our purpose, $\rho = ar$ and $u = \cos \theta$. We do not go into all the details of the proof of relation (2.10), but show only the last step of the induction method summarized above. Thus we have to prove that $Y_{l+1,m}((1/\alpha)\nabla)g_0(r) = \psi_{l+1,m}^+(r)$ assuming that this relation is valid for the indices $(l,m)$ and $(l-1,m)$. We apply the substitution defined in Eq. (2.9) to a relation expressing the spherical harmonic $Y_{l+1,m}$ in terms of $Y_{l,m}$ and $Y_{l-1,m}$

\[
n_{l+1,m} Y_{l+1,m}(\theta, \varphi) = \frac{(2l+1)}{(l-m+1)} n_{lm} \cos \theta Y_{l,m}(\theta, \varphi) - \frac{(l+m)}{(l-m+1)} n_{l-1,m} Y_{l-1,m}(\theta, \varphi),
\]

which can be derived from recursion relation (2.14), and the result is then

\[
n_{l+1,m} Y_{l+1,m} \left( -\frac{1}{\alpha} \nabla \right) g_0(r) = \left[ \frac{(2l+1)}{(l-m+1)} n_{lm} \frac{\partial}{\partial z} \left[ Y_{l,m} \left( -\frac{1}{\alpha} \nabla \right) \right] - \frac{(l+m)}{(l-m+1)} n_{l-1,m} Y_{l-1,m} \left( -\frac{1}{\alpha} \nabla \right) \right] g_0(r).
\]
To derive a final expression we have to determine $(\partial/\partial z) \psi^+_{lm}(r)$ in terms of other regular spherical wave solutions. First we express $\partial/\partial z$ in terms of spherical coordinates

$$\frac{\partial}{\partial z} = \cos \theta \frac{\partial}{\partial r} - \frac{\sin \theta}{r} \frac{\partial}{\partial \theta}. \quad (2.18)$$

It is not very difficult to show, using the recursion relations for the modified spherical Bessel functions and those of the associated Legendre polynomials [Eqs. (2.12)–(2.15)], that we can obtain the following result:

$$n_{lm} \frac{\partial}{\partial z} \psi^+_{lm}(r) = n_{l+1,m} \frac{(l-m+1)}{(2l+1)} \psi^+_{l+1,m}(r) + n_{l-1,m} \frac{(l+m)}{(2l+1)} \psi^+_{l-1,m}(r). \quad (2.19)$$

Substitution of this result into Eq. (2.17) for $(\partial/\partial z) \psi^+_{lm}(r)$ leads directly to the final relation,

$$Y_{l+1,j}(\frac{i}{k} \nabla) f_0(kr) = (-i)^l Y_{l,m}(\theta, \phi) f_j(kr). \quad (2.20)$$

In this case the recursion relations for the spherical Bessel functions should be used. Also the direct relations between the spherical Bessel functions and the modified spherical Bessel functions might be used, of course.

Finally we want to emphasize that our relations (2.10), (2.11), and (2.20) might be reduced to special cases of the symbolic form of Gegenbauer’s equation which generate the (modified) spherical Bessel functions themselves. We give only the results here, but it is not difficult to prove them with the use of the appropriate recurrence relations. A direct but less elegant approach to show these relations is via inspection of Eqs. (2.10), (2.11), and (2.20), respectively. By considering the special case $\theta \rightarrow 0$, $r \rightarrow z$ (and $\alpha = 1$) the following results are obtained:

$$g_i(r) = P_j \left( \frac{d}{dr} \right) g_0(r), \quad (2.21)$$

$$k_i(r) = (-1)^l P_j \left( \frac{d}{dr} \right) k_0(r), \quad (2.22)$$

$$f_i(r) = i^l P_j \left( i \frac{d}{dr} \right) f_0(r). \quad (2.23)$$

In the latter equation $f_i \in \{j_i, y_i, h_i^{(1)}, h_i^{(2)}\}$.

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III. THE DERIVATION OF THE ADDITION THEOREM

Consider two points 0 and 0' as the origins of two coordinate systems with parallel axes and a point P denoted by the vector \( r = (r, \theta, \varphi) \) and \( r' = (r', \theta', \varphi') \), respectively. The vector pointing from 0' to 0 is denoted by \( \mathbf{Z} \). To express the spherical wave solutions \( \psi_{lm}(r) \), defined with respect to the origin 0, in terms of the spherical wave solutions \( \psi_{lm}'(r') \), defined with respect to the origin 0', we need only the addition theorem of the modified spherical Bessel function \( k_0(\alpha r) \). However, the addition theorem of \( k_0(\alpha r) \) which we have at our disposal is the one where \( \varphi \) is parallel to the z axis:

\[
k_0(\alpha r) = \sum_{s \geq 0} (-1)^s (2s+1) k_s(\alpha R) P_s(\cos \theta') g_s(\alpha r'), \quad |r'| < R,
\]

with \( R = |\mathbf{R}| \). It expresses \( k_0(\alpha r) \) in terms of modified regular spherical Bessel functions defined with respect to another origin. We want to emphasize that this expression has a slightly different form in comparison with the generally used addition theorem. In Eq. (3.1) \( \theta' \) (the polar angle of the coordinate system in 0') represents an outer angle of the triangle OPO' instead of the inner angle \( \gamma = \pi - \theta' \) which is generally used in the addition theorems. Use of \( \theta' \) leads to the appearance of the factor \( (-1)^s \). For our purpose we need a generalized version of Eq. (3.1) where \( R \) has an arbitrary direction with respect to the coordinate systems defined with 0 and 0'. Thus we have to rotate both coordinate systems, keeping the axes parallel, and to use the addition theorem for spherical harmonics. The rotation of the coordinate system defined with 0 does not affect the left hand side of Eq. (3.1). Finally we obtain

\[
k_0(\alpha r) = 4\pi \sum_{s \geq 0} (-1)^s k_s(\alpha R) Y_{st}(\theta', \varphi') Y^*_s(\xi, \eta) g_s(\alpha r'), \quad |r'| < R,
\]

with, of course, \( |r'| < R \). The azimuthal index \( t \) runs over all allowed values. The polar and azimuthal angles \( \xi \) and \( \eta \) belong to the vector \( R \). The addition theorems for the singular wave solutions \( \psi_{lm}^-(r) = Y_{lm}(\theta, \varphi) k_l(\alpha r) \) are now

\[
Y_{lm}(\theta, \varphi) k_l(\alpha r) = (-1)^{t} Y_{lm} \left( \frac{1}{\alpha} \nabla \right) k_0(\alpha r)
= 4\pi (-1)^{t} Y_{lm} \left( \frac{1}{\alpha} \nabla \right) \sum_{s \geq 0} (-1)^s k_s(\alpha R) Y^*_s(\xi, \eta) Y_{st} \left( \frac{1}{\alpha} \nabla' \right) g_s(\alpha r'),
\]

(3.3)

Keeping the separation vector \( R \) constant we can interchange both differential operators and obtain the following result:

\[
\psi_{lm}^-(r) = 4\pi (-1)^{t} \left( \sum_{s \geq 0} (-1)^s k_s(\alpha R) Y^*_s(\xi, \eta) Y_{st} \left( \frac{1}{\alpha} \nabla' \right) \right) \psi_{lm}^+(r').
\]

(3.4)

This expression can be simplified by introducing explicit expressions for the remaining differential operator.

Using the recursion relations for the modified spherical Bessel functions and the associated Legendre polynomials [see Eqs. (2.12)-(2.15)] we can easily obtain the following matrix relations:
with the differential operators $M^\alpha$ defined in Eq. (2.9) and

$$
M^0_{lm,pq} = \frac{n_{l-1,m} (l+m)}{n_{lm}} \frac{n_{l+1,m+1} (l-m+1)}{(2l+1)} \delta_{p,l-1} \delta_{q,m} + \frac{n_{l+1,m} (l-m+1)}{n_{lm}} \delta_{p,l+1} \delta_{q,m},
$$

$$
M^+_{lm,pq} = \frac{n_{l-1,m+1} (l+m+1)}{n_{lm}} \frac{n_{l+1,m+1} (l-m+2)}{(2l+1)} \delta_{p,l-1} \delta_{q,m+1},
$$

$$
M^-_{lm,pq} = -\frac{n_{l-1,m-1} (l+m) (l+m-1)}{n_{lm}} \delta_{p,l-1} \delta_{q,m-1} + \frac{n_{l+1,m-1} (l-m+1) (l-m+2)}{n_{lm}} \delta_{p,l+1} \delta_{q,m-1}.
$$

The constants $n_{lm}$ are defined in Eq. (2.7). Furthermore, using the fact that the differential operators commute, it can be shown that

$$
(M^\alpha M^\beta) \psi_{im}^+ (r) = (M^\beta M^\alpha) \psi_{im}^+ (r) = \sum_{p>0} (M^\alpha M^\beta)_{lm,pq} \psi_{pq}^+ (r).
$$

Consequently we can write

$$
Y_{st} \left( \frac{1}{\alpha} \nabla \right) \psi_{im}^+ (r) = \sum_{p>0} \left[ Y_{st}(M) \right]_{lm,pq} \psi_{pq}^+ (r),
$$

where $Y_{st}$ is a combination of the matrices $M^0$ and $M^+$ (if $t>0$) or $M^-$ (if $t<0$) following the definition (2.8). Finally we obtain for the addition theorem

$$
\psi_{\gamma m}^+ (r) = 4\pi (-1)^t \sum_{p>0} \left( \sum_{q>0} \left( -1 \right)^t k_z(\alpha r) Y_{st}(\xi,\eta) Y_{st}(M) \right)_{lm,pq} \psi_{pq}^+ (r').
$$

In an analogous way it is possible to express $\psi_{\gamma m}^-(r')$ in terms of $\psi_{pq}^+(r)$, or even simpler, by interchanging the role of $r$ and $r'$ in Eq. (3.11) and replacing $(\xi,\eta)$ by $(\pi - \xi, \eta + \pi)$.

The familiar form of the addition theorem for $f_z(kr) Y_{lm}(\theta,\phi)$ [Eq. (1.5)] can be transformed into an addition theorem of $\psi_{\gamma m}^-(r)$ by means of the relations between the spherical Bessel functions and the modified spherical Bessel functions\(^10\)

$$
k_z(z) = -\frac{\pi}{2} \iota h_1^{(1)}(iz),
$$

$$
g_z(z) = -\frac{1}{2} j_1(iz).
$$

In both cases the argument of $z$ is restricted to $-\pi < \text{arg}(z) < \frac{\pi}{2}$. This requirement is in our case satisfied because $\text{Re}(z) = \text{Re}(\alpha r) > 0$ (see Ref. 2). The transformation is straightforward and the result is
where the $C$ symbols are defined in Eq. (1.6). Comparison with our expression leads to the conclusion that the following equality should exist:

$$\left[ Y_{st}(M) \right]_{lm,pq} = \frac{(-1)^q}{\sqrt{4\pi}} \sqrt{(2l+1)(2s+1)(2p+1)} \begin{pmatrix} l & s & p \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & s & p \\ m & t & -q \end{pmatrix}$$

$$= \int Y_{lm}(\theta,\varphi) Y_{st}(\theta,\varphi) Y_{pq}^*(\theta,\varphi) d\Omega,$$  \hspace{1cm} (3.15)

i.e., an explicit matrix formulation exists for Gaunt's integral. Such a matrix formulation has already been acknowledged implicitly by the notation $\langle lm | Y_{st} | pq \rangle$. However, as far as we know, the formulation presented above has not been given before. In the following section we give a simple proof of Eq. (3.15) which directly relates the product of 3-j symbols with the matrix $Y_{st}(M)$.

In our opinion the presented formulation of the addition theorem is easier to use in numerical calculations because it is not necessary to introduce special computer programs to calculate 3-j symbols of Wigner like, e.g., the Root-Rational-Fraction package of Stone and Wood,\textsuperscript{11} which in the first instance we used to check our expression numerically.\textsuperscript{2} Furthermore it is more convenient to use a matrix notation because many physical problems as described in Ref. 2 or problems appearing in electromagnetic theory can be solved by using a matrix formulation. We should especially think of the case when accurate numerical calculations are needed. In that situation large values of the indices $l$, $p$, and $s$ are necessary. In this context it is important to emphasize that the matrix $Y_{st}(M)$ is in some sense sparse and banded, so it is not a very difficult task to determine the sum in the addition theorem (3.11). As far as we know there exist no derivations as presented here, but in an article by Gérardy and Ausloos\textsuperscript{12} similar methods are used starting with a method previously presented by Langbein\textsuperscript{13}. However, two important differences exist. First, they do not express their differential operators in a special combination as in this article (i.e., they did not use operators like $P_s(M)$, with $P_s$ a Legendre polynomial), but only derive a recursion relation for a so-called Langbein function [see Eq. (40) Ref. 12]. Second, they reversed the order of the differential operators and the rotation of the interparticle axis to an arbitrary orientation $R$. For this reason their expression is very complicated.

IV. PROOF OF THE RELATION BETWEEN THE RECURSION MATRIX AND THE INTEGRAL OF PRODUCTS OF THREE SPHERICAL HARMONICS

In this section we present an outline of the proof of Eq. (3.15). We restrict ourselves to azimuthal indices $\tau \geq 0$. The derivation of the addition theorem is, of course, an indirect proof of that relation, but we prefer to present also a direct proof. We can proceed in the same way as in Sec. II, i.e., use the method of induction. The first step is a simple one

$$\left[ Y_{00}(M) \right]_{lm,pq} = \int Y_{lm}(\theta,\varphi) Y_{00}(\theta,\varphi) Y_{pq}^*(\theta,\varphi) d\Omega = \frac{\delta_{l0} \delta_{m0} \delta_{p0}}{\sqrt{4\pi}}.$$  \hspace{1cm} (4.1)

From the theory of spherical harmonics we know

$$Y_{ss}(\theta,\varphi) = -\left( \frac{2s+1}{2s} \right)^{1/2} \sin \theta e^{i\varphi} Y_{s-1,s-1}(\theta,\varphi).$$  \hspace{1cm} (4.2)
Suppose Eq. (3.15) is valid for the indices \((s-1,s-1)\) for some \(s\geq 1\). Prove then that this equation is valid for the indices \((s,s)\). From our definition of \(Y_{st}(M)\) we may write

\[
[Y_{st}(M)]_{lm;pq} = -\left(\frac{2s+1}{2s}\right)^{1/2} \sum_{\rho,\sigma} M^\rho_{lm,po} [Y_{s-1,s-1}(M)]_{po;pq}
\]

\[
= -\left(\frac{2s+1}{2s}\right)^{1/2} \left(\frac{n_{l-1,m+1}}{n_{lm}} \frac{1}{(2l+1)} [Y_{s-1,s-1}(M)]_{l-1,m+1;pq}
\right.
\]

\[
- \left. \frac{n_{l+1,m+1}}{n_{lm}} \frac{1}{(2l+1)} [Y_{s-1,s-1}(M)]_{l+1,m+1;pq} \right)
\]

\[
= -\left(\frac{2s+1}{2s}\right)^{1/2} \int \sin \theta \epsilon^p Y_{lm}(\theta,\phi) Y_{s-1,s-1}(\theta,\phi) Y^*_p(\theta,\phi) d\Omega
\]

\[
= \langle lm | Y_{st} | pq \rangle, \tag{4.3}
\]

where we have used a composition relation for spherical harmonics,\(^3\) and Eq. (4.2). The following step is to show that \([Y_{s+1,s}(M)]_{lm;pq} = \langle lm | Y_{s+1,s} | pq \rangle\) if Eq. (4.3) is valid. This step can be seen to follow from

\[
[Y_{s+1,s}(M)]_{lm;pq} = \sqrt{2s+3} \sum_{\rho,\sigma} M^\rho_{lm,po} [Y_{st}(M)]_{po;pq}, \tag{4.4}
\]

which is based on the relation: \(Y_{s+1,s}(\theta,\phi) = \sqrt{2s+3} \cos \theta Y_{st}(\theta,\phi)\). We do not present details, the proof is analogous to the one presented above. From the theory of spherical harmonics we also know

\[
Y_{s+1,s}(\theta,\phi) = \frac{(2s+1)}{(s-t+1)} \frac{n_{st}}{n_{s+1,t}} \cos \theta Y_{st}(\theta,\phi) - \frac{(s+t)}{(s-t+1)} \frac{n_{s-1,t}}{n_{s+1,t}} Y_{s-1,t}(\theta,\phi). \tag{4.5}
\]

If we can show the validity of an equivalent relation for \(Y_{s+1,s}(M)\) in terms of \(Y_{s-1,s}(M)\) and the product of \(M^0\) with \(Y_{st}(M)\), respectively, then we have proven Eq. (3.15) for \(t>0\). We want to emphasize that we use the method of induction, thus we assume that Eq. (3.15) is valid for \(Y_{st}(M)\) and \(Y_{s-1,s}(M)\). We have met this condition by proving Eqs. (4.1), (4.3), and (4.4). We proceed in the following way. With Eq. (3.6) we may write

\[
\sum_{\rho,\sigma} M^0_{lm,po} [Y_{st}(M)]_{po;pq} = \frac{n_{l-1,m}}{n_{lm}} \frac{(l+m)}{(2l+1)} [Y_{st}(M)]_{l-1,m;pq}
\]

\[
+ \frac{n_{l+1,m}}{n_{lm}} \frac{(l-m+1)}{(2l+1)} [Y_{st}(M)]_{l+1,m;pq}
\]

\[
= \int \cos \theta Y_{lm}(\theta,\phi) Y_{st}(\theta,\phi) Y^*_p(\theta,\phi) d\Omega, \tag{4.6}
\]

where Eq. (4.5) has been used. We have also used the equivalence between \([Y_{st}(M)]_{l\pm 1,m;pq}\) and \(\langle l\pm 1,m | Y_{st} | pq \rangle\). Then we substitute this expression into the matrix analog of Eq. (4.5)

\[
[Y_{s+1,s}(M)]_{lm;pq} = \frac{(2s+1)}{(s-t+1)} \frac{n_{st}}{n_{s+1,t}} \sum_{\rho,\sigma} M^\rho_{lm,po} [Y_{st}(M)]_{po;pq}
\]

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\[
\frac{(s+t)}{(t+1)} n_{s-1,t} \left[ Y_{s-1,t}(M) \right]_{lm,pq}
\]

\[
\frac{(2s+1)}{(s-t+1)} n_{st} \left( \langle lm | \cos \theta Y_{st} | pq \rangle - \frac{(s+t)}{(t+1)} n_{s-1,t} \langle lm | Y_{s-1,t} | pq \rangle \right)
\]

\[
= \int Y_{lm}(\theta,\varphi) Y_{s+1,t}(\theta,\varphi) Y_{pq}^*(\theta,\varphi) d\Omega. \tag{4.7}
\]

The last step is again application of Eq. (4.5). In the same way it is possible to prove Eq. (3.15) for \( t < 0 \).

The expression of the integral of the product of three spherical harmonics in terms of the components of the matrix \( Y_{st}(M) \) has some further implications. Consider the product of these matrices

\[
\sum_{\rho,\sigma} [ Y_{ab}(M) ]_{lm,\rho\sigma} [ Y_{st}(M) ]_{\rho\sigma,pq} = \int \int Y_{lm}(\theta,\varphi) Y_{ab}(\theta,\varphi)
\times \left( \sum_{\rho,\sigma} Y_{\rho\sigma}^*(\theta,\varphi) Y_{\rho\sigma}(\theta',\varphi') \right) Y_{st}(\theta',\varphi')
\times Y_{pq}^*(\theta',\varphi') d\Omega \ d\Omega'
\]

\[
= \int Y_{lm}(\theta,\varphi) Y_{ab}(\theta,\varphi) Y_{st}(\theta,\varphi) Y_{pq}^*(\theta,\varphi) d\Omega. \tag{4.8}
\]

where we have used \( \Sigma_{\rho,\sigma} Y_{\rho\sigma}^*(\theta,\varphi) Y_{\rho\sigma}(\theta',\varphi') = \delta(\Omega - \Omega') \). It is obvious that an integral of a product of \( N \) spherical harmonics can be expressed as a specific component of the matrix obtained by the product of \( N-2 \) matrices \( Y_{st}(M) \). In implicit notation Eq. (4.8) is nothing else than the application of the orthonormal projection operator \( \Sigma_{\rho,\sigma} | \rho\sigma \rangle \langle \rho\sigma | \), or

\[
\langle lm | Y_{ab} Y_{st} | pq \rangle = \sum_{\rho,\sigma} \langle lm | Y_{ab} | \rho\sigma \rangle \langle \rho\sigma | Y_{st} | pq \rangle. \tag{4.9}
\]

It should be noted that the derivation of Eqs. (3.15) and (4.8) cannot be directly generalized to include the so-called vector addition theorems.\(^{1,4}\)

V. CONCLUSION

In this article we have presented an alternative method to obtain addition theorems which seems easier to implement in numerical calculations because it is not necessary to introduce explicitly the 3-\( j \) symbols of Wigner. Furthermore we have been able to show a simple relation between products of the matrices \( Y(M) \) on the one hand, and the integral of a product of spherical harmonics, the so-called generalized form of Gaunt's integral, on the other hand. Also this expression and its possible applications are interesting topics for further exploration. It remains an open question how the presented method might be extended to the so-called vector addition theorems.\(^{1,4}\)

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