A simple derivation of the addition theorems of the irregular solid harmonics, the Helmholtz harmonics, and the modified Helmholtz harmonics

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In this article a simple derivation of the addition theorems of the irregular solid harmonics, the Helmholtz harmonics, and the modified Helmholtz harmonics is presented. Our derivation is based upon properties of the differential operator $\mathscr{Y}_l^m(\nabla)$, which is obtained from the regular solid harmonic $\mathscr{Y}_l^m(\mathbf{r})$ by replacing the Cartesian components of $\mathbf{r}$ by the Cartesian components of ∇. With the help of this differential operator $\mathscr{Y}_l^m(\nabla)$, which is an irreducible spherical tensor of rank l, the addition theorems of the anisotropic functions are obtained by differentiating the addition theorems of the isotropic functions. The performance of the necessary differentiations is greatly facilitated by a systematic exploitation of the tensorial nature of the differential operator $\mathscr{Y}_l^m(\nabla)$.

I. INTRODUCTION

In molecular and solid state physics, systems with more than one electron and with more than one atomic nucleus are treated. Consequently, it frequently happens that the eigenfunctions or operators which occur there have arguments that are given as sums or differences of two vectors that represent the coordinates of electrons and nuclei. Since quantum mechanical computational procedures usually involve integrations, the dependence of eigenfunctions and operators on the sum or difference of two vectors may be very inconvenient and it is often imperative to obtain a separation of variables, which can be achieved with the help of addition theorems. The probably best-known example of such an addition theorem is the Laplace expansion of the Coulomb potential in spherical coordinates,

$$\frac{1}{|\mathbf{r}-\mathbf{R}|} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{4\pi}{2l+1} \frac{r_<^l}{r_>^{l+1}} Y_l^{m*}\left(\frac{\mathbf{r}}{r}\right) Y_l^m\left(\frac{\mathbf{R}}{R}\right),$$
$$r_< = \min(r,R), \quad r_> = \max(r,R). \tag{1.1}$$

There is an extensive literature on addition theorems. Particularly well-studied are the addition theorems of those solutions of the homogeneous Laplace, Helmholtz, and modified Helmholtz equations that are also eigenstates of the orbital angular momentum operators. The addition theorems of the regular and irregular solid harmonics which are solutions of the homogeneous Laplace equation were studied by Hobson,[1] Rose,[2] Chiu,[3] Sack,[4,5] Dahl and Barnett,[6] Steinborn,[7] Steinborn and Ruedenberg[8] and by Tough and Stone.[9] The addition theorems of the Helmholtz harmonics which are products of Bessel functions and spherical harmonics were studied by Friedman and Russek,[10] Stein,[11] Cruzan,[12] Sack,[5] Danos and Maximon,[13] Nozawa,[14] and by Steinborn and Filter.[15] The addition theorems of the modified Helmholtz harmonics which are products of modified Bessel functions and spherical harmonics were studied by Buttle and Goldfarb[16] and by Steinborn and Filter.[15]

In the articles cited a multitude of different methods was used for the derivation of these addition theorems. Most of these approaches, however, are relatively complicated and sometimes rather lengthy and are based upon some special properties of the functions under consideration. Therefore, it is the intention of this article to demonstrate that the addition theorems of the irregular solid harmonics, the Helmholtz harmonics, and the modified Helmholtz harmonics can be derived in a very simple and unified way. Our method has the additional advantage that it can also be applied in the case of other functions.

Our derivation is based upon some special differential operator, which we call the spherical tensor gradient $\mathscr{Y}_l^m(\nabla)$. It is obtained from the regular solid harmonic $\mathscr{Y}_l^m(\mathbf{r})$ by replacing the Cartesian components of $\mathbf{r}$—x, y, and z—by the differentials $\partial/\partial x$, $\partial/\partial y$, and $\partial/\partial z$. The properties of the spherical tensor gradient, which was in principle already used by Hobson,[1] were investigated by Santos,[17] Rowe,[18] Bayman,[19] Stuart,[20] and recently by Níukkanen[21,22] and ourselves.[23,24] We shall show that there exists an intimate relationship between the spherical tensor gradient and irregular solid harmonics of (modified) Helmholtz harmonics, respectively, which can be employed profitably for the derivation of addition theorems.

II. DEFINITIONS

For the commonly occurring special functions of mathematical physics we shall use the notations and conventions of Magnus, Oberhettinger, and Soni[25] unless explicitly stated. Hereafter, this reference will be denoted as MOS in the text.

For the spherical harmonics $Y_l^m(\theta,\phi)$ we use the phase convention of Condon and Shortley,[26] i.e., they are defined by the expression

$$Y_l^m(\theta,\phi) = i^{m+|m|} \left[\frac{(2l+1)}{4\pi} \frac{(l-|m|)!}{(l+|m|)!}\right]^{1/2} \times P_l^{|m|}(\cos\theta) e^{im\phi}. \tag{2.1}$$

Here, $P_l^{|m|}(\cos\theta)$ is an associated Legendre polynomial

$$P_l^m(x) = (1-x^2)^{m/2} \frac{d^{l+m}}{dx^{l+m}} \frac{(x^2-1)^l}{2^l l!} = (1-x^2)^{m/2} \frac{d^m}{dx^m} P_l(x). \tag{2.2}$$

For the regular and irregular solid harmonics we use the notation

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$$\mathcal{Y}_l^m(\mathbf{r}) = r^l Y_l^m(\theta,\phi), \tag{2.3}$$

$$\mathcal{Z}_l^m(\mathbf{r}) = r^{-l-1} Y_l^m(\theta,\phi). \tag{2.4}$$

For the integral of the product of three spherical harmonics over the surface of the unit sphere in $\mathbb{R}^3$ we write

$$\langle l_3 m_3 | l_2 m_2 | l_1 m_1 \rangle = \int Y_{l_3}^{m_3 *}(\Omega) Y_{l_2}^{m_2}(\Omega) Y_{l_1}^{m_1}(\Omega) d\Omega. \tag{2.5}$$

These Gaunt coefficients may be expressed in terms of Clebsch–Gordan coefficients[27] or $3jm$ symbols

$$\langle l_3 m_3 | l_2 m_2 | l_1 m_1 \rangle = (-1)^{m_3} \left[\frac{(2l_1+1)(2l_2+1)(2l_3+1)}{4\pi} \right]^{1/2} \times \begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & -m_3 \end{pmatrix}. \tag{2.6}$$

With the help of the Gaunt coefficients the product of two spherical harmonics can be linearized

$$Y_{l_1}^{m_1}(\theta,\phi) Y_{l_2}^{m_2}(\theta,\phi) = \sum_{l=l_{\min}}^{l_{\max}}{}^{(2)} \langle l m_1 + m_2 | l_1 m_1 | l_2 m_2 \rangle Y_l^{m_1+m_2}(\theta,\phi). \tag{2.7}$$

The symbol $\Sigma^{(2)}$ indicates that the summation is to be performed in steps of two. The summation limits in Eq. (2.7) are direct conseqences of the selection rules satisfied by the Gaunt coefficient and are given by[28]

$$l_{\max} = l_1 + l_2, \tag{2.8a}$$

$$l_{\min} = \begin{cases} \max(|l_1 - l_2|, |m_1 + m_2|), \\ \quad \text{if } l_{\max} + \max(|l_1 - l_2|, |m_1 + m_2|) \text{ is even,} \\ \text{and} \\ \max(|l_1 - l_2|, |m_1 + m_2|) + 1, \\ \quad \text{if } l_{\max} + \max(|l_1 - l_2|, |m_1 + m_2|) \text{ is odd.} \end{cases} \tag{2.8b}$$

III. SOME PROPERTIES OF THE SPHERICAL TENSOR GRADIENT

In this section we shall review only those properties of the spherical tensor gradient $\mathcal{Y}_l^m(\nabla)$ which are needed for our derivation of the addition theorems of the irregular solid harmonics and the (modified) Helmholtz harmonics. Further properties can be found elsewhere.[17–24]

The spherical tensor gradient is an irreducible spherical tensor of rank l.[29] Therefore, if the spherical tensor gradient is applied to a function $\phi(r)$ which only depends upon the distance r, i.e., to an irreducible spherical tensor of rank zero, we obtain in agreement with the angular momentum coupling rules an irreducible spherical tensor of rank l, which is given by

$$\mathcal{Y}_l^m(\nabla)\phi(r) = \left[\left(\frac{1}{r} \frac{d}{dr} \right)^l \phi(r) \right] \mathcal{Y}_l^m(\mathbf{r}). \tag{3.1}$$

As we showed recently[30] this relationship can be derived quite easily with the help of a theorem on differentiation which was published by Hobson[31] already in 1892. Equation (3.1) can also be obtained by considering special cases in more recent publications by Santos,[32] Bayman,[33] Stuart,[34] and Niukkanen[35] who, however, apparently were not aware of Hobson's theorem.[31] If the spherical tensor gradient is applied to another spherical tensor of nonvanishing rank, i.e., to a function that can be written as

$$F_{l_2}^{m_2}(\mathbf{r}) = f_{l_2}(r) Y_{l_2}^{m_2}(\theta,\phi), \tag{3.2}$$

the structure of the resulting expression can also be understood in terms of angular momentum coupling,[36]

$$\mathcal{Y}_{l_1}^{m_1}(\nabla) F_{l_2}^{m_2}(\mathbf{r}) = \sum_{l=l_{\min}}^{l_{\max}}{}^{(2)} \langle l m_1 + m_2 | l_1 m_1 | l_2 m_2 \rangle \times \gamma_{l_1 l_2}^l(r) Y_l^{m_1+m_2}(\theta,\phi). \tag{3.3}$$

For the functions $\gamma_{l_1 l_2}^l$ in Eq. (3.3) various representations could be derived, for instance[37]

$$\gamma_{l_1 l_2}^l(r) = \sum_{q=0}^{\Delta l} \frac{(-\Delta l)_q (-\sigma(l) - \frac{1}{2})_q}{q!} 2^q r^{l_1 + l_2 - 2q} \times \left(\frac{1}{r} \frac{d}{dr} \right)^{l_1 - q} \frac{f_{l_2}(r)}{r^{l_2}} \tag{3.4}$$

$$= \sum_{s=0}^{\Delta l_2} \frac{(-\Delta l_2)_s (\Delta l_1 + \frac{1}{2})_s}{s!} 2^s r^{l_1 - l_2 - 2s - 1} \times \left(\frac{1}{r} \frac{d}{dr} \right)^{l_1 - s} r^{l_2 + 1} f_{l_2}(r), \tag{3.5}$$

$$\Delta l = (l_1 + l_2 - l)/2, \quad \Delta l_1 = (l - l_1 + l_2)/2,$$
$$\Delta l_2 = (l + l_1 - l_2)/2, \quad \sigma(l) = (l_1 + l_2 + l)/2. \tag{3.6}$$

It is a direct consequence of the selection rules satisfied by the Gaunt coefficient in Eq. (3.3) that $\Delta l, \Delta l_1, \Delta l_2$, and $\sigma(l)$ are always either positive integers or zero.

Since the spherical tensor gradient is obtained from the regular solid harmonic by replacing the Cartesian components of $\mathbf{r}$ by the Cartesian components of ∇ we may conclude that the spherical tensor gradient and the regular solid harmonics must obey the same coupling law. Hence we obtain from Eq. (2.7) (see Refs. 38 and 39)

$$\mathcal{Y}_{l_1}^{m_1}(\nabla) \mathcal{Y}_{l_2}^{m_2}(\nabla) = \sum_{l=l_{\min}}^{l_{\max}}{}^{(2)} \langle l m_1 + m_2 | l_1 m_1 | l_2 m_2 \rangle \times \nabla^{l_1 + l_2 - l} \mathcal{Y}_l^{m_1+m_2}(\nabla). \tag{3.7}$$

Let us now assume that a spherical tensor $F_{l_2}^{m_2}(\mathbf{r})$ and a radially symmetric function $\phi(r)$ are known, which satisfy

$$F_{l_2}^{m_2}(\mathbf{r}) = \mathcal{Y}_{l_2}^{m_2}(\nabla)\phi(r). \tag{3.8}$$

If the spherical tensor gradient $\mathcal{Y}_{l_1}^{m_1}(\nabla)$ is applied to $F_{l_2}^{m_2}(\mathbf{r})$ we then can couple the two spherical tensor gradients according to Eq. (3.7) and finally obtain with the help of Eq. (3.1)

$$\mathcal{Y}_{l_1}^{m_1}(\nabla) F_{l_2}^{m_2}(\mathbf{r}) = \mathcal{Y}_{l_1}^{m_1}(\nabla) \mathcal{Y}_{l_2}^{m_2}(\nabla)\phi(r) = \sum_{l=l_{\min}}^{l_{\max}}{}^{(2)} \langle l m_1 + m_2 | l_1 m_1 | l_2 m_2 \rangle \nabla^{l_1 + l_2 - l} \times \left[\left(\frac{1}{r} \frac{d}{dr} \right)^l \phi(r) \right] \mathcal{Y}_l^{m_1+m_2}(\mathbf{r}). \tag{3.9}$$

This relationship is particularly well-suited for the functions which are treated in this article since in these cases the differential operators which occur in Eq. (3.9) can be applied quite easily. Under these circumstances Eq. (3.9) is in our opinion preferable to other, more general expressions which were, for instance, given by Santos,[17] Niukkanen,[21] and ourselves.[24] Relationships of the type of Eq. (3.9) were already used by Novosadov[40] and ourselves[41] in connection with functions related to modified Bessel functions.

IV. THE ADDITION THEOREM OF THE IRREGULAR SOLID HARMONICS

Our derivation of the addition theorem of the irregular solid harmonics will be based upon the fact that the addition theorem of the Coulomb potential, Eq. (1.1), is known and that the application of the spherical tensor gradient to the Coulomb potential yields the irregular solid harmonic

$$\mathscr{Z}_l^m(\mathbf{r}) = [(-1)^l/(2l-1)!!]\,\mathscr{Y}_l^m(\nabla)(1/r). \tag{4.1}$$

This relationship, which was already known to Hobson,[1,31] can be proved quite easily with the help of Eq. (3.1). In order to facilitate the application of the spherical tensor gradient we rewrite the Laplace expansion of the Coulomb potential, Eq. (1.1), in the following way, which is more convenient for our purposes:

$$\frac{1}{|\mathbf{r}_< + \mathbf{r}_>|} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{(-1)^l}{2l+1} \mathscr{Y}_l^{m*}(\mathbf{r}_<)\mathscr{Z}_l^m(\mathbf{r}_>). \tag{4.2}$$

Here, $\mathbf{r}_<$ is the vector with the smaller magnitude and $\mathbf{r}_>$ is the vector with the greater magnitude.

The spherical tensor gradient is invariant with respect to translation. Consequently, Eq. (4.1) can be rewritten in the following ways:

$$\mathscr{Z}_l^m(\mathbf{r}_< + \mathbf{r}_>) = \frac{(-1)^l}{(2l-1)!!} \mathscr{Y}_l^m(\nabla_<) \frac{1}{|\mathbf{r}_< + \mathbf{r}_>|}, \tag{4.3}$$

$$= \frac{(-1)^l}{(2l-1)!!} \mathscr{Y}_l^m(\nabla_>) \frac{1}{|\mathbf{r}_< + \mathbf{r}_>|}. \tag{4.4}$$

Here, $\nabla_<$ implies a differentiation with respect to $\mathbf{r}_<$ and $\nabla_>$ implies a differentiation with respect to $\mathbf{r}_>$. If we combine Eqs. (4.2) and (4.4) we find

$$\mathscr{Z}_l^m(\mathbf{r}_< + \mathbf{r}_>) = \frac{(-1)^l 4\pi}{(2l-1)!!} \sum_{l_1=0}^{\infty} \sum_{m_1=-l_1}^{l_1} \frac{(-1)^{l_1}}{2l_1+1} \times \mathscr{Y}_{l_1}^{m_1*}(\mathbf{r}_<)\mathscr{Y}_l^m(\nabla_>)\mathscr{Z}_{l_1}^{m_1}(\mathbf{r}_>). \tag{4.5}$$

The remaining differentiation can be performed quite easily. The easiest way would be the use of Eqs. (3.8) and (3.9) in connection with Eq. (4.1). We then obtain

$$\mathscr{Y}_{\lambda_1}^{\mu_1}(\nabla)\mathscr{Z}_{\lambda_2}^{\mu_2}(\mathbf{r}) = (-1)^{\lambda_1} \sum_{\lambda=\lambda_{\min}}^{\lambda_{\max}}{}^{(2)} \frac{(2\lambda-1)!!}{(2\lambda_2-1)!!} \times \langle \lambda\mu_1+\mu_2|\lambda_1\mu_1|\lambda_2\mu_2\rangle \nabla^{\lambda_1+\lambda_2-\lambda} \mathscr{Z}_{\lambda}^{\mu_1+\mu_2}(\mathbf{r}). \tag{4.6}$$

If we take into account that the irregular solid harmonics are solutions of the homogeneous Laplace equation we see that in Eq. (4.6) only the term with $l = l_1 + l_2$ can be different from zero. This implies

$$\mathscr{Y}_{\lambda_1}^{\mu_1}(\nabla)\mathscr{Z}_{\lambda_2}^{\mu_2}(\mathbf{r}) = (-1)^{\lambda_1}(2\lambda_1+2\lambda_2-1)!!/(2\lambda_2-1)!! \times \langle \lambda_1+\lambda_2\mu_1+\mu_2|\lambda_1\mu_1|\lambda_2\mu_2\rangle \mathscr{Z}_{\lambda_1+\lambda_2}^{\mu_1+\mu_2}(\mathbf{r}). \tag{4.7}$$

Inserting this result into Eq. (4.5) yields the addition theorem for the irregular solid harmonics

$$\mathscr{Z}_l^m(\mathbf{r}_< + \mathbf{r}_>) = 4\pi \sum_{l_1=0}^{\infty} \sum_{m_1=-l_1}^{l_1} (-1)^{l_1} \frac{(2l+2l_1-1)!!}{(2l_1+1)!!(2l-1)!!} \times \langle l+l_1 m+m_1|lm|l_1m_1\rangle \mathscr{Y}_{l_1}^{m_1*}(\mathbf{r}_<)\mathscr{Z}_{l+l_1}^{m+m_1}(\mathbf{r}_>). \tag{4.8}$$

The Gaunt coefficient in Eq. (4.8) can be expressed in closed form. In that case one obtains the factorless form of the addition theorem which was given by Steinborn[7] and by Steinborn and Ruedenberg.[8]

If we now combine Eqs. (4.2) and (4.3) we find

$$\mathscr{Z}_l^m(\mathbf{r}_< + \mathbf{r}_>) = \frac{(-1)^l 4\pi}{(2l-1)!!} \sum_{l_1=0}^{\infty} \sum_{m_1=-l_1}^{l_1} \frac{(-1)^{l_1}}{2l_1+1} \times \mathscr{Y}_l^m(\nabla_<)\mathscr{Y}_{l_1}^{m_1*}(\mathbf{r}_<)\mathscr{Z}_{l_1}^{m_1}(\mathbf{r}_>). \tag{4.9}$$

The remaining differentiation again poses no problems. With the help of Eqs. (3.3) and (3.4) we obtain after some algebra

$$\mathscr{Y}_{\lambda_1}^{\mu_1}(\nabla)\mathscr{Y}_{\lambda_2}^{\mu_2}(\mathbf{r}) = \frac{(2\lambda_2+1)!!}{(2\lambda_2-2\lambda_1+1)!!} \langle \lambda_2-\lambda_1\mu_1+\mu_2|\lambda_1\mu_1|\lambda_2\mu_2\rangle \times \mathscr{Y}_{\lambda_2-\lambda_1}^{\mu_1+\mu_2}(\mathbf{r}). \tag{4.10}$$

If we insert this result into Eq. (4.9) we find another version of the addition theorem of the irregular solid harmonics

$$\mathscr{Z}_l^m(\mathbf{r}_< + \mathbf{r}_>) = 4\pi \sum_{l_1=l}^{\infty} \sum_{m_1=-l_1}^{l_1} \frac{(2l_1-1)!!}{(2l-1)!!(2l_1-2l+1)!!} \times \langle l_1m_1|lm|l_1-l m_1-m\rangle \times (-1)^{l_1+l} \mathscr{Y}_{l_1-l}^{m_1-m*}(\mathbf{r}_<)\mathscr{Z}_{l_1}^{m_1}(\mathbf{r}_>). \tag{4.11}$$

In order to prove the equivalence of Eqs. (4.8) and (4.11) we introduce new summation variables in Eq. (4.11)

$$l_2 = l_1 - l, \quad m_2 = m_1 - m. \tag{4.12}$$

With these definitions we find for Eq. (4.11)

$$\mathscr{Z}_l^m(\mathbf{r}_< + \mathbf{r}_>) = 4\pi \sum_{l_2=0}^{\infty} \sum_{m_2=-l_2}^{l_2} (-1)^{l_2} \frac{(2l+2l_2-1)!!}{(2l-1)!!(2l_2+1)!!} \times \langle l+l_2 m+m_2|lm|l_2m_2\rangle \mathscr{Y}_{l_2}^{m_2*}(\mathbf{r}_<)\mathscr{Z}_{l+l_2}^{m+m_2}(\mathbf{r}_>). \tag{4.13}$$

Obviously, Eqs. (4.8) and (4.13) are identical.

V. THE ADDITION THEOREMS OF THE HELMHOLTZ HARMONICS

In this section $C_\nu(z)$ stands for any of the Bessel functions $J_\nu(z)$ and $Y_\nu(z)$ or Hankel functions $H_\nu^{(1)}(z)$ and $H_\nu^{(2)}(z)$, which are defined by (MOS, pp. 65–66)

$$J_\nu(z) = \sum_{m=0}^{\infty} \frac{(-1)^m (z/2)^{\nu+2m}}{m!\,\Gamma(\nu+m+1)} = \frac{(z/2)^\nu}{\Gamma(\nu+1)}\, {}_0F_1\left(\nu+1; -\frac{z^2}{4}\right), \tag{5.1}$$

$$Y_\nu(z) = [1/\sin(\pi\nu)]\,[\cos(\pi\nu) J_\nu(z) - J_{-\nu}(z)], \tag{5.2}$$

$$H_\nu^{(1)}(z) = J_\nu(z) + iY_\nu(z), \tag{5.3}$$

$$H_\nu^{(2)}(z) = J_\nu(z) - iY_\nu(z). \tag{5.4}$$

This generalization is possible because for our derivation of the addition theorems we shall only need the following differential formulas and the recurrence relationship of these functions (MOS, p.67)

$$\left(\frac{1}{z}\frac{d}{dz}\right)^m z^\nu C_\nu(z) = z^{\nu-m} C_{\nu-m}(z), \tag{5.5}$$

$$\left(\frac{1}{z}\frac{d}{dz}\right)^m z^{-\nu} C_\nu(z) = (-1)^m z^{-\nu-m} C_{\nu+m}(z), \tag{5.6}$$

$$C_{\nu-1}(z) + C_{\nu+1}(z) = (2\nu/z) C_\nu(z). \tag{5.7}$$

With the help of these formulas the following relationships can be proved quite easily:

$$[1+\alpha^{-2}\nabla^2](\alpha r)^{-l-1/2} C_{l+1/2}(\alpha r)\mathcal{Y}_l^m(\alpha\mathbf{r}) = 0, \tag{5.8}$$

$$[1+\alpha^{-2}\nabla^2](\alpha r)^{-l-1/2} C_{-l-1/2}(\alpha r)\mathcal{Y}_l^m(\alpha\mathbf{r}) = 0. \tag{5.9}$$

The functions in Eqs. (5.8) and (5.9) are usually called Helmholtz harmonics. It seems that we have obtained two different classes of solutions of the homogeneous three-dimensional Helmholtz equation. However, in the case of half-integral orders $\nu = n + \frac{1}{2}$, $n \in \mathbb{Z}$, there exist symmetry relationships among Bessel functions, for instance (MOS, p. 72)

$$Y_{-n-1/2}(z) = (-1)^n J_{n+1/2}(z), \quad n \in \mathbb{N}. \tag{5.10}$$

Hence, if $C_{n+1/2}$ stands for one of the Bessel functions $J_{n+1/2}$, $Y_{n+1/2}$, $H_{n+1/2}^{(1)}$, and $H_{n+1/2}^{(2)}$, then $C_{-n-1/2}$ can also be expressed in terms of one of these functions. Consequently, it would in principle be sufficient to derive the addition theorems for either the functions in Eq. (5.8) or those in Eq. (5.9). However, since the derivation is in either case quite simple we shall derive the addition theorems for the functions in Eqs. (5.8) and (5.9) independently.

In Eqs. (5.5) and (5.6) the differential operator $z^{-1}\, d/dz$ acts as a kind of a shift operator for the order ν. Hence, if we combine Eq. (3.1) with either Eq. (5.5) or (5.6) we immediately find

$$(\alpha r)^\nu C_\nu(\alpha r)\mathcal{Y}_l^m(\alpha\mathbf{r}) = \alpha^{-l}\mathcal{Y}_l^m(\nabla)(\alpha r)^{\nu+l} C_{\nu+l}(\alpha r), \tag{5.11}$$

$$(\alpha r)^{-\nu} C_\nu(\alpha r)\mathcal{Y}_l^m(\alpha\mathbf{r}) = (-\alpha)^{-l}\mathcal{Y}_l^m(\nabla)(\alpha r)^{l-\nu} C_{\nu-l}(\alpha r). \tag{5.12}$$

Bessel and Hankel functions with orders $\nu = \pm\frac{1}{2}$ are essentially trigonometric functions, for instance (MOS, p. 73)

$$J_{1/2}(z) = [2/\pi z]^{1/2} \sin z. \tag{5.13}$$

Therefore, we see that the Helmholtz harmonics with higher angular momentum quantum numbers may be generated by applying the spherical tensor gradient to some trigonometric functions,

$$(\alpha r)^{-l-1/2} C_{-l-1/2}(\alpha r)\mathcal{Y}_l^m(\alpha\mathbf{r}) = \alpha^{-l}\mathcal{Y}_l^m(\nabla)(\alpha r)^{-1/2} C_{-1/2}(\alpha r), \tag{5.14}$$

$$(\alpha r)^{-l-1/2} C_{l+1/2}(\alpha r)\mathcal{Y}_l^m(\alpha\mathbf{r}) = (-\alpha)^{-l}\mathcal{Y}_l^m(\nabla)(\alpha r)^{-1/2} C_{1/2}(\alpha r). \tag{5.15}$$

These relationships suggest that the addition theorems of the Helmholtz harmonics can be derived in exactly the same way as we derived the addition theorem of the irregular solid harmonics in Sec. IV. We only have to apply the spherical tensor gradient to the addition theorems of the relatively simple functions $(\alpha r)^{-1/2} C_{\pm 1/2}(\alpha r)$, which are usually called Gegenbauer addition theorems (MOS, p. 107), and which can be compactly written as

$$(\alpha|\mathbf{r}_< + \mathbf{r}_>|)^{-1/2} C_{-1/2}(\alpha|\mathbf{r}_< + \mathbf{r}_>|) = (2\pi)^{3/2} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} (\alpha r_<)^{-l-1/2} J_{l+1/2}(\alpha r_<)\mathcal{Y}_l^{m*}(\alpha\mathbf{r}_<)(\alpha r_>)^{-l-1/2} C_{-l-1/2}(\alpha r_>)\mathcal{Y}_l^m(\alpha\mathbf{r}_>), \tag{5.16}$$

$$(\alpha|\mathbf{r}_< + \mathbf{r}_>|)^{-1/2} C_{1/2}(\alpha|\mathbf{r}_< + \mathbf{r}_>|) = (2\pi)^{3/2} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} (-1)^l (\alpha r_<)^{-l-1/2} J_{l+1/2}(\alpha r_<)\mathcal{Y}_l^{m*}(\alpha\mathbf{r}_<)(\alpha r_>)^{-l-1/2} C_{l+1/2}(\alpha r_>)\mathcal{Y}_l^m(\alpha\mathbf{r}_>). \tag{5.17}$$

Again, $\mathbf{r}_<$ is the vector with the smaller and $\mathbf{r}_>$ is the vector with the greater magnitude. Following our procedure in Sec. IV we differentiate Eq. (5.16) with respect to $\mathbf{r}_>$ and obtain with the help of Eq. (5.14)

$$\begin{aligned}(\alpha|\mathbf{r}_< + \mathbf{r}_>|)^{-l-1/2} C_{-l-1/2}(\alpha|\mathbf{r}_< + \mathbf{r}_>|)\mathcal{Y}_l^m(\alpha[\mathbf{r}_< + \mathbf{r}_>]) &= \alpha^{-l}\mathcal{Y}_l^m(\nabla_>)(\alpha|\mathbf{r}_< + \mathbf{r}_>|)^{-1/2} C_{-1/2}(\alpha|\mathbf{r}_< + \mathbf{r}_>|) \\ &= (2\pi)^{3/2} \sum_{l_1=0}^{\infty} \sum_{m_1=-l_1}^{l_1} (\alpha r_<)^{-l_1-1/2} J_{l_1+1/2}(\alpha r_<)\mathcal{Y}_{l_1}^{m_1*}(\alpha\mathbf{r}_<)\alpha^{-l}\mathcal{Y}_l^m(\nabla_>)(\alpha r_>)^{-l_1-1/2} C_{-l_1-1/2}(\alpha r_>)\mathcal{Y}_{l_1}^{m_1}(\alpha\mathbf{r}_>).\end{aligned} \tag{5.18}$$

The remaining differentiation can be done quite easily. With the help of Eqs. (3.8), (3.9), (5.8), and (5.14) we obtain immediately

$$\alpha^{-\lambda_1}\mathcal{Y}_{\lambda_1}^{\mu_1}(\nabla)(\alpha r)^{-\lambda_2-1/2} C_{-\lambda_2-1/2}(\alpha r)\mathcal{Y}_{\lambda_2}^{\mu_2}(\alpha\mathbf{r}) = \sum_{\lambda=\lambda_{\min}}^{\lambda_{\max}}{}^{(2)} (-1)^{\Delta\lambda} \langle \lambda\mu_1+\mu_2|\lambda_1\mu_1|\lambda_2\mu_2\rangle (\alpha r)^{-\lambda-1/2} C_{-\lambda-1/2}(\alpha r)\mathcal{Y}_\lambda^{\mu_1+\mu_2}(\alpha\mathbf{r}), \quad \Delta\lambda = (\lambda_1+\lambda_2-l)/2. \tag{5.19}$$

If we insert this relationship into Eq. (5.18) we obtain the addition theorem

$$(\alpha|\mathbf{r}_< + \mathbf{r}_>|)^{-l-1/2} C_{-l-1/2}(\alpha|\mathbf{r}_< + \mathbf{r}_>|)\mathscr{Y}_l^m(\alpha[\mathbf{r}_< + \mathbf{r}_>])$$

$$= (2\pi)^{3/2} \sum_{l_1=0}^{\infty} \sum_{m_1=-l_1}^{l_1} (\alpha r_<)^{-l-1/2} J_{l_1+1/2}(\alpha r_<) \mathscr{Y}_{l_1}^{m_1^*}(\alpha \mathbf{r}_<) \sum_{l_2=l_2^{\min}}^{l_2^{\max}} {}^{(2)} (-1)^{\Delta l_2}$$

$$\times \langle l_2 m + m_1 | l m | l_1 m_1 \rangle (\alpha r_>)^{-l_2-1/2} C_{-l_2-1/2}(\alpha r_>) \mathscr{Y}_{l_2}^{m+m_1}(\alpha \mathbf{r}_>), \quad \Delta l_2 = (l + l_1 - l_2)/2. \qquad (5.20)$$

This addition theorem can also be derived by differentiating Eq. (5.16) with respect to $\mathbf{r}_<$. We only need

$$(-\alpha)^{-\lambda_1} \mathscr{Y}_{\lambda_1}^{\mu_1}(\nabla)(\alpha r)^{-\lambda_2-1/2} C_{\lambda_2+1/2}(\alpha r) \mathscr{Y}_{\lambda_2}^{\mu_2}(\alpha \mathbf{r})$$

$$= \sum_{\lambda=\lambda_{\min}}^{\lambda_{\max}} {}^{(2)} (-1)^{\Delta\lambda} \langle \lambda \mu_1 + \mu_2 | \lambda_1 \mu_1 | \lambda_2 \mu_2 \rangle (\alpha r)^{-\lambda-1/2} C_{\lambda+1/2}(\alpha r) \mathscr{Y}_{\lambda}^{\mu_1+\mu_2}(\alpha \mathbf{r}), \quad \Delta\lambda = (\lambda_1 + \lambda_2 - \lambda)/2, \qquad (5.21)$$

which can be proved with the help of Eqs. (3.8), (3.9), (5.9), and (5.15) to obtain a somewhat different representation of the addition theorem,

$$(\alpha|\mathbf{r}_< + \mathbf{r}_>|)^{-l-1/2} C_{-l-1/2}(\alpha|\mathbf{r}_< + \mathbf{r}_>|)\mathscr{Y}_l^m(\alpha[\mathbf{r}_< + \mathbf{r}_>])$$

$$= (2\pi)^{3/2} \sum_{l_1=0}^{\infty} \sum_{m_1=-l_1}^{l_1} (\alpha r_>)^{-l_1-1/2} C_{-l_1-1/2}(\alpha r_>) \mathscr{Y}_{l_1}^{m_1}(\alpha \mathbf{r}_>) \sum_{l_2=l_2^{\min}}^{l_2^{\max}} {}^{(2)} (-1)^{\Delta l_1}$$

$$\times \langle l_1 m_1 | l m | l_2 m_1 - m \rangle (\alpha r_<)^{-l_2-1/2} J_{l_2+1/2}(\alpha r_<) \mathscr{Y}_{l_2}^{m_1-m^*}(\alpha \mathbf{r}_<), \quad \Delta l_1 = (l - l_1 + l_2)/2. \qquad (5.22)$$

To prove the equivalence of Eqs. (5.20) and (5.22) we only have to introduce in Eq. (5.22) the new summation variable $\mu_2 = m_1 - m$ and to change the order of the two l summations.

The addition theorem of the function $(\alpha r)^{-l-1/2} C_{l+1/2}(\alpha r)\mathscr{Y}_l^m(\alpha \mathbf{r})$ can be derived in exactly the same way. If we differentiate Eq. (5.17) with respect to $\mathbf{r}_>$ we find

$$(\alpha|\mathbf{r}_< + \mathbf{r}_>|)^{-l-1/2} C_{l+1/2}(\alpha|\mathbf{r}_< + \mathbf{r}_>|)\mathscr{Y}_l^m(\alpha[\mathbf{r}_< + \mathbf{r}_>])$$

$$= (2\pi)^{3/2} \sum_{l_1=0}^{\infty} \sum_{m_1=-l_1}^{l_1} (-1)^{l_1} (\alpha r_<)^{-l_1-1/2} J_{l_1+1/2}(\alpha r_<) \mathscr{Y}_{l_1}^{m_1^*}(\alpha \mathbf{r}_<)$$

$$\times \sum_{l_2=l_2^{\max}}^{l_2^{\min}} {}^{(2)} (-1)^{\Delta l_2} \langle l_2 m + m_1 | l m | l_1 m_1 \rangle (\alpha r_<)^{-l_2-1/2} C_{l_2+1/2}(\alpha r_>) \mathscr{Y}_{l_2}^{m+m_1}(\alpha \mathbf{r}_>), \quad \Delta l_2 = (l + l_1 - l_2)/2. \qquad (5.23)$$

If we differentiate Eq. (5.17) with respect to $\mathbf{r}_<$, we find

$$(\alpha|\mathbf{r}_< + \mathbf{r}_>|)^{-l-1/2} C_{l+1/2}(\alpha|\mathbf{r}_< + \mathbf{r}_>|)\mathscr{Y}_l^m(\alpha[\mathbf{r}_< + \mathbf{r}_>])$$

$$= (2\pi)^{3/2} \sum_{l_1=0}^{\infty} \sum_{m_1=-l_1}^{l_1} (-1)^{l_1} (\alpha r_>)^{-l_1-1/2} C_{l_1+1/2}(\alpha r_>) \mathscr{Y}_{l_1}^{m_1}(\alpha \mathbf{r}_>)$$

$$\times \sum_{l_2=l_2^{\min}}^{l_2^{\max}} {}^{(2)} (-1)^{\Delta l_2} \langle l_1 m_1 | l m | l_2 m - m_1 \rangle (\alpha r_<)^{-l_2-1/2} J_{l_2+1/2}(\alpha r_<) \mathscr{Y}_{l_2}^{m-m_1^*}(\alpha \mathbf{r}_<). \qquad (5.24)$$

The equivalence of Eqs. (5.23) and (5.24) can be proved by introducing the new summation variable $\mu_2 = m - m_1$ into (5.24) and by changing the order of the two l summations.

VI. THE ADDITION THEOREM OF THE MODIFIED HELMHOLTZ HARMONICS

The differential operator of the modified Helmholtz equation, $1 - \alpha^{-2}\nabla^2$, can be obtained from the differential operator of the Helmholtz equation, $1 + \alpha^{-2}\nabla^2$, if the parameter α is replaced by $i\alpha$. Consequently, the solutions of the homogeneous modified Helmholtz equations can be expressed in terms of modified Bessel functions. This follows also from the following relationships, which can be proved quite easily using known differential and recursive properties of the modified Bessel functions,

$$[1 - \alpha^{-2}\nabla^2](\alpha r)^{-l-1/2} I_{-l-1/2}(\alpha r)\mathscr{Y}_l^m(\alpha \mathbf{r}) = 0, \qquad (6.1)$$

$$[1 - \alpha^{-2}\nabla^2](\alpha r)^{-l-1/2} I_{l+1/2}(\alpha r)\mathscr{Y}_l^m(\alpha \mathbf{r}) = 0, \qquad (6.2)$$

$$[1 - \alpha^{-2}\nabla^2](\alpha r)^{-l-1/2} K_{l+1/2}(\alpha r)\mathscr{Y}_l^m(\alpha \mathbf{r}) = 0. \qquad (6.3)$$

Here, $I_\nu(z)$ is a modified Bessel function of the first kind (MOS, p. 66),

$$I_\nu(z) = \sum_{m=0}^{\infty} \frac{(z/2)^{\nu+2m}}{m!\Gamma(\nu+m+1)}$$
$$= \frac{(z/2)^\nu}{\Gamma(\nu+1)} {}_0F_1\left(\nu+1; \frac{z^2}{4}\right), \tag{6.4}$$

and $K_\nu(z)$ is a modified Bessel function of the second kind (MOS, p. 66),

$$K_\nu(z) = \pi/[2\sin(\pi\nu)][I_{-\nu}(z) - I_\nu(z)]. \tag{6.5}$$

The functions of the first kind, $I_\nu(z)$, increase exponentially for large arguments z whereas the functions of the second kind, $K_\nu(z)$, decline exponentially (MOS, p. 139). Consequently, it is not surprising that only the modified Helmholtz harmonics which occur in Eq. (6.3) have been of physical interest so far.

The modified Helmholtz harmonics in Eq. (6.3) may be considered to be some special B functions which are defined by[42]

$$B^m_{n,l}(\alpha,\mathbf{r}) = (2/\pi)^{1/2}/[2^{n+l}(n+l)!](\alpha r)^{n-1/2} \times K_{n-1/2}(\alpha r)\mathscr{Y}^m_l(\alpha\mathbf{r}). \tag{6.6}$$

Because of the factorial in the denominator, B functions are only defined in the sense of classical analysis if the inequality $n + l \geqslant 0$ holds. However, it can be shown that the definition of the B functions, Eq. (6.6), remains meaningful even if n is a negative integer such that $n + l < 0$ holds. In those cases B functions are distributions which can be identified with derivatives of the delta function.[24]

If B functions are used Eq. (6.3) can be rewritten as

$$[1 - \alpha^{-2}\nabla^2]B^m_{-l,l}(\alpha,\mathbf{r}) = 0. \tag{6.7}$$

If the spherical tensor gradient is applied to a scalar B function, one obtains[43]

$$B^m_{n,l}(\alpha,\mathbf{r}) = (4\pi)^{1/2}(-\alpha)^{-l}\mathscr{Y}^m_l(\nabla)B^0_{n+l,0}(\alpha,\mathbf{r}). \tag{6.8}$$

If we set in Eq. (6.8) $n = -l$ we find

$$B^m_{-l,l}(\alpha,\mathbf{r}) = (4\pi)^{1/2}(-\alpha)^{-l}\mathscr{Y}^m_l(\nabla)B^0_{0,0}(\alpha,\mathbf{r}). \tag{6.9}$$

However, the function $B^0_{0,0}$ is proportional to the Yukawa potential,

$$B^0_{0,0}(\alpha,\mathbf{r}) = (4\pi)^{-1/2}e^{-\alpha r}/(\alpha r), \tag{6.10}$$

for which an addition theorem is known (MOS, p. 107). We rewrite this addition theorem in the following way:

$$B^0_{0,0}(\alpha,\mathbf{r}_< + \mathbf{r}_>) = (2\pi^2)^{1/2}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}(-1)^l(\alpha r_<)^{-l-1/2} \times I_{l+1/2}(\alpha r_<)\mathscr{Y}^{m*}_l(\alpha\mathbf{r}_<)B^m_{-l,l}(\alpha,\mathbf{r}_>). \tag{6.11}$$

Again, $\mathbf{r}_<$ is the vector with the smaller and $\mathbf{r}_>$ is the vector with the greater magnitude.

The derivation of the addition theorems of the modified Helmholtz harmonics can now be done in exactly the same way as the derivation of the addition theorems of the irregular solid harmonics and of the Helmholtz harmonics. If we differentiate Eq. (6.11) with respect to $\mathbf{r}$, we find

$$B^m_{-l,l}(\alpha,\mathbf{r}_< + \mathbf{r}_>) = (4\pi)^{1/2}(-\alpha)^{-l}\mathscr{Y}^m_l(\nabla_>)B^0_{0,0}(\alpha,\mathbf{r}_< + \mathbf{r}_>)$$
$$= (2\pi)^{3/2}\sum_{l_1=0}^{\infty}\sum_{m_1=-l_1}^{l_1}(-1)^{l_1}(\alpha r_<)^{-l_1-1/2} \times I_{l_1+1/2}(\alpha r_<)\mathscr{Y}^{m_1*}_{l_1}(\alpha\mathbf{r}_<) \times (-\alpha)^{-l}\mathscr{Y}^m_l(\nabla_>)B^{m_1}_{-l_1,l_1}(\alpha,\mathbf{r}_>). \tag{6.12}$$

Now we only have to insert the relationship[44]

$$(-\alpha)^{\lambda_1}\mathscr{Y}^{\mu_1}_{\lambda_1}(\nabla)B^{\mu_2}_{-\lambda_2,\lambda_2}(\alpha,\mathbf{r}) = \sum_{\lambda=\lambda_{\min}}^{\lambda_{\max}}{}^{(2)}\langle\lambda\mu_1+\mu_2|\lambda_1\mu_1|\lambda_2\mu_2\rangle B^{\mu_1+\mu_2}_{-\lambda,\lambda}(\alpha,\mathbf{r}) \tag{6.13}$$

into Eq. (6.12) to obtain the addition theorem of the modified Helmholtz harmonics,

$$B^m_{-l,l}(\alpha,\mathbf{r}_< + \mathbf{r}_>) = (2\pi)^{3/2}\sum_{l_1=0}^{\infty}\sum_{m_1=-l_1}^{l_1}(-1)^{l_1}(\alpha r_<)^{-l_1-1/2} \times I_{l_1+1/2}(\alpha r_<)\mathscr{Y}^{m_1*}_{l_1}(\alpha\mathbf{r}_<) \times \sum_{l_2=l_2^{\min}}^{l_2^{\max}}{}^{(2)}\langle l_2 m+m_1|lm|l_1m_1\rangle \times B^{m+m_1}_{-l_2,l_2}(\alpha,\mathbf{r}_>). \tag{6.14}$$

This addition theorem can also be derived by differentiating Eq. (6.11) with respect to $\mathbf{r}_<$. We then obtain

$$B^m_{-l,l}(\alpha,\mathbf{r}_< + \mathbf{r}_>) = (4\pi)^{1/2}(-\alpha)^{-l}\mathscr{Y}^m_l(\nabla_<)B^0_{0,0}(\alpha,\mathbf{r}_< + \mathbf{r}_>)$$
$$= (2\pi)^{3/2}\sum_{l_1=0}^{\infty}\sum_{m_1=-l_1}^{l_1}(-1)^{l_1}(-\alpha)^{-l} \times \mathscr{Y}^m_l(\nabla_<)(\alpha r_<)^{-l_1-1/2}I_{l_1+1/2}(\alpha r_<)\mathscr{Y}^{m_1*}_{l_1}(\alpha\mathbf{r}_<) \times B^{m_1}_{-l_1,l_1}(\alpha,\mathbf{r}_>). \tag{6.15}$$

To perform the remaining differentiation we use (MOS, p. 67)

$$\left(\frac{1}{z}\frac{d}{dz}\right)^m z^{-\nu}I_\nu(z) = z^{-\nu-m}I_{\nu+m}(z) \tag{6.16}$$

in connection with Eq. (3.1) to obtain

$$(\alpha r)^{-l-1/2}I_{l+1/2}(\alpha r)\mathscr{Y}^m_l(\alpha\mathbf{r}) = \alpha^{-l}\mathscr{Y}^m_l(\nabla)(\alpha r)^{-1/2}I_{1/2}(\alpha r). \tag{6.17}$$

If we now combine Eqs. (3.9), (6.2), and (6.17) we find

$$\alpha^{-\lambda_1}\mathscr{Y}^{\mu_1}_{\lambda_1}(\nabla)(\alpha r)^{-\lambda_2-1/2}I_{\lambda_2+1/2}(\alpha r)\mathscr{Y}^{\mu_2}_{\lambda_2}(\alpha\mathbf{r}) = \sum_{\lambda=\lambda_{\min}}^{\lambda_{\max}}{}^{(2)}\langle\lambda\mu_1+\mu_2|\lambda_1\mu_1|\lambda_2\mu_2\rangle(\alpha r)^{-\lambda-1/2} \times I_{\lambda+1/2}(\alpha r)\mathscr{Y}^{\mu_1+\mu_2}_\lambda(\alpha\mathbf{r}). \tag{6.18}$$

If we insert this result into Eq. (6.15) we obtain a somewhat different representation of the addition theorem of the modified Helmholtz harmonics,

$$B^m_{-l,l}(\alpha,\mathbf{r}_< + \mathbf{r}_>) = (2\pi)^{3/2}\sum_{l_1=0}^{\infty}\sum_{m_1=-l_1}^{l_1}B^{m_1}_{-l_1,l_1}(\alpha,\mathbf{r}_>) \times \sum_{l_2=l_2^{\min}}^{l_2^{\max}}{}^{(2)Y}(-1)^{l_2}\langle l_1m_1|lm|l_2m_1-m\rangle \times(\alpha r_<)^{-l_2-1/2}I_{l_2+1/2}(\alpha r_<)\mathscr{Y}^{m_1-m*}_{l_2}(\alpha\mathbf{r}_<). \tag{6.19}$$

To prove the equivalence of Eqs. (6.14) and (6.19) we only have to introduce the new summation variable $\mu_2 = m_1 - m$

into Eq. (6.19) and to change the order of the two l summations.

VII. SUMMARY AND CONCLUSIONS

In this article simple and unified derivations of the addition theorems of the irregular solid harmonics, the Helmholtz harmonics, and the modified Helmholtz harmonics are presented. Our derivations are based upon differential relationships of the following type:

$$F_l^m(\mathbf{r}) = \mathcal{Y}_l^m(\nabla)\phi(r). \tag{7.1}$$

Here, $F_l^m(\mathbf{r})$ is an irreducible spherical tensor, $\phi(r)$ is a function that only depends upon the distance r, i.e., a spherical tensor of rank zero, and $\mathcal{Y}_l^m(\nabla)$ is the spherical tensor gradient which is obtained from the regular solid harmonic $\mathcal{Y}_l^m(\mathbf{r})$ by replacing the Cartesian components of $\mathbf{r}$ by the Cartesian components of ∇.

The differential relationship (7.1) assumes a particularly simple form for the functions under consideration because in these cases the application of the spherical tensor gradient merely leads to a shift of angular momentum quantum numbers. If the spherical tensor gradient $\mathcal{Y}_l^m(\nabla)$ acts upon the Coulomb potential which is the irregular solid harmonic of rank zero we obtain $\mathcal{Z}_l^m(\mathbf{r})$. In the same way we obtain the (modified) Helmholtz harmonics of rank l by differentiating the (modified) Helmholtz harmonics of rank zero.

The remarkable differential properties of the irregular solid harmonics and the (modified) Helmholtz harmonics can be employed profitably for the derivation of addition theorems. We simply have to apply the spherical tensor gradient to the addition theorems of the Coulomb potential or the (modified) Helmholtz harmonics of rank zero and obtain the addition theorems of the anisotropic functions.

The idea of applying differentiation methods for the derivation of addition theorems is not at all new. Methods that are in some sense equivalent or closely related to our method, which is based upon the spherical tensor gradient and its tensor character, have already been employed by Hobson,[1] Rose,[2] Chiu,[3] Dahl and Barnett,[6] Steinborn and Ruedenberg,[8] Tough and Stone,[9] and Nozawa.[14] However, in the references cited the differential operators were applied in their Cartesian form and the tensorial nature of the differential operators was not exploited systematically. The direct application of differential operators, which involve differentiations with respect to x, y, and z to irreducible spherical tensors, leads to relatively complicated and sometimes rather messy expressions which cannot be manipulated easily. In our approach we utilize the fact that the application of the spherical tensor gradient to an irreducible spherical tensor leads to an angular momentum coupling. Therefore, only differentiations with respect to the radial variable r have to be done. It is the systematic exploitation of the tensor character of the differential operator $\mathcal{Y}_l^m(\nabla)$ which makes our derivation of the addition theorems almost trivial.

It should be noted that our method for the derivation of the addition theorem of an anisotropic function is not restricted to irregular solid harmonics and (modified) Helmholtz harmonics. If the addition theorem of an isotropic function $\phi(r)$ is known one only has to apply the spherical tensor gradient $\mathcal{Y}_l^m(\nabla)$ to it. According to Eq. (7.1) one then obtains the addition theorem of the anisotropic function $F_l^m(\mathbf{r})$.

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