Addition Theorems as Three-Dimensional Taylor Expansions.
II. $B$ Functions and Other Exponentially Decaying Functions

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Abstract
Addition theorems can be constructed by doing three-dimensional Taylor expansions according to $f(r + r') = \exp(r' \cdot \nabla)f(r)$. Since, however, one is normally interested in addition theorems of irreducible spherical tensors, the application of the translation operator in its Cartesian form $\exp(x'\partial/\partial x)\exp(y'\partial/\partial y)\exp(z'\partial/\partial z)$ would lead to enormous technical problems. A better alternative consists in using a series expansion for the translation operator $\exp(r' \cdot \nabla)$ involving powers of the Laplacian $\nabla^2$ and spherical tensor gradient operators $Y^m_\ell(r)$, which are irreducible spherical tensors of ranks zero and $\ell$, respectively [F.D. Santos, Nucl. Phys. A 212, 341 (1973)]. In this way, it is indeed possible to derive addition theorems by doing three-dimensional Taylor expansions [E.J. Weniger, Int. J. Quantum Chem. 76, 280 (2000)]. The application of the translation operator in its spherical form is particularly simple in the case of $B$ functions and leads to an addition theorem with a comparatively compact structure. Since other exponentially decaying functions like Slater-type functions, bound-state hydrogenic eigenfunctions, and other functions based on generalized Laguerre polynomials can be expressed by simple finite sums of $B$ functions, the addition theorems for these functions can be written down immediately.

1 Introduction

In many branches of physics and physical chemistry – for example in electrodynamics [1], in classical field theory [2], or in the theory of intermolecular forces [3] – an essential step towards a solution of the problem under consideration consists in a separation of the variables.

Principal tools, which can accomplish such a separation of variables, are addition theorems: These are expansions of a given function $f(r + r')$ with $r, r' \in \mathbb{R}^3$ in terms of other functions that only depend on either $r$ or $r'$.

In atomic and molecular calculations, one is usually interested in irreducible spherical tensors which can be partitioned into a radial part and an angular part that is given by a spherical harmonic:

$$F^m_\ell(r) = f_\ell(r)Y^m_\ell(r/r).$$

Thus, the function $f(r + r')$, which is to be expanded, as well as the functions, that only depend on either $r$ or $r'$, should be irreducible spherical...
tensors.

The best known example of such an addition theorem is the Laplace expansion of the Coulomb potential in terms of spherical harmonics:

\[
\frac{1}{|r-r'|} = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{4\pi}{2\ell+1} Y_\ell^m(\mathbf{r}_< / \mathbf{r}_>) Y_\ell^m(\mathbf{r}_> / \mathbf{r}_>) \times \frac{r_\ell}{r_{\ell+1}}, \quad r_< = \min(r, r') \quad r_> = \max(r, r').
\]

(1.2)

The Laplace expansion leads to a separation of the variables \(r\) and \(r'\). However, the right-hand side of this expansion depends on \(r\) and \(r'\) only indirectly via the vectors \(\mathbf{r}_<\) and \(\mathbf{r}_>\) which satisfy \(|\mathbf{r}_<| < |\mathbf{r}_>\). Hence, the Laplace expansion has a two-range form, depending on the relative size of \(r\) and \(r'\). This is a complication which occurs frequently among addition theorems.

There is an extensive literature on addition theorems. Since addition theorems can be viewed as expansions in terms of spherical harmonics with arguments \(r/r\) and \(r'/r'\), they are often treated in books on angular momentum theory or on related topics (see for example pp. 163 - 169 of [1] or Appendix H.4 of [5]).

Particularly well studied are the addition theorems of the solutions of the homogeneous Laplace equation, of the homogeneous Helmholtz equation, and of the homogeneous modified Helmholtz equation. This large number of references does not only reflect the importance of these functions, but also the relative ease with which their addition theorems can be derived. The derivation of addition theorems for other functions, which are not solutions of the equations listed above, is according to experience significantly more difficult.

In the context of atomic and molecular electronic structure calculations, addition theorems have traditionally been used for the separation of the variables of interelectronic repulsion integrals and of other multicenter integrals. For that purpose, one also needs addition theorems for the so-called basis functions. Probably the oldest attempt is the zeta function method of Barnett and Coulson [31] which tries to obtain addition theorems for exponentially decaying functions by applying suitable generating differential operators to the well-known addition theorem of the Yukawa potential \(e^{-\alpha r}/r\). In the case of Slater-type functions, this approach did not lead to a complete success: It was not possible to do the differentiations in closed form, and the coefficients occurring in the zeta function expansion had to be computed recursively [32].

Another general method for the derivation of addition theorems is the alpha function method, which was introduced by Per-Olof Löwdin in his seminal paper on the quantum theory of cohesive properties of solids [33], and which was later used and extended by numerous other authors [34 - 50].

In 1967, Ruedenberg [31] and Silverstone [32] suggested independently to derive addition theorems via Fourier transformation. If the function \(f(r \pm r')\) is an irreducible spherical tensor of the type of (1.1), then the angular integrations can be done in closed form, and there only remain some radial integrals in momentum space containing two spherical Bessel functions (see for example Eq. (7.5) of [53]). Unfortunately, these integrals can be very difficult. There is the additional complication that even if explicit expressions for these integrals can be found, the radial variables \(r\) and \(r'\) need not be separated in the final result. Thus, the success of this approach depends crucially upon one’s ability of handling complicated integrals containing products of spherical Bessel functions.

Addition theorems can be defined as three-dimensional Taylor expansions (see for example p. 181 of [54]):

\[
f(r + r') = \sum_{n=0}^{\infty} \frac{\left(r' \cdot \nabla\right)^n}{n!} f(r)
\]

(1.3)

Thus, the translation operator \(e^{r' \cdot \nabla}\) generates \(f(r + r')\) by doing a three-dimensional Taylor expansion of \(f\) around \(r\).

From a practical point of view, three-dimensional Taylor expansions do not seem to be
very useful for the derivation of addition theorems. In atomic and molecular physics, one is usually interested in addition theorems of irreducible spherical tensors of the type of \((1.1)\) which are defined in terms of spherical polar coordinates \(r, \theta,\) and \(\phi.\) Accordingly, differentiations with respect to the Cartesian components \(x, y,\) and \(z\) of \(r\) would lead to extremely messy expressions. Moreover, it is highly desirable to express the angular part of the addition theorem in terms of the spherical harmonics \(Y_{\ell_m}^m(r/r)\) and \(Y_{\ell_n}^{m_n}(r'/r').\) Thus, any attempt to derive an addition theorem for an irreducible spherical tensor via a straightforward application of the translation operator in its Cartesian form \(e^{x^2/\partial x}e^{y^2/\partial y}e^{z^2/\partial z}\) would lead to enormous technical problems.

Nevertheless, it is not only possible to obtain addition theorems via three-dimensional Taylor expansions, but this approach may even be the most natural and the most widely applicable technique \([55]\). This is accomplished by expanding the translation operator \(e^{r \cdot \nabla}\) in terms of differential operators that are irreducible spherical tensors. Then, the angular part of the addition theorem is obtained via angular momentum coupling, and only radial differentiations have to be done explicitly. Obviously, this leads to a significant simplification \([55]\).

In \([55]\), it was shown how the Laplace expansion \((1.4)\) of the Coulomb potential and the addition theorems of the regular and irregular solid harmonics and of the Yukawa potential \(e^{-\alpha r}/r\) can be derived by applying the translation operator in its spherical form. Of course, these addition theorems are all comparatively simple, and they do not necessarily provide convincing evidence that the Taylor expansion method is indeed a useful tool for the derivation of more complicated addition theorems. However, on p. 293 of \([55]\), it was emphasized that this method had been applied successfully also in the case of other functions of physical interest. Thus, it is the intention of this article to provide some evidence that these claims are indeed true (further articles on additions theorems are in preparation \([54]\)). Moreover, in \([57]\) the addition theorem of the so-called spherical Laguerre Gaussian functions was derived by applying the techniques described in \([55]\).

Currently, the vast majority of molecular electronic structure calculations use Gaussian basis functions although these functions are neither able to reproduce the cusps \([58]\) of the exact solutions of molecular Schrödinger equations at the nuclei nor their exponential decay \([59, 60]\). The only, but nevertheless decisive advantage of Gaussian functions has been the relative ease, with which the molecular multicenter integrals can be computed. Nevertheless, there are still many researchers who hope that ultimately the unphysical Gaussian functions can be replaced by the physically better motivated exponentially decaying functions and who are doing research in this direction. Accordingly, there is a large number of recent articles on molecular multicenter integrals of exponentially decaying functions \([31, 38]\).

So far, Slater-type functions \([33]\) have been the most important and most widely used exponentially decaying basis functions in atomic, molecular, and solid state calculations. Unfortunately, the molecular multicenter integrals of Slater-type functions are notoriously difficult, and so is its addition theorem which can be used for the separation of variables in multicenter integrals. Over the years, a large variety of different techniques were used for the construction of addition theorems for Slater-type functions \([31, 38, 39, 42, 52, 54, 71]\), and most likely there is still room for improvements.

The topic of this article is not the derivation of addition theorems for Slater-type functions but for another class of exponentially decaying functions, the so-called \(B\) functions \([54]\). At first sight, this may look surprising since \(B\) functions have a comparatively complicated mathematical structure, and it is by no means obvious that anything can be gained by considering \(B\) functions instead of the apparently much simpler Slater-type functions. However, \(B\) functions have some remarkable mathematical properties which give them a unique position among exponentially decaying functions and make them especially useful for molecular calculations. Due to these advan-
tageous properties it is not only relatively easy to derive an addition theorem with the help of three-dimensional Taylor expansions as described in [53], but the addition theorems for \( B \) functions also have comparatively simple structures [83].

Moreover, all the commonly used exponentially declining functions as for example Slater-type functions or bound-state hydrogenic eigenfunctions can be expressed as simple finite sums of \( B \) functions (see for example Section III of [93] and references therein). These advantageous features have led to a considerable amount of recent research on \( B \) functions and their multicenter integrals [24, 65, 81, 87, 88].

Addition theorems for \( B \) functions have already been derived in [83] by applying techniques that closely resemble the zeta function method of Barnett and Coulson [31]. So, the emphasis of this article is not so much on the derivation of new results but on the discussion of methodological questions related to the application of the translation operator in its spherical form to exponentially decaying functions.

In Section 2, the definitions and conventions used in this article are listed. In Section 3, the expansion of the translation operator in terms of irreducible spherical tensors is reviewed, and the properties of the differential operator \( \mathcal{Y}_m^m(\nabla) \), which is the key quantity in this expansion, are discussed. Section 4 covers \( B \) functions and their mathematical properties, and in Section 5, an addition theorem for \( B \) functions is derived by doing a three-dimensional Taylor expansion. Finally, in Section 6 there is a short discussion of the results presented in this article.

### 2 Definitions

For the commonly occurring special functions of mathematical physics we use the notation of Magnus, Oberhettinger, and Soni [94] unless explicitly stated.

For the set of positive and negative integers, we write \( \mathbb{Z} = \{0, \pm 1, \pm 2, \ldots \} \), for the set of positive integers, we write \( \mathbb{N} = \{1, 2, 3, \ldots \} \), and for the set of non-negative integers, we write \( \mathbb{N}_0 = \{0, 1, 2, \ldots \} \). The real numbers are denoted by \( \mathbb{R} \), and for the set of three-dimensional vectors with real components we write \( \mathbb{R}^3 \).

For the spherical harmonics \( Y_{\ell}^m(\theta, \phi) \), we use the phase convention of Condon and Shortley [95], i.e., they are defined by (p. 69 of [54])

\[
Y_{\ell}^m(\theta, \phi) = \frac{i^{m+|m|}}{4\pi(\ell + |m|)!} \times P_{\ell}^{|m|}(\cos \theta) e^{im\phi}.
\] (2.1)

Here, \( P_{\ell}^{|m|}(\cos \theta) \) is an associated Legendre polynomial (p. 155 of [93]):

\[
P_{\ell}^{|m|}(x) = (1 - x^2)^{m/2} \frac{d^{\ell+m} (x^2 - 1)^{\ell}}{2^{\ell} \ell!} = (1 - x^2)^{m/2} \frac{d^m}{dx^m} P_\ell(x).
\] (2.2)

Under complex conjugation, the spherical harmonics satisfy (p. 69 of [54]):

\[
[Y_{\ell}^m(\theta, \phi)]^* = (-1)^m Y_{\ell}^{-m}(\theta, \phi).
\] (2.3)

For the regular solid harmonics, which is a solution of the homogeneous Laplace equation, we write:

\[
\mathcal{Y}_m^m(\mathbf{r}) = r^\ell \mathcal{Y}_m^m(\theta, \phi).
\] (2.4)

The regular solid harmonic is a homogeneous polynomial of degree \( \ell \) in the Cartesian components \( x, y, \) and \( z \) of \( \mathbf{r} \) (p. 71 of [54]):

\[
\mathcal{Y}_m^m(\mathbf{r}) = \frac{[(2\ell + 1)(\ell + m)!(\ell - m)!]^{1/2}}{4\pi} \times \sum_{k \geq 0} \frac{(-ix - iy)^{m+k}(x - iy)^{z}(\ell - m - 2k)}{2^{m+2k}(m + k)!k!(\ell - m - 2k)!}.
\] (2.5)

This formula holds for the Cartesian components of an arbitrary three-dimensional vector. Consequently, it can be used to define the differential operator \( \mathcal{Y}_m^m(\nabla) \) by replacing in (2.3) the Cartesian components \( \partial/\partial x, \partial/\partial y, \) and \( \partial/\partial z \) of \( \nabla \).
For the integral of the product of three spherical harmonics over the surface of the unit sphere in \( \mathbb{R}^3 \), the so-called Gaunt coefficient [97], we write

\[
\langle \ell_3 m_3 | \ell_2 m_2 | \ell_1 m_1 \rangle = \int \left[ Y_{\ell_3}^{m_3} (\Omega) \right]^* Y_{\ell_2}^{m_2} (\Omega) Y_{\ell_1}^{m_1} (\Omega) \, d\Omega . \tag{2.6}
\]

The Gaunt coefficient can be expressed in terms of \( 3jm \) symbols (see for example p. 168 of [96]):

\[
\langle \ell_3 m_3 | \ell_2 m_2 | \ell_1 m_1 \rangle = (-1)^{m_3} \frac{(2\ell_1+1)(2\ell_2+1)(2\ell_3+1)}{4\pi} \times \left( \begin{array}{ccc}
\ell_1 & \ell_2 & \ell_3 \\
0 & 0 & 0
\end{array} \right) \left( \begin{array}{ccc}
\ell_1 & \ell_2 & \ell_3 \\
m_1 & m_2 & -m_3
\end{array} \right). \tag{2.7}
\]

It follows from the orthonormality of the spherical harmonics that the Gaunt coefficients linearize the product of two spherical harmonics:

\[
Y_{\ell_1}^{m_1} (\Omega) Y_{\ell_2}^{m_2} (\Omega) = \sum_{\ell=\ell_{\text{min}}}^{\ell_{\text{max}}} \langle \ell m_1 + m_2 | \ell_1 m_1 | \ell_2 m_2 \rangle Y_{\ell}^{m_1 + m_2} (\Omega). \tag{2.8}
\]

The symbol \( \sum^{(2)} \) indicates that the summation proceeds in steps of two. The summation limits given in (2.8), which follow from the selection rules satisfied by the \( 3jm \) symbols, are given by [98]

\[
\ell_{\text{max}} = \ell_1 + \ell_2 \quad \text{and} \quad \ell_{\text{min}} = \begin{cases}
\lambda_{\text{min}}, & \text{if } \ell_{\text{max}} + \lambda_{\text{min}} \text{ is even}, \\
\lambda_{\text{min}} + 1, & \text{if } \ell_{\text{max}} + \lambda_{\text{min}} \text{ is odd},
\end{cases} \tag{2.9}
\]

where

\[
\lambda_{\text{min}} = \max(|\ell_1 - \ell_2|, m_1 + m_2). \tag{2.10}
\]

It may be of interest to note that several articles on Gaunt coefficients have appeared recently [99] [104].

In the sequel, the following abbreviations will be used:

\[
\Delta \ell = (\ell_1 + \ell_2 - \ell)/2, \tag{2.11}
\]

\[
\Delta \ell_1 = (\ell - \ell_1 - \ell_2)/2, \tag{2.12}
\]

\[
\Delta \ell_2 = (\ell + \ell_1 - \ell_2)/2, \tag{2.13}
\]

\[
\sigma (\ell) = (\ell_1 + \ell_2 + \ell)/2. \tag{2.14}
\]

If the three orbital angular momentum quantum numbers \( \ell_1, \ell_2, \) and \( \ell \) satisfy the summation limits (2.9), then these quantities are always positive integers or zero.

### 3 The Translation Operator in Spherical Form

In this Section, the expansion of the translation operator \( e^{r \cdot \nabla} \) in terms of irreducible spherical tensors will be reviewed. Moreover, the for our purposes most important properties of the differential operator \( Y_{\ell}^{m} (\nabla) \), which is the key quantity in the expansion mentioned above, will be discussed shortly. Additional details be found in Sections 3 and 4 of [53].

If we want to derive an addition theorem for some function \( f \) by applying the translation operator according to (1.3), \( f \) has to be analytic at the expansion point \( r \) as well as at the shifted argument \( r + r' \). Consequently, (1.3) is in general not symmetric with respect to an interchange of \( r \) and \( r' \). Thus, if the three-dimensional Taylor expansion (1.3) converges, it is in general not possible to expand \( f \) around \( r' \) and use \( r \) as the shift vector according to

\[
f(r + r') = \sum_{n=0}^{\infty} \frac{(r \cdot \nabla')^n}{n!} f(r')
\]

\[
= e^{r \cdot \nabla'} f(r'), \tag{3.1}
\]

The reason is that (1.3) and (3.1) can only hold simultaneously for essentially arbitrary vectors \( r, r' \in \mathbb{R}^3 \) if \( f \) is analytic at \( r, r', \) and at \( r + r' \). However, most functions, that are of interest in
the context of atomic and molecular quantum mechanics, are either singular at the origin or are not analytic at the origin. Obvious examples are the Coulomb potential, which is singular at the origin, or the 1s hydrogen eigenfunction, which possesses a cusp at the origin \([B^{38}]\). In fact, all the commonly used exponentially decaying functions as for example Slater-type functions or also \(B\) functions are not analytic at the origin.

The reason for the non-analyticity is that the three-dimensional distance \(r = [x^2 + y^2 + z^2]^{1/2}\) is not analytic with respect to \(x, y,\) and \(z\) at the origin \(r = 0\). In contrast, \(r^2 = x^2 + y^2 + z^2\) and the regular solid harmonic \(Y_n^m(\mathbf{r})\) are analytic since they are polynomial in \(x, y,\) and \(z\). Consequently, a 1s Gaussian function \(\exp(-\alpha r^2)\) is analytic at \(r = 0\), but a 1s Slater-type function \(\exp(-\alpha r)\) is not.

Thus, for the derivation of addition theorems for \(B\) functions, which are not analytic at the origin, we have to use the translation operator in the following form,

\[
f(\mathbf{r}_< + \mathbf{r}_>) = \sum_{n=0}^{\infty} \frac{(\mathbf{r}_< \cdot \nabla_>)^n}{n!} f(\mathbf{r}_>) = e^{\mathbf{r}_< \cdot \nabla_>} f(\mathbf{r}_>) , \tag{3.2}
\]

where \(0 \leq |\mathbf{r}_<| < |\mathbf{r}_>|\). In this way, the convergence of the Taylor expansion is guaranteed provided that \(f\) is analytical everywhere except at the origin. Thus, the non-analyticity at the origin explains why \(B\) functions as well as all the other commonly occurring exponentially decaying functions have addition theorems with a two-range form of the type of the Laplace expansion \([12]\) of the Coulomb potential.

The crucial step, which ultimately makes the Taylor expansion method practically useful, is the expansion of the translation operator \(e^{\mathbf{r}_< \cdot \nabla_>}\) in terms of differential operators which are irreducible spherical tensors. The starting point is an expansion of \(e^{\mathbf{a} \cdot \mathbf{b}}\) with \(\mathbf{a}, \mathbf{b} \in \mathbb{R}^3\) in terms of modified Bessel functions and Legendre polynomials \((p.\ 108\ of\ [94]):\)

\[
e^{\mathbf{a} \cdot \mathbf{b}} = e^{|\mathbf{a}| \cos \theta} = \left( \frac{\pi}{2ab} \right)^{1/2} \times \sum_{\ell=0}^{\infty} (2\ell + 1) I_{\ell+1/2}(ab) P_\ell(\cos \theta) . \tag{3.3}
\]

Next, the series expansion for the modified Bessel function \(I_{\ell+1/2}(p.\ 66\ of\ [94])\) is inserted into \((3.3)\), and the Legendre polynomials are replaced by spherical harmonics. This yields the following expansion of \(e^{\mathbf{a} \cdot \mathbf{b}}\) in terms of regular solid harmonics, which are irreducible spherical tensors of rank \(\ell\), and even powers of the vectors \(\mathbf{a}\) and \(\mathbf{b}\), which are irreducible spherical tensors of rank zero:

\[
e^{\mathbf{a} \cdot \mathbf{b}} = 2\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \left[ Y_\ell^m(\mathbf{a}) \right]^* Y_\ell^m(\mathbf{b})
\times \sum_{k=0}^{\infty} \frac{a^{2k} b^{2k}}{2^{\ell+2k} k! (1/2)^{\ell+k+1}} . \tag{3.4}
\]

This relationship is obtained from \([3.3]\) by rearranging the Cartesian components of the vectors \(\mathbf{a}\) and \(\mathbf{b}\). Accordingly, it holds for essentially arbitrary vectors \(\mathbf{a}\) and \(\mathbf{b}\) and we can choose \(\mathbf{a} = \mathbf{r}_<\) and \(\mathbf{b} = \mathbf{n}_>\), yielding

\[
e^{\mathbf{r}_< \cdot \nabla_>} = 2\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \left[ Y_\ell^m(\mathbf{r}_<) \right]^* Y_\ell^m(\mathbf{n}_>)
\times \sum_{k=0}^{\infty} \frac{r_<^{2k} \nabla_2^{2k}}{2^{\ell+2k} k! (1/2)^{\ell+k+1}} . \tag{3.5}
\]

It seems that \((3.3)\) was first published by Santos (Eq. (A.6) of \([105]\)). Santos also emphasized that this expansion should be useful for the derivation of addition theorems, but apparently did not use it for that purpose.

The only non-standard quantity in \((3.5)\) is the differential operator \(Y_\ell^m(\nabla)\). Therefore, we will now discuss those properties of \(Y_\ell^m(\nabla)\) that are needed for the derivation of addition theorems for \(B\) functions. Other properties as well as numerous applications – mainly in the context of multicenter integrals – are described in the literature \([1, 13, 29, 53, 71, 103, 105, 135]\).

The spherical tensor gradient operator \(Y_\ell^m(\nabla)\) is an irreducible spherical tensor of rank \(\ell\) (p. 312

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of \([\ref{14}]\). Consequently, its application to a function \(\phi(r)\), which only depends on the distance \(r\) and therefore is an irreducible spherical tensor of rank zero, yields an irreducible spherical tensor of rank \(\ell\) according to

\[
\mathcal{Y}_\ell^m(\nabla) \phi(r) = \left[ \left( \frac{1}{r} \frac{d}{dr} \right)^\ell \phi(r) \right] \mathcal{Y}_\ell^m(r). \tag{3.6}
\]

As discussed in Section IV of \([\ref{12}]\), this relationship can be derived with the help of a theorem on differentiation which was published by Hobson already in the late 19th century \([\ref{10}]\). Further details can be found on pp. 124 - 129 of Hobson’s book \([\ref{3}]\) which was first published in 1931.

If the spherical tensor gradient operator is applied to a spherical tensor of nonzero rank, i.e., to a function that can be written as

\[
F_{\ell_2}^{m_2}(r) = f_{\ell_2}(r) Y_{\ell_2}^{m_2}(r/r), \tag{3.7}
\]

the structure of the resulting expression can be understood in terms of angular momentum coupling (Eq. (3.9) of \([\ref{13}]\)):

\[
\mathcal{Y}_{\ell_1}^{m_1}(\nabla) F_{\ell_2}^{m_2}(r) = \sum_{\ell=\ell_{\text{min}}}^{\ell=\ell_{\text{max}}} \langle \ell m_1 + m_2 | \ell_1 m_1 \ell_2 m_2 \rangle \times \gamma_{\ell_1 \ell_2}^{\ell}(r) Y_{\ell}^{m_1 + m_2}(r/r). \tag{3.8}
\]

For the radial functions \(\gamma_{\ell_1 \ell_2}^{\ell}(r)\) in \((3.8)\), various representations could be derived, for example (Eqs. (3.29) and (4.24) of \([\ref{13}]\))

\[
\gamma_{\ell_1 \ell_2}^{\ell}(r) = \sum_{q=0}^{\Delta \ell} \binom{-\Delta \ell}{q} (-\sigma(\ell - 1/2))_q \frac{1}{q!} 2^{\ell_1 + \ell_2 - 2q} r^{\ell_1 - q} \times \left( \frac{1}{r} \frac{d}{dr} \right)^{\ell_1 - q} f_{\ell_2}(r/r) \tag{3.9}
\]

\[
= \sum_{s=0}^{\Delta \ell_2} \binom{-\Delta \ell_2}{s} (-\Delta \ell_1 + 1/2)_s \frac{1}{s!} 2^{\ell_1 - \ell_2 - 2s - 1} \times \left( \frac{1}{r} \frac{d}{dr} \right)^{\ell_1 - s} r^{\ell_2 + 1} f_{\ell_2}(r). \tag{3.10}
\]

The abbreviations \(\Delta \ell, \Delta \ell_1, \Delta \ell_2, \sigma(\ell)\) are defined in \((2.11) - (2.14)\).

These two as well as analogous other expressions for \(\gamma_{\ell_1 \ell_2}^{\ell}(r)\) can be used for the derivation of addition theorems of \(B\) functions. However, in the case of \(B\) functions more convenient expressions are available. Consequently, the general expressions \((3.9)\) and \((3.10)\) will actually not be used at all in this article.

As mentioned before, \(\mathcal{Y}_\ell^m(\nabla)\) is obtained from the regular solid harmonic \(\mathcal{Y}_\ell^m(r)\) by replacing the Cartesian components \(x, y, z\) of \(r\) by the Cartesian components \(\partial/\partial x, \partial/\partial y, \text{ and } \partial/\partial z\) of \(\nabla\). Consequently, \(\mathcal{Y}_\ell^m(\nabla)\) must obey the same coupling law. Hence, \((3.8)\) implies (Eq. (6.24) of \([\ref{13}]\)):

\[
\mathcal{Y}_{\ell_1}^{m_1}(\nabla) \mathcal{Y}_{\ell_2}^{m_2}(\nabla) = \sum_{\ell=\ell_{\text{min}}}^{\ell=\ell_{\text{max}}} \langle \ell m_1 + m_2 | \ell_1 m_1 \ell_2 m_2 \rangle \times \nabla^{\ell_1 + \ell_2 - \ell} \mathcal{Y}_\ell^{m_1 + m_2}(\nabla). \tag{3.11}
\]

It follows from the summation limits \((2.3)\) that the power \(\ell_1 + \ell_2 - \ell = 2\Delta \ell\) of \(\nabla\) is either zero or an even positive integer.

Let us now assume that a spherical tensor \(F_{\ell_2}^{m_2}(r)\) and a radially symmetric function \(\Phi_{\ell_2}(r)\) exist which satisfy

\[
F_{\ell_2}^{m_2}(r) = \mathcal{Y}_{\ell_2}^{m_2}(\nabla) \Phi_{\ell_2}(r). \tag{3.12}
\]

If we apply \(\mathcal{Y}_{\ell_1}^{m_1}(\nabla)\) to \(F_{\ell_2}^{m_2}(r)\), then the two differential operators can be coupled according to \((3.11)\). With the help of \((3.6)\), we then obtain (Eq. (3.9) of \([\ref{19}]\)):

\[
\mathcal{Y}_{\ell_1}^{m_1}(\nabla) F_{\ell_2}^{m_2}(r) = \mathcal{Y}_{\ell_1}^{m_1}(\nabla) \mathcal{Y}_{\ell_2}^{m_2}(\nabla) \Phi_{\ell_2}(r)
= \sum_{\ell=\ell_{\text{min}}}^{\ell=\ell_{\text{max}}} \langle \ell m_1 + m_2 | \ell_1 m_1 \ell_2 m_2 \rangle \nabla^{\ell_1 + \ell_2 - \ell} \times \left[ \left( \frac{1}{r} \frac{d}{dr} \right)^\ell \Phi_{\ell_2}(r) \right] \mathcal{Y}_{\ell}^{m_1 + m_2}(r). \tag{3.13}
\]
This relationship is particularly well suited for \(B\) functions. In this case, \([142]\) is more convenient than other, more general expressions for the product \(Y_{\ell_1}^m(\nabla) F_{\ell_2}^{m_2}(r)\) which can for instance be found in articles by Santos \([105]\), Bayman \([107]\), Stuart \([111]\), Niukkanen \([115]\), Weniger and Steinborn \([113]\), and Rashid \([120]\).

4 \(B\) Functions

In this Section, those mathematical properties of \(B\) functions, that are relevant for the derivation of an addition theorem via three-dimensional Taylor expansion, will be reviewed. More complete treatments can be found in \([12, 122, 136, 110]\).

If \(K_\nu(z)\) is a modified Bessel function of the second kind (p. 66 of \([94]\)), the reduced Bessel function is defined by (Eqs. (3.1) and (3.2) of \([138]\):

\[
\hat{K}_\nu(z) = (2/\pi)^{1/2} z^\nu K_\nu(z). \tag{4.1}
\]

If the order \(\nu\) of a reduced Bessel function is half-integral, \(\nu = n+1/2\) with \(n \in \mathbb{N}_0\), the reduced Bessel function can be written as an exponential multiplied a terminating confluent hypergeometric series \(1F_1\) (Eq. (3.7) of \([138]\)):

\[
\hat{k}_{n+1/2}(z) = 2^n (1/2)_n e^{-z} 1F_1(-n; -2n; 2z). \tag{4.2}
\]

The polynomial part in \([12]\) was also treated independently in the mathematical literature \([142]\), where the notation

\[
\Theta_n(z) = e^z \hat{k}_{n+1/2}(z), \quad n \in \mathbb{N}_0, \tag{4.3}
\]

is used. Together with some other, closely related polynomials, the \(\Theta_n(z)\) are called Bessel polynomials. They are applied in such diverse fields as number theory, statistics, and the analysis of complex electrical networks \([142]\).

The so-called \(B\) function was introduced by Filter and Steinborn as an anisotropic generalization of the reduced Bessel function (Eq. (2.14) of \([92]\)),

\[
B_{n,\ell}^m(\alpha, r) = [2^{n+\ell}(n+\ell)!]^{-1} \hat{k}_{n-1/2}(\alpha r) Y_\ell^m(\alpha r), \tag{4.4}
\]

where \(\alpha > 0\) and \(n \in \mathbb{Z}\). Because of the factorial \((n + \ell)!\) in the denominator, \(B\) functions are defined in the sense of classical analysis only if \(n + \ell \geq 0\) holds. However, the definition of a \(B\) function remains meaningful even for \(n + \ell < 0\). If \(r \neq 0\), \(B_{n-\ell,\ell}^m(r)\) with \(n \in \mathbb{N}\) is zero, but for \(r = 0\), its value is \(\infty/\infty\) and therefore undefined.

In fact, such a \(B\) function can be interpreted as a derivative of the three-dimensional Dirac delta function (Eq. (6.20) of \([113]\)):

\[
B_{n-\ell,\ell}^m(r) = \frac{(2\ell-1)!!}{\alpha^{\ell+3}} \frac{4\pi}{\ell^{\ell+3}} \times \left[1 - \alpha^{-2} \nabla^2\right] \delta_\ell^m(r), \quad n \in \mathbb{N}. \tag{4.5}
\]

The spherical delta function \(\delta_\ell^m\) is defined by

\[
\delta_\ell^m(r) = \frac{(-1)^\ell}{(2\ell-1)!!} \frac{\nabla Y_\ell^m(\nabla)}{Y_\ell^m(\nabla)} \delta(r). \tag{4.6}
\]

If follows from (4.1) - (4.4) that \(B\) functions are relatively complicated mathematical objects. Nevertheless, all the commonly occurring exponentially decaying functions can be expressed as simple finite sums of \(B\) functions. For example, if

\[
\chi_{n,\ell}^m(\alpha, \mathbf{r}) = (\alpha r)^{n-1} e^{-\alpha r} Y_\ell^m(\theta, \phi) \tag{4.7}
\]

is an (unnormalized) Slater-type function with \(\alpha > 0\) and \(n \geq \ell + 1\), then (Eqs. (3.3) and (3.4) of \([92]\))

\[
\chi_{n,\ell}^m(\alpha, \mathbf{r}) = \sum_{p=p_{\text{min}}}^{n-\ell} (-1)^{n-1-p} \frac{(n-\ell)!2^{\ell+p}(\ell+p)!}{(2p-n+\ell)!(2n-2\ell-2p)!!} B_{p,\ell}^m(\alpha, r), \tag{4.8}
\]

where \(p_{\text{min}} = \lceil(n-\ell)/2\rceil\). Here, \(\lfloor x \rfloor\) stands for the integral part of \(x\), i.e., for the largest integer \(\nu\) satisfying \(\nu \leq x\).

As is well known, the bound-state eigenfunctions of a hydrogen-like ion with nuclear charge \(Z\) can be expressed as follows:

\[
W_{n,\ell}(Z, r) = \left(\frac{2Z}{n}\right)^{3/2} \left[\frac{(n-\ell-1)!}{2n(n+\ell)!}\right]^{3/2} \times e^{-Zr/n} \int_{n-\ell-1}^{2(n+\ell)} f_{n-\ell-1}(2Zr/n) Y_\ell^m(2Zr/n), \tag{4.9}
\]
where \( t_{n-\ell-1}^{(2\ell+1)} \) is a generalized Laguerre polynomial. Then (Eq. (3.16) of \([53]\)),

\[
W_{n,\ell}^{m}(Z, r) = \left( \frac{2Z}{n} \right)^{3/2} \times \frac{2^{\ell+1}}{(2\ell+1)!!} \left[ \frac{n(n + \ell)!}{2(n - \ell - 1)!} \right]^{1/2} \times \sum_{t=0}^{n-\ell-1} \frac{(-n + \ell + 1)_{t}(n + \ell + 1)_{t}}{t!(\ell + 3/2)_{t}} \times B_{t+1,\ell}^{m}(Z/n, r). \tag{4.10}
\]

The bound-state hydrogenic eigenfunctions are orthonormal, but not complete in the Hilbert space \( L^2(\mathbb{R}^3) \). This incompleteness is sometimes overlooked (see for example the discussion in \([143]\)).

The following set of functions, which was introduced by Hylleraas \([144]\) and by Shull and Löwdin \([145, 146]\), is complete and orthonormal in the Hilbert space \( L^2(\mathbb{R}^3) \):

\[
\Lambda_{n,\ell}^{m}(\alpha, R) = (2\alpha)^{3/2} \frac{(n - \ell - 1)!}{(n + \ell + 1)!} \times e^{-\alpha r} L_{n-\ell-1}^{(2\ell+2)}(2\alpha r) \gamma_{\ell}^{m}(2\alpha r). \tag{4.11}
\]

Then (Eq. (3.18) of \([147]\)),

\[
\Lambda_{n,\ell}^{m}(\alpha, r) = (2\alpha)^{3/2} \times 2^\ell \frac{(2n + 1)}{(2\ell + 3)!!} \left[ \frac{(n + \ell + 1)!}{(n - \ell - 1)!} \right]^{1/2} \times \sum_{t=0}^{n-\ell-1} \frac{(-n + \ell + 1)_{t}(n + \ell + 2)_{t}}{t!(\ell + 5/2)_{t}} \times B_{t+1,\ell}^{m}(\alpha, r). \tag{4.12}
\]

Closely related to the bound-state hydrogenic eigenfunctions is the following set of functions which were already used in 1928 by Hylleraas \([148]\) and which are commonly called Coulomb Sturmians or simply Sturmians \([149]\):

\[
\Psi_{n,\ell}^{m}(\alpha, r) = (2\alpha)^{3/2} \left[ \frac{(n - \ell - 1)!}{2n(n + \ell)!} \right]^{3/2} \times e^{-\alpha r} \gamma_{n-\ell-1}^{(2\ell+1)}(2\alpha r) \gamma_{\ell}^{m}(2\alpha r). \tag{4.13}
\]

Comparison of (4.9) and (4.13) yields

\[
\Psi_{n,\ell}^{m}(Z/n, r) = W_{n,\ell}^{m}(Z, r). \tag{4.14}
\]

The fact, that bound-state hydrogenic eigenfunctions and Sturmians have the same normalization constant, is actually by no means obvious. The \( W_{n,\ell}^{m}(Z, r) \) are normalized with respect to norm of the Hilbert space \( L^2(\mathbb{R}^3) \), whereas the \( \Psi_{n,\ell}^{m}(\alpha, r) \) are normalized with respect to the norm of the Sobolev space \( W^{2}_{2}(\mathbb{R}^3) \) \([150]\). Further details can be found in \([53]\).

In (4.10), we only have to replace \( Z/n \) by \( \alpha \) to obtain the following representation of Sturmians in terms of \( B \) functions (Eq. (4.19) of \([53]\)):

\[
\Psi_{n,\ell}^{m}(\alpha, r) = (2\alpha)^{3/2} \times \frac{(2^{\ell+1})}{(2\ell + 1)!!} \left[ \frac{n(n + \ell)!}{2(n - \ell - 1)!} \right]^{1/2} \times \sum_{t=0}^{n-\ell-1} \frac{(-n + \ell + 1)_{t}(n + \ell + 1)_{t}}{t!(\ell + 3/2)_{t}} \times B_{t+1,\ell}^{m}(\alpha, r). \tag{4.15}
\]

The linear combinations \([1.8], (4.10), (4.12), \) and \([4.13]\) imply that mathematical results for \( B \) functions can be translated immediately to analogous results for Slater-type functions, bound-state hydrogenic eigenfunctions, Lambda functions, and Sturmians.

In view of the fact that \( B \) functions have a relatively complicated mathematical structure, it is by no means trivial that the linear combinations \([1.8], (4.10), (4.12), \) and \([4.13]\) could be derived at all. However, these relationships as well as other advantageous properties of \( B \) functions can be explained via their Fourier transform, which is of exceptional simplicity among exponentially declining functions (Eq. (7.1-6) of \([139]\) or Eq. (3.7) of \([114]\)):

\[
\tilde{B}_{n,\ell}^{m}(p) = (2\pi)^{-3/2} \int e^{-ip \cdot r} B_{n,\ell}^{m}(r) \, d^3r
= (2/\pi)^{1/2} \frac{\alpha^{2n+\ell-1}}{[\alpha^2 + p^2]^{n+1/2}} \gamma_{\ell}^{m}(-i\alpha). \tag{4.16}
\]

The linear combinations \([1.8], (4.10), (4.12), \) and \([4.13]\) imply that the Fourier transforms of Slater-type functions, of the bound-state hydrogenic
eigenfunctions, of Lambda functions, and of Sturmians can be expressed as simple linear combinations of Fourier transforms of $B$ functions.

If we want to derive an addition theorem for some function via the translation operator in its spherical form (3.3), then the application of higher powers of the Laplacian and of the spherical tensor gradient operator to this function must lead to expressions of manageable complexity. On the basis of the Fourier transform (4.16), it can be seen that these expressions are indeed very simple in the case of $B$ functions.

The differential operator $1 - \nabla^2/\alpha^2$, which is typical of the modified Helmholtz equation, acts on $B$ functions as a ladder operator for the order $n$ (Eq. (5.6) of [113]):

$$[1 - \nabla^2/\alpha^2] B_{n,\ell}^m(r) = B_{n-1,\ell}^m(r).$$

(4.17)

This follows at once from the Fourier transform (4.16) in combination with the fact that in momentum space the differential operator $[1 - \nabla^2/\alpha^2]$ is transformed into the multiplicative operator $[\alpha^2 + p^2]/\alpha^2$.

With the help of this relationship, the application of the higher powers of the Laplacian $\nabla^2$ can be expressed quite easily in closed form. Combination of (4.17) with the binomial theorem yields (Eq. (5.7) of [113]):

$$\alpha^{-2\nu} \nabla^{2\nu} B_{n,\ell}^m(r)$$

$$= \sum_{t=0}^\nu (-1)^t \binom{\nu}{t} B_{n-t,\ell}^m(r).$$

(4.18)

The remarkably simple Fourier transform (4.16) also explains why the application of the spherical tensor gradient operator to a $B$ function produces particularly compact expressions. For example, if we combine

$$\mathcal{Y}_\ell^m(\nabla) e^{\pm ip \cdot r} = \mathcal{Y}_\ell^m(\pm ip)e^{\pm ip \cdot r}$$

(4.19)

with the Fourier transform (4.16), we find that a nonscalar $B$ function can be obtained by applying the corresponding spherical tensor gradient operator to a scalar $B$ function (Eq. (4.12) of [112]):

$$B_{n,\ell}^m(r) = \frac{(4\pi)^{1/2}}{(-\alpha)^{\ell}} \mathcal{Y}_\ell^m(\nabla) B_{n+\ell,0}^0(r).$$

(4.20)

This relationship can also be obtained in a straightforward way with the help of (4.6). The differential operator $\left(r^{-1}d/dr\right)^t$ in (4.6) is a simple operator for modified Bessel functions, but not for the other exponentially decaying functions considered in this article. It acts as a shift operator for reduced Bessel functions according to

$$\left(\frac{1}{z} \frac{d}{dz}\right)^{m} \check{k}_\nu(z) = (-1)^m \check{k}_{\nu-m}(z).$$



Similarly, the application of the spherical tensor gradient operator to a nonscalar $B$ function with $\ell > 0$ yields a simple linear combination of $B$ functions (Eq. (6.25) of [113]):

$$\mathcal{Y}_{\ell_1}^{m_1}(\nabla) B_{n_2,\ell_2}^{m_2}(r)$$

$$= (-\alpha)^{\ell_1} \sum_{t=0}^{\ell = \ell_{\text{max}}} \binom{2\ell}{\ell_1 m_1 + m_2 | 1 \ell_1 | \ell_2 m_2}$$

$$\times \sum_{t=0}^{\Delta \ell} (-1)^t \binom{\Delta \ell}{t} B_{n_2+\ell_2-\ell-t,\ell}^{m_1+m_2}(r).$$

(4.22)

This relationship follows at once from (3.13), (4.18), and (4.20).

## 5 An Addition Theorem for $B$ Functions

We now want to derive an addition theorem for $B$ functions via three-dimensional Taylor expansion. For that purpose, we apply the translation operator in its spherical form (3.5) to a $B$ function:

$$B_{n,\ell}^m(\alpha, r_++r)$$

$$= 2\pi \sum_{\ell_1=0}^\infty \sum_{m=-\ell_1}^{\ell_1} \left[ \mathcal{Y}_{\ell_1}^{m_1}(r_<) \right]^{*} \mathcal{Y}_{\ell_1}^{m_1}(\nabla_<)$$

$$\times \sum_{q=0}^\infty \frac{r^{2q} \nabla^{2q}}{r^{2q} + 2q!(1/2)_{\ell_1+q+1}} B_{n,\ell}^m(\alpha, r_<).$$

(5.1)
Now, we want to apply the powers of the Laplacian $\nabla^2_\nu$ to the $B$ functions in (5.1). This can be done with the help of (4.18), yielding

$$B_{n,\ell}(\alpha, r_\nu + r_\rho) = 2\pi \sum_{\ell_1=-\ell}^{\ell_1=\ell} \sum_{m=-\ell_1}^{m=\ell_1} \left[ \mathcal{Y}_{\ell_1}^{m_1}(r_\nu) \right]^* \mathcal{Y}_{\ell_1}^{m_1}(\nabla_\rho)$$

$$\times \frac{(\alpha r_\nu)^{2q}}{2^{\ell_1+2q}q!(1/2)_{\ell_1+q+1}} \times \sum_{t=0}^{q} (-1)^t \left( \frac{q}{t} \right) B_{n-t,\ell}(\alpha, r_\rho). \quad (5.2)$$

It follows from the definition of a $B$ function according to (1.14) that $B_{n,\ell}(r_\nu)$ with $r_\nu \neq 0$ is zero for $n < -\ell$. Thus, the summation limit of the innermost summation in (5.2) is not $q$ but $\min(q, n + \ell)$. Hence, if we introduce a new summation variable $s = q - t$, we obtain for the two innermost summations in (5.2):

$$\sum_{q=0}^{\infty} \frac{(\alpha r_\nu)^{2q}}{2^{\ell_1+2q}q!(1/2)_{\ell_1+q+1}} \times \sum_{t=0}^{\min(q, n + \ell)} (-1)^t \left( \frac{q}{t} \right) B_{n-t,\ell}(\alpha, r_\rho)$$

$$= \sum_{q=0}^{\infty} \frac{(\alpha r_\nu)^{2q}}{2^{\ell_1+2q}q!(1/2)_{\ell_1+q+1}} \times \sum_{t=0}^{\min(q, n + \ell)} (-1)^t \left( \frac{q}{t} \right) B_{n-t,\ell}(\alpha, r_\rho) \quad (5.3)$$

$$= 2^{-(\ell_1+1)} \sum_{t=0}^{n+\ell} \frac{(-1)^t}{t!} B_{n-t,\ell}(\alpha, r_\rho)$$

$$\times \sum_{s=0}^{\infty} \frac{(\alpha r_\nu)^{2s+2t}}{s!(1/2)_{s+t+1}} \quad (5.4)$$

$$= 2^{-(\ell_1+1)} \sum_{t=0}^{n+\ell} \frac{(-1)^t (\alpha r_\nu)^{2t}}{t!(1/2)_{t+1}} B_{n-t,\ell}(\alpha, r_\rho)$$

$$\times 0 F_1 \left( \ell_1 + t + 3/2; (\alpha r_\nu)^2/4 \right) \quad (5.5)$$

The generalized hypergeometric series $0 F_1$ can be replaced by a modified Bessel function of the first kind according to (p. 66 of [14])

$$0 F_1 (\nu + 1; z^2/4) = \frac{\Gamma(\nu + 1)}{(z/2)^\nu} I_\nu(z). \quad (5.6)$$

By combining (5.3) and (5.6) we obtain

$$\sum_{q=0}^{\infty} \frac{(\alpha r_\nu)^{2q}}{2^{\ell_1+2q}q!(1/2)_{\ell_1+q+1}} \times \sum_{t=0}^{q} (-1)^t \left( \frac{q}{t} \right) B_{n-t,\ell}(\alpha, r_\rho)$$

$$= \pi^{-1/2} \sum_{t=0}^{n+\ell} \frac{(-1)^t (2^{1-t})}{t!(\alpha r_\nu)^{2t-1}} I_{\ell_1+t+1/2}(\alpha r_\nu)$$

$$\times B_{n-t,\ell}(\alpha, r_\rho). \quad (5.7)$$

Inserting (5.7) into (5.2) yields:

$$B_{n,\ell}(\alpha, r_\nu + r_\rho) = (2\pi)^{3/2} \sum_{\ell_1=0}^{\ell_1=\ell} \sum_{m=-\ell_1}^{m=\ell_1} \left[ \mathcal{Y}_{\ell_1}^{m_1}(r_\nu) \right]^* \mathcal{Y}_{\ell_1}^{m_1}(\nabla_\rho)$$

$$\times \sum_{t=0}^{\min(n+\ell, q, m+\ell)} (-1)^t \left( \frac{q}{t} \right) B_{n-t,\ell}(\alpha, r_\rho) \quad (5.8)$$

Now, all that remains to be done is the application of the spherical tensor gradient operator to the $B$ functions. This can be done with the help of (4.22), yielding

$$\mathcal{Y}_{\ell_1}^{m_1}(\nabla_\rho) B_{n-t,\ell}(r_\rho)$$

$$= (-\alpha)^{\ell_1} \sum_{\ell_2=\ell_1}^{\ell_2=\ell_2^{\max}} \left( \frac{2}{m_1} \right) \sum_{m=\ell_1 m_1}^{m=\ell_2 m_1} \sum_{s=0}^{\Delta \ell_2} (-1)^s \left( \frac{\Delta \ell_2}{s} \right) B_{n+\ell_2,\ell-\ell_2-s-t_2}(r_\rho) \quad (5.9)$$

The summation limit $\Delta \ell_2$ in (5.9) is defined in (2.13). By inserting (5.9) into (5.8), we finally...
obtain an addition theorem for $B$ functions:

\[
B_{n,\ell}^m(\alpha, r_\prec + r_\succ) = (2\pi)^{3/2} \sum_{\ell_1=0}^{\ell} \sum_{m=-\ell_1}^{\ell_1} (-1)^{\ell_1} \left[ \gamma_{\ell_1}^{m_1}(r_\prec) \right]^* \\
\times \sum_{\ell_2=0}^{\ell_2=\ell_\max} (\alpha r_\prec)^{l-\ell_1-1/2} I_{l_1+t+1/2}(\alpha r_\prec) \\
\times \sum_{\ell_2=\ell_2=\ell_\min}^{\ell_2=\ell_\max} (2) \langle \ell_2 m + m_1 | \ell_1 m_1 | \ell m \rangle \\
\times \sum_{s=0}^{\Delta \ell_2} (-1)^s \left( \Delta \ell_2 \right) B_{n+\ell_2-s-t,\ell_2}^m(r_\succ). (5.10)
\]

This expression is not yet completely satisfactory from a formal point of view. We have to take into account that the $B$ functions in the innermost sum are zero if $n + \ell - \ell_2 - s - t < -\ell_2$. For that purpose, we introduce a new summation variable $q = n + \ell - t$. This yields:

\[
B_{n,\ell}^m(\alpha, r_\prec + r_\succ) = (2\pi)^{3/2} (\frac{1}{2})^{n+\ell} \\
\times \sum_{\ell_1=0}^{\ell} \sum_{m=-\ell_1}^{\ell_1} (-1)^{\ell_1} \left[ \gamma_{\ell_1}^{m_1}(r_\prec) \right]^* \\
\times \sum_{q=0}^{\ell_2=\ell_\max} (\alpha r_\prec)^{n+\ell_1-1/2} \\
\times I_{n+\ell_1+1/2}(\alpha r_\prec) \\
\times \sum_{\ell_2=\ell_\min}^{\ell_2=\ell_\max} (2) \langle \ell_2 m + m_1 | \ell_1 m_1 | \ell m \rangle \\
\times \sum_{s=0}^{\Delta \ell_2} (-1)^s \left( \Delta \ell_2 \right) B_{q-\ell_2-s,\ell_2}^m(r_\succ). (5.11)
\]

This addition theorem is identical to the addition theorem (4.27) of [34] which was derived with the help of techniques that closely resemble the zeta function method of Barnett and Coulson [31]. Other addition theorems for $B$ functions and for reduced Bessel functions can be found in Sections IV and V of [34].

### 6 Summary and Conclusions

Addition theorems are expansions of a given function $f(r + r')$ with $r, r' \in \mathbb{R}^3$ in terms of other functions that only depend on either $r$ or $r'$. As discussed in Section 1, many different techniques for the construction of addition theorems are known. Examples are the zeta function method of Barnett and Coulson [31], Löwdin’s alpha function method [34], or the Fourier transform method suggested independently by Ruedenberg [51] and Silverstone [52].

Addition theorems can also be defined as three-dimensional Taylor expansions according to (1.3). In this approach, the translation operator $e^{r_\cdot \nabla}$ generates $f(r + r')$ by doing a three-dimensional Taylor expansion of $f$ around $r$. In the context of atomic and molecular calculations, one is normally interested in addition theorems of irreducible spherical tensors of the type of (1.1). In such a case, the straightforward application of the translation operator $e^{r_\cdot \nabla}$ would lead to enormous technical problems. Consequently, it was generally believed that three-dimensional Taylor expansions constitute essentially a formal solution, but cannot be used for the actual derivation of addition theorems of irreducible spherical tensors. However, the Taylor expansion method is indeed a practically useful tool if the translation operator is expanded in terms of differential operators that are irreducible spherical tensors according to (3.3). This was demonstrated in [55] by constructing the Laplace expansion of the Coulomb potential as well as the addition theorems of the regular and irregular solid harmonics and of the Yukawa potential.

Since the addition theorems mentioned above are all comparatively simple, their successful construction does not necessarily guarantee that the Taylor expansion method is also practically useful if more complicated addition theorems are to be constructed. Consequently, the topic of the present article is the construction of addition theorems for exponentially decaying functions which are notoriously complicated.
Slater-type functions have the simplest structure of all the commonly occurring exponentially decaying functions. Consequently it looks like an obvious idea to concentrate on addition theorems of Slater-type functions, and to express the addition theorems for other exponentially decaying functions in terms of addition theorems for Slater-type functions.

However, the addition theorems for Slater-type functions are notoriously difficult. Moreover, Slater-type functions have a simple analytical structure only in the coordinate representation. In momentum space, which is probably more important in the case of multicenter problems, the simplest exponentially decaying functions are the so-called $B$ functions. Their extremely simple Fourier transform (4.16) as well as some other advantageous mathematical properties give $B$ functions a unique position among exponentially decaying functions. Moreover, as discussed in Section 7, all the commonly occurring exponentially decaying functions can be expressed as simple finite sums of $B$ functions. This implies that the addition theorems of Slater-type functions, of bound-state hydrogenic eigenfunctions, and of other functions based on Laguerre polynomials can be expressed in terms of the addition theorems of $B$ functions.

So, this article focuses on the derivation of an addition theorem for $B$ functions by doing a three-dimensional Taylor expansion in its spherical form (3.5). The relative ease, with which the addition theorem (5.11) can be constructed, and its comparatively compact structure indicate once more that $B$ functions have in the context of multicenter problems considerable advantages over other exponentially decaying functions.

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