Clebsch-Gordan-type linearisation relations for the products of Laguerre polynomials and hydrogen-like functions

1985 J. Phys. A: Math. Gen. 18 1399

(http://iopscience.iop.org/0305-4470/18/9/022)

J. Phys. A: Math. Gen. 18 (1985) 1399-1417. Printed in Great Britain

Clebsch–Gordan-type linearisation relations for the products of Laguerre polynomials and hydrogen-like functions

A W Niukkanen

Laboratory of Molecular Spectroscopy and Quantum Chemistry, V I Vernadsky Institute of Geochemistry and Analytical Chemistry, Academy of Sciences of the USSR, Moscow 117334, USSR

Received 5 August 1982, in final form 7 June 1984

Abstract. Two series of Clebsch–Gordan type are derived for the most general product of the Laguerre polynomials, $L_{n_1}^{\alpha_1}(u_1x)L_{n_2}^{\alpha_2}(u_2x)$, which differ in orders, n, weights, α, and scaling multipliers, u. The general form and particular cases of coefficients in the expansion of the polynomial $x^kL_{n_1}^{\alpha_1}(u_1x)\ldots L_{n_N}^{\alpha_N}(u_Nx)$ in terms of the Laguerre polynomials are established. The applications to hydrogen-like functions and Morse oscillators are indicated. Connection with an earlier Carlitz expansion, the technical links with the hyperspherical harmonics formalism and different approaches to the important Koornwinder's positivity theorems are discussed briefly.

1. Introduction

The Laguerre and Jacobi polynomials, which virtually cover all the classical orthogonal polynomials, play an important role in various physical applications. In many cases, the solutions of the Schrödinger equation for simple systems are expressed directly in terms of such polynomials; for example, hydrogen-like functions via the Laguerre polynomials, rotator functions via the Jacobi polynomials, etc. Since the Hermite and Bessel polynomials are particular cases of the Laguerre polynomials, and the Legendre and Gegenbauer polynomials are particular cases of the Jacobi polynomials, the numbers of such examples may be easily extended.

The Laguerre and Jacobi polynomials also play an important role in approximate variational solutions of complex many-electron systems, because basis functions in variational methods are frequently connected with these two classes of special functions.

It is convenient (and, as a rule, such a procedure cannot be avoided in practice) to represent the product of polynomials, $p_n(x)p_m(x)$, arising in quantum mechanical applications, as a linear combination of some functions p'_k, i.e. to use some linearisation theorem. If p_k polynomials of the same type, as in the initial product, are used as the elements of such a linear combination, then the corresponding expansion is of Clebsch–Gordan type (it is just this structure which is peculiar to the Clebsch–Gordan series for spherical functions). Sometimes it is more suitable to use in linear combination some functions p'_k which differ from p_k. We call such an expansion the (modified) series of Clebsch–Gordan type.

Another important class of relations for classical polynomials is constituted by addition theorems which either relate to an expansion of $f(x+y)$, as in elliptic functions, or to an expansion of $f(g(x_1,\ldots,x_N))$ where $g(x_1,\ldots,x_N)$ is an appropriate function of some variables that are usually related to a distance function on a homogeneous space. There are a number of addition formulae for the Jacobi and Laguerre polynomials (Erdelyi 1953, Vilenkin 1965). Some new addition formulae for the Laguerre polynomials were given by Koornwinder (1977) and Durand (1977).

As regards the linearisation theorems, they are rather numerous for the Jacobi polynomials (Vilenkin 1965) or, equivalently, for the Wigner D functions (Varshalovich *et al* 1975). However, in the case of the Laguerre polynomials the linearisation theorems, except for one general theorem of the modified type (Carlitz 1957)†, relate to special cases rather than to a general case. For example, for a product $L_{n_1}^{\alpha_1}(u_1x)L_{n_2}^{\alpha_2}(u_2x)$ the following particular cases of modified linearisation theorems have been considered: the case $\alpha_1=\alpha_2$, $n_1=n_2$ has been studied by Bailey (1936) (see also equation 10.12 (42), Erdélyi 1953), and the case $\alpha_1=\alpha_2$, $u_1=u_2$ by Howell (1937)‡. The usual (non-modified) Clebsch-Gordan type expansions have not been, to the author's knowledge, considered so far in explicit form.

The need for the Laguerre polynomials in more general linearisation theorems is implied by their importance in atomic and nuclear shell theories. One more reason is that the hydrogen-like functions have been intensively advanced in recent years as perspective basis functions for variational calculations of molecular electron wavefunctions.

Some interesting mathematical problems arise in connection with the linearisation relations§. For example, in particular cases the coefficients C in Clebsch-Gordan type expansions satisfy some important inequalities. Very interesting results were found by Koornwinder (1978). He showed that for integral k, l

$$L_m^k(x)L_n^l(x)=\sum_i(-1)^iC_iL_{m+n-i}^{k+l}(x) \tag{1}$$

where $C_i\geqslant 0$, and

$$L_m^\alpha(\lambda x)L_n^\alpha((1-\lambda)x)=\sum_k C_k(\lambda)L_{m+n-k}^\alpha(x) \tag{2}$$

with $C_k(\lambda)\geqslant 0$ when $0\leqslant\lambda\leqslant 1$ and $\alpha\geqslant 0$. These relations are useful for computational purposes. For example, if $\alpha=0$ then $\Sigma_kC_k(\lambda)=1$ (set $x=0$ in equation (2)), so the computation with these coefficients will be very stable for many problems. The coefficients $C_k(\lambda)$ also have an interesting combinational meaning (Askey *et al* 1978). Since Koornwinder (1978) did not give explicit expressions for C_i and $C_k(\lambda)$ and his original positivity proofs seem to be very cumbersome (especially for $C_k(\lambda)$), it would be interesting to see whether the positivity of C_i and $C_k(\lambda)$ follow directly from explicit algebraic formulae. This problem is discussed briefly in § 6‖.

† This theorem is a particular case of more general expansion given in § 7. This particular expansion has been intensively studied in nuclear physics in recent years (the references are given in § 7).

‡ The expansion of the product $\Phi(a,c;x)\Phi(a',c;x)$, which is equivalent to Howell's expansion, is presented in equation 6.15 (29) by Erdélyi (1953) with some misprints, as well as Howell's expansion (1937). The correct forms of the expansions are given by Burchnall and Chaundy (1941) (relations (72) and (98), respectively).

§ The author is indebted to the referee for the comments which are used in the rest of this section.

‖ It is shown that simple positivity proofs for C_i and $C_k(\lambda)$ based on explicit algebraic expressions are, actually, possible. However, we give in the following only sketches of the proofs rather than the proofs themselves in full detail. The reason is that a number of other interesting properties of $C_k(\lambda)$, including generating functions, addition and linearisation theorems, etc, are implied by our approach. The presentation of these results would therefore lead to a conspicuous deviation from the initial objectives of the present investigation. The corresponding results will be presented in a separate publication.

2. Expansion of $x^k L_m^\beta(\tau x)$ in terms of the Laguerre polynomials

Consider the expansion

$$x^k L_m^\beta(\tau x) = \sum_n C_{m,n}^{\beta,\alpha}(k, \tau, \sigma) L_n^\alpha(\sigma x). \tag{3}$$

Since $x^k = (-1)^k k! L_k^{-k}(x)$, expansion (3) may be considered as a special form of linearisation theorem for the Laguerre polynomials. Without a loss in generality, we may confine ourselves to the case $\sigma = 1$,

$$x^k L_m^\beta(\tau x) = \sum_n C_{m,n}^{\beta,\alpha}(k, \tau) L_n^\alpha(x) \tag{4}$$

because

$$C_{m,n}^{\beta,\alpha}(k, \tau, \sigma) = \sigma^{-k} C_{m,n}^{\beta,\alpha}(k, \tau/\sigma). \tag{5}$$

Introducing the notation for the scalar product

$$(f, \varphi)_\alpha = \int_0^\infty \mathrm{d}x\, x^\alpha \exp(-x) f(x)\varphi(x) \tag{6}$$

and taking into account the orthogonality relation for the Laguerre polynomials

$$(L_m^\alpha, L_n^\alpha)_\alpha = \delta(m, n)\Gamma(\alpha + 1 + n)/n! \tag{7}$$

we obtain

$$C_{m,n}^{\beta,\alpha}(k, \tau) = n!/\Gamma(\alpha + 1 + n) \int_0^\infty \mathrm{d}x\, x^{\alpha+k} \exp(-x) L_n^\alpha(x) L_m^\beta(\tau x). \tag{8}$$

Prior to using equation (8) for establishing the algebraic expression for $C(k, \tau)$ coefficients, we shall make two general remarks.

The first observation concerns 'selection rules'. The scalar product of a classical polynomial (with 'its own' weight function) of degree n by any polynomial p_N of degree N is not zero only if $n \leq N$ (see § 10.3 in Erdélyi (1953)), i.e. for example:

$$(L_n^\alpha, p_N)_\alpha \neq 0 \qquad \text{if } n \leq N. \tag{9}$$

Presenting equation (8) in the form

$$C(k, \tau) = n!/\Gamma(\alpha + 1 + n)(L_n^\alpha, x^k L_m^\beta(\tau x))_\alpha \tag{10}$$

we obtain in the case of integer $k \geq 0$ (the polynomiality condition for $x^k L_m^\beta$) the evident selection rule

$$0 \leq n \leq m + k. \tag{11}$$

If $\tau = 1$ (the case frequently arising in applications), there is an alternative expression:

$$C(k, \tau) = n!/\Gamma(\alpha + 1 + n(L_m^\beta, x^{\alpha-\beta+k} L_n^\alpha)_\beta. \tag{12}$$

This means, by virtue of equation (9), that if $\alpha - \beta + k$ is non-negative integer (the polynomiality condition for the second multiplier in equation (12)), then there exists the supplementary selection rule and, then, in the case $\alpha - \beta + k < m$, the number of terms in the sum (3) is determined not by condition (11), but obeys a stronger inequality

$$m - \alpha + \beta - k \leq n \leq m + k. \tag{13}$$

In particular, if $\alpha-\beta+k=0$, then $m\leqslant n\leqslant m+k$. Thus, in the case of k and $\alpha-\beta$ integers, with fixed values of m, β and k in the left-hand side of equation (3), by choosing a parameter α one may control the number of terms in the right-hand side of equation (3). Evidently, the least possible number of terms corresponds to the case $\alpha=\beta-k$.

The second remark concerns the orthogonality relation and the sum rule for $C(k, \tau)$. Applying the scaling transformations, one may easily show that

$$L_n^\alpha(x)=\sum_q \tau^k C_{n,q}^{\alpha,\beta}(-k, 1/\tau)x^k L_q^\beta(\tau x). \tag{14}$$

Substituting equation (14) into equation (4), we obtain

$$L_m^\beta(\tau x)=\sum_q \tau^k \sum_n C_{m,n}^{\beta,\alpha}(k, \tau)C_{n,q}^{\alpha,\beta}(-k, 1/\tau)L_q^\beta(\tau x)$$

and, hence,

$$\sum_n C_{m,n}^{\beta,\alpha}(k, \tau)C_{n,q}^{\alpha,\beta}(-k, 1/\tau)=\tau^{-k}\delta(m, q). \tag{15}$$

Note that in the case $k=1,2,\ldots,$ the orthogonality relation links the coefficients $C(k, \tau)$ in expansion (4) of polynomial type ($k>0$) with coefficients $C(-k, 1/\tau)$ of the corresponding expansion of non-polynomial type. In the case $k=0$ both sets of coefficients in equation (15) pertain to polynomial expansions of the same type.

Multiplying both sides of equation (3) by the power x^q and using, one the one hand, the expansion of type (3) for the expression arising on the left-hand side of the equation

$$x^{k+q}L_m^\beta(\tau x)=\sum_n C_{m,r}^{\beta,\gamma}(k+q, \tau, t)L_r^\gamma(tx)$$

and, on the other hand, the expansion of the same type for the expressions arising on the right-hand side of the equation

$$x^q L_n^\alpha(\sigma x)=\sum_r C_{n,r}^{\alpha,\gamma}(q, \sigma, t)L_r^\gamma(tx)$$

we obtain, after obvious manipulations,

$$C_{m,r}^{\beta,\gamma}(k+q, \tau t)=\sum_n C_{m,n}^{\beta,\alpha}(k, \tau)t^{-k}C_{n,r}^{\alpha,\gamma}(q, t). \tag{16}$$

The 'sum rule' (16) can also be interpreted as an argument multiplication theorem for the function $C(k, \tau)$, or alternatively, as an addition theorem for the index k. One may also easily show that the orthogonality relation (15) is a particular case of the addition theorem (16).

3. Algebraic representation for coefficients $C(k, \tau)$—particular cases

In order to obtain 'explicit expressions' for the coefficients C, we use the integral representation equation (8). Writing down the Laguerre polynomials in equation (8) in the form of a hypergeometric series, F_1^1, we obtain the expression for $C(k, \tau)$ as an

Appell function, F_2†:

$$C_{m,n}^{\beta,\alpha}(k,\tau)=\frac{(\beta+1)_m}{m!}(\alpha+1)_k{}^2F_{0,1}^{1,1}\left[\begin{matrix}\alpha+1+k;\ -m,-n;\ \tau,1\\ \varnothing;\ \beta+1,\alpha+1\end{matrix}\right] \tag{17}$$

where $(a)_n$ is the Pochhammer symbol.

Using the reduction formula for the corresponding Lauricella function, F_A, with the unit argument (see equation (16) in Niukkanen (1983)), we have

$$C_{m,n}^{\beta,\alpha}(k,\tau)=\frac{(\alpha+1)_k(\beta+1)_m(-k)_n}{m!(\alpha+1)_n}F_2^3\left[\begin{matrix}\alpha+1+k,k+1,-m;\tau\\ k+1-n,\beta+1\end{matrix}\right]. \tag{18}$$

Expression (18) is fallacious in some cases. Indeed, for the value $n\geqslant k+1$, allowed by selection rule (11), the quantity $(-k)_n$ in equation (18) assumes zero value, and the series F_2^3 tends to infinity, since the parameter $k+1-n$ in F_2^3 is a non-positive integer and, hence, the coefficients of τ^i in the sum F_2^3, in the case $i\geqslant n-k$, contain zero denominators, $(k+1-n)$; therefore, the condition $i\leqslant m$ does not lead to termination of the series before the 'dangerous denominators' appear. Consequently, in the case of $n\geqslant k+1$ expression (18) is formal, and to make it sensible it is necessary to use some limiting transition or to apply some other calculation procedure that would not result in the appearance of 'dangerous denominators'.

Since the hypergeometric series in equation (18) is a finite sum, it may be written in 'inverse order' by reordering it in descending rather than ascending powers of argument. Using for this purpose the general formula (35) from Niukkanen (1983), we obtain the expression for the coefficient $C(k,\tau)$ in terms of the Appell function, F_3:

$$\begin{aligned}C_{m,n}^{\beta,\alpha}(k,\tau)&=(-1)^{m+n}\frac{(\alpha+1)_k(\alpha+k+1)_{n+m}}{m!(\alpha+1)_n}\tau^m\\ &\quad\times{}^2F_{1,0}^{0,2}\left[\begin{matrix}\varnothing;-m,-m-\beta;-n,-n-\alpha;1/\tau,1\\ -\alpha-k-n-m,\varnothing,\varnothing\end{matrix}\right].\end{aligned} \tag{19}$$

Applying the reduction formula (17) from Niukkanen (1983), to the corresponding Lauricella function F_B, with the unit argument, we have

$$\begin{aligned}C_{m,n}^{\beta,\alpha}(k,\tau)&=(-1)^m\frac{1}{m!}(\alpha+n+1)_{k+m-n}(-k-m)_n\tau^m\\ &\quad\times F_2^3\left[\begin{matrix}-m,-m-\beta,-k-m+n;1/\tau\\ -m-\alpha-k,-k-m\end{matrix}\right].\end{aligned} \tag{20}$$

Obviously, expression (20) is correct for any n such that $0\leqslant n\leqslant m+k$. Really, in spite of negative integer denominators, the negative integer numerators assure the termination of the series before the diverging coefficients appear in the sum F_2^3. In the case $\tau=1$ the coefficient $C(k,\tau)$ is expressed in terms of $F_2^3(1)$.

In turn, any finite series $F_2^3(1)$ is equivalent to a Clebsch-Gordan coefficient (Smorodinsky and Shelepin 1972), which indicates an indirect link of the problem under consideration with the linearisation theorem for spherical functions.

Let us consider some particular cases of expansion (4). In the case $k=0$ we obtain the expansion of the Laguerre polynomial $L_m^\beta(\tau x)$ over the Laguerre polynomials of

† We use in equation (17) and hereafter the notation accepted in Niukkanen (1983)). $\varnothing$ indicates an empty set.

different weight with unit scaling multiplier

$$L_m^\beta(\tau x)=\sum_n C_{m,n}^{\beta,\alpha}(0,\tau)L_n^\alpha(x) \tag{21}$$

the corresponding function F_2^3 in equation (20) being reduced to the function F_1^2 due to cancellation of numerator and denominator parameters, i.e.

$$C_{m,n}^{\beta,\alpha}(0,\tau)=\frac{(-1)^m}{m!}(\alpha+n+1)_{m-n}(-m)_n\tau^m F_1^2\left[\begin{matrix}-m-\beta,\ -m+n;\ 1/\tau\\ -m-\alpha\end{matrix}\right]. \tag{22}$$

If, in addition, $\alpha=\beta$ or $\tau=1$, then further reduction of the series F_1^2 takes place: in the first case due to additional cancellation of numerator and denominator parameters, and in the second case as a consequence of the Gauss theorem (Erdélyi 1953, equation 2.1 (14)). As a result, we obtain, as particular cases of equation (21), two standard expansions (Erdélyi 1953, equations 10.12 (40, 39)):

$$L_m^\beta(\tau x)=\sum_n C_{m,n}^{\beta,\beta}(0,\tau)L_n^\beta(x)=\sum_n\binom{\beta+m}{m-n}\tau^n(1-\tau)^{m-n}L_n^\beta(x) \tag{23}$$

and

$$L_m^\beta(x)=\sum_n C_{m,n}^{\beta,\alpha}(0,1)L_n^\alpha(x)=\sum_n\frac{(\beta-\alpha)_{m-n}}{(m-n)!}L_n^\alpha(x). \tag{24}$$

Other cases of reduction of F_2^3 to F_1^2 in equation (20), which we shall not write down in explicit form, correspond to $k=\beta$, $k=-\alpha$ and $k=\beta-\alpha$, which shows a particular simplicity of expansions with functions of $x^\alpha L_n^\alpha$ form on the left- and/or right-hand side of an expansion. The case $m=0$ or $\beta=-m$ corresponds to the expansion of an exponential function over the Laguerre polynomials (in this case $F_2^3(1)=1$ in equation (20)). In some particular cases the series $F_2^3(1)$ can be written as a simple Γ product with the aid of the well known summation theorems (see § 4.4 in Erdélyi (1953)). The case $\beta=-2m-1$ leads to expansion of the Bessel polynomial over the Laguerre polynomials.

It is worth mentioning that there are alternative methods of obtaining equation (20) directly†. First, one can combine the known formulae (23) and (24) to obtain an expansion with coefficients ${}_2F_1(z)$ where $z=\tau(\tau-1)^{-1}$. Applying the analytical continuation formula $z\to 1-z^{-1}$ (see equation 2.10(4), Erdélyi 1953), one can derive equation (22) independently of (20). Differentiating equation (22) k times with respect to τ, we obtain, eventually, equation (20). Another approach is to use the explicit algebraic expressions for Laguerre polynomials in equation (8) to obtain C as a double sum. Expressing the resulting integrals in terms of the Γ functions and transforming the double sum to a one-fold one with the help of the Gauss summation theorem‡ for ${}_2F_1(1)$ one can prove equation (18) directly. Moreover, equation (18) can be transformed into equation (20) by ordering the sum F in descending rather than ascending powers of the argument τ. Therefore one can proceed without the use of the general formulae (Niukkanen 1983) in this relatively simple case. Nevertheless the use of the reduction formulae may serve as a paradigm for more complicated cases (see § 5), where it allows us to save much calculational effort.

† The author is indebted to the referee for this indication.

‡ The use of the Gauss theorem is, actually, equivalent to what is partially implied by 'reduction rules'.

4. Coefficients $C(k, \tau)$: physical and formal applications

Using the coefficients $C(k, \tau)$ of the particular types (22), (23) and (24), one may easily obtain alternative forms of expansions of the general coefficients $C(k, \tau)$ in equation (20), in terms of simpler functions. For this purpose the polynomial multipliers in the integrand of equation (8) should be grouped in such a way that it would be possible to use any two of the three particular expansions indicated in § 3, as well as the orthonormality integral (7). Using, for example, in equation (8), the expansions

$$L_n^{\alpha}(x) = \sum_r C_{n,r}^{\alpha,\alpha+k}(0, 1) L_r^{\alpha+k}(x)$$

$$L_m^{\beta}(\tau x) = \sum_s C_{m,s}^{\beta,\alpha+k}(0, \tau) L_s^{\alpha+k}(x)$$

we obtain, with the help of equation (7),

$$C_{m,n}^{\beta,\alpha}(k, \tau) = \frac{n!}{\Gamma(\alpha+1+n)} \sum_r \frac{\Gamma(\alpha+k+1+r)}{r!} C_{n,r}^{\alpha,\alpha+k}(0, 1) C_{m,r}^{\beta,\alpha+k}(0, \tau). \tag{25}$$

By virtue of relations (24) and (22), equation (25) yields an expansion of $F_2^3(1/\tau)$ in terms of the Gauss functions, $F_1^2(1/\tau)$. In the case $\tau = 1$ equation (25) results in one of the Thomae relations between $F_2^3(1)$ series (Bailey 1935a) which can be used, in particular, for transition to a more symmetric (by n, α and m, β parameters) form for $F_2^3(1)$ series. Another representation of similar type arises when the functions $x^k L_n^{\alpha}(x)$ and $L_m^{\beta}(\tau x)$ in equation (8) are expanded over the Laguerre polynomials, $L_r^{\alpha}(x)$.

The coefficients $C(k, \tau)$ also allow a number of straightforward physical applications. For example, when the Morse oscillator eigenfunctions (Wallace 1976, Ephremov 1977) or the eigenfunctions of the Strum–Liouville equation for the Morse oscillator (Ephremov 1978) are used as a basis set in the variational theory of oscillations of polyatomic molecules, 'a great many matrix elements involving these eigenfunctions must be evaluated. That theory would not be practical if analytic expressions for the matrix elements could not be found' (Wallace 1976). The matrix elements in this quote have the following form in Wallace's (1976) notation:

$$I_{n+j,n}^{\alpha-2j,\alpha}[f] = \int_0^{\infty} \mathrm{d}x\, x^{\alpha-j} \exp(-x) L_{n+j}^{\alpha-2j}(x) f(x) L_n^{\alpha}(x) \tag{26}$$

where $f(x) = 1$, x, $x\mathrm{d}/\mathrm{d}x$. Analytical expressions for integrals (26) were given by Wallace (1976), depending on the form of the operator f, as a combination of some cumbersome sums. With the aid of coefficients $C(k, \tau)$ one may obtain a much more compact expression for integrals (26) both in the case $f = 1$, x, $x\mathrm{d}/\mathrm{d}x$, and for a wider class of operators $f = x^r(\mathrm{d}/\mathrm{d}x)^s$. Indeed, using the differentiation formula for the Laguerre polynomials and taking into account equation (8), we obtain

$$I_{n+j,n}^{\alpha-2j,\alpha}\left[x^r \frac{\mathrm{d}^s}{\mathrm{d}x^s}\right] = (-1)^a \frac{\Gamma(\alpha-j+n+1)}{(n+j)!} C_{n-s,n+j}^{\alpha+s,\alpha-2j}(j+r, 1).$$

By virtue of equation (20) the integral I is expressed as a finite sum $F_2^3(1)$.

The coefficients $C(k, \tau)$ also arise in the theory of molecular electronic states when calculating matrix elements with hydrogen-like functions, $H(\boldsymbol{r})$:

$$H_{\omega nlm}(\boldsymbol{r}) = h_{\omega nl}(r) Y_{lm}(\boldsymbol{r}) \tag{27}$$

$$h_{\omega nl}(r) = (2\omega r)^l L_{n-l-1}^{2l+1}(2\omega r) \exp(-\omega r) \tag{28}$$

where $Y_{lm}(\boldsymbol{r})$ is the spherical function. The case $\omega = 1/n$ corresponds to a hydrogen atom, and $\omega = Z/n$ to a hydrogen-like atom with nuclear charge, Z. Introducing the reduced density

$$\rho_{lm}^{12}(\boldsymbol{r}) = \{H_{\omega_1 n_1 l_1}(\boldsymbol{r}) \otimes H_{\omega_2 n_2 l_2}(\boldsymbol{r})\}_{lm} \tag{29}$$

where the symbol $\{\otimes\}$ denotes the irreducible tensor product (Varshalovich *et al* 1975), one may easily show, for example, that the probability of an electrical 2^l-pole transition is associated with the integral

$$T_l^{12} = \int \mathrm{d}\boldsymbol{r}\, \{\mathcal{Y}_l^0(\boldsymbol{r}) \otimes \rho_l^{12}(\boldsymbol{r})\}_{00}$$

where $\mathcal{Y}_{lm}^0(\boldsymbol{r}) = r^l Y_{lm}(\boldsymbol{r})$ is the regular solid harmonic. Taking into account that (Varshalovich *et al* 1975)

$$\{Y_{l_1}(\boldsymbol{r}) \otimes Y_{l_2}(\boldsymbol{r})\}_{lm} = \left(\frac{(2l_1+1)(2l_2+1)}{4\pi(2l+1)}\right)^{1/2} \langle l_1 0 l_2 0 | l 0\rangle Y_{lm}(\boldsymbol{r}) = H(l_1, l_2, l)\, Y_{lm}(\boldsymbol{r}) \tag{30}$$

where $\langle a\alpha b\beta | c\gamma\rangle$ is the Clebsch-Gordan coefficient, we obtain

$$T_l^{12} = (4\pi)^{1/2} H(l_1, l_2, l) H(l, l, 0)(2\omega_1)^{l_1}(2\omega_2)^{l_2} I_l^{12}/(\omega_1+\omega_2)^{l_1+l_2+l+3}$$

$$I_l^{12} = \int_d^\infty \mathrm{d}r\, r^{l_1+l_2+l+3} \exp(-r) L_{\nu_1}^{2l_1+1}(x_1 r) L_{\nu_2}^{2l_2+1}(x_2 r) \tag{31}$$

where

$$l_2 = |l_1 - l|, |l_1 - l| + 2, \ldots, l_1 + l,$$

$$x_1 = 1 + \nu \qquad x_2 = 1 - \nu \qquad \nu = (\omega_1 - \omega_2)(\omega_1 + \omega_2)^{-1}$$

$$\nu_1 = n_1 - l_1 - 1 \qquad \nu_2 = n_2 - l_2 - 1.$$

Generally, the integral (31) is expressed in terms of the Appell function, F_2,

$$I_l^{12} = \frac{(2l+1)_{\nu_1}(2l_2+1)_{\nu_2}}{\nu_1!\,\nu_2!} \Gamma(l_1+l_2+l+3)^2 F_{0,1}^{1,1}\left[\begin{matrix} l_1+l_2+l+3;\, -\nu_1, -\nu_2;\, x_1, x_2 \\ \varnothing;\, 2l_1+1, 2l_2+1 \end{matrix}\right].$$

For $nl_1 \to nl_2$ transitions a more simple expression via the $C(k, \tau)$ coefficient takes place:

$$I_l^{12} = \frac{\Gamma(n+l_1+1)}{(n-l_1-1)!} C_{n-l_2-1, n-l_1-1}^{2l_2+1, 2l_1+1}(l_2+l-l_1+1, 1)$$

i.e. in accordance with equation (20), the probability of any multipole transitions, in which the principal quantum number does not change, is expressed in terms of the Clausen function, $F_2^3(1)$.

Transforming a part of the polynomial multipliers in the integrand (31) with the help of equation (4),

$$r^{l_2+l-l_1+1} L_{\nu_2}^{2l_2+1}(x_2 r) = \sum_n C_{\nu_2, n}^{2l_2+1, 2l_1+1}(l_2+l-l_1+1, 1) L_n^{2l_1+1}(x_2 r)$$

and taking into account the reduction formula (Erdélyi 1953, equation 5.10 (3))

$$^2F_{0,1}^{1,1}\left[\begin{matrix} 2l_1+2;\, -\nu_1, -n;\, x_1, x_2 \\ \varnothing;\, 2l_1+2, 2l_1+2 \end{matrix}\right] = (1-x_1)^{\nu_1}(1-x_2)^n F_1^2\left[\begin{matrix} -\nu_1, -n;\, \dfrac{x_1 x_2}{(1-x_1)(1-x_2)} \\ 2l_1+2 \end{matrix}\right]$$

we obtain in the general case

$$I_l^{12}=\frac{(2l_1+2)_{\nu_1}}{\nu_1!}\Gamma(2l_1+2)\sum_n C^{2l_2+1,2l_1+1}_{\nu_2,n}(l_2+l-l_1+1,1)$$

$$\times\frac{(2l_1+2)_n}{n!}(1-x_1)^{\nu_1}(1-x_2)^{n_2}F_1^2\left[\begin{matrix}-\nu_1,-n;\dfrac{x_1x_2}{(1-x_1)(1-x_2)}\\ 2l_1+2\end{matrix}\right]. \tag{32}$$

By virtue of the selection rule (13):

$$\nu_2+l_2-l_1-l-1\leqslant n\leqslant\nu_2+l_2+l_1+1$$

the number of terms in the right-hand side of equation (32) is $2l+3$, i.e. increases proportionally to the transition orbital moment. The formulae obtained in this section provide a convenient generalisation of expressions for the probability of dipole electrical transitions (see earlier works on the hydrogen atom cited by Condon and Shortley (1935)) for the case of any multipole transitions.

It is worth noting that expansion (4) also proves to be very useful in calculations of the Fourier transforms of atomic orbitals in the MO LCAO SCF method (Niukkanen 1984a).

5. Generalisation for the case of N variables

The reduced density, equation (29), also enters, as a typical integrand structure, in more complicated four-centre integrals with hydrogen-like functions in variational calculations of molecular electronic structure. The calculation of these integrals is simplified if the irreducible product of the functions H, appearing in equation (29), is expressed as a linear combination of functions H. With due respect to equations (27) and (28) such a linearisation relation should have the form

$$\{H_{\omega_1n_1l_1}(\boldsymbol{r})\otimes H_{\omega_2n_2l_2}(\boldsymbol{r})\}_{lm}=\sum_n Q^{l_1l_2l}_{n_1n_2n}(\omega_1,\omega_2)H_{\omega_1+\omega_2,nlm}(\boldsymbol{r})$$

where coefficients $Q(\omega_1,\omega_2)$ are related to the coefficients $R(\omega_1,\omega_2)$ in the expansion

$$r^{l_1+l_2-l}L^{2l_1+1}_{n_1-l_1-1}(2\omega_1r)L^{2l_2+1}_{n_2-l_2-1}(2\omega_2r)=\sum_n R^{l_1l_2l}_{n_1n_2n}(\omega_1,\omega_2)L^{2l+1}_{n-l-1}[2(\omega_1+\omega_2)r] \tag{33}$$

by

$$(2\omega_1+2\omega_2)^lQ^{l_1l_2l}_{n_1n_2n}(\omega_1,\omega_2)=(2\omega_1)^{l_1}(2\omega_2)^{l_2}H(l_1,l_2,l)R^{l_1l_2l}_{n_1n_2n}(\omega_1,\omega_2).$$

In turn, relation (33) is an obvious generalisation of expansion (3) for the case of two Laguerre polynomials in the left-hand side of the equation. Since general formulae have a similar structure for any number of the Laguerre polynomials, we consider the most general expansion of this type

$$t^kL^{\alpha_1}_{n_1}(x_1t)\dots L^{\alpha_N}_{n_N}(x_Nt)=\sum_n C^{\alpha_1\dots\alpha_N\alpha}_{n_1\dots n_Nn}(k;x_1,\dots,x_N;x)L^{\alpha}_n(xt). \tag{34}$$

Obviously, the coefficients R in equation (33) are a particular case of the coefficients C:

$$R^{l_1l_2l}_{n_1n_2n}(\omega_1,\omega_2)=C^{2l_1+1,2l_2+1,2l+1}_{n_1-l_1-1,n_2-l_2-1,n-l-1}(l_1+l_2-l;2\omega_1,2\omega_2;2\omega_1+2\omega_2). \tag{35}$$

General properties of the coefficients C in equation (34) may be easily obtained by analogy with the reasoning given in §§ 2 and 3. In particular, just as in the case of equations (4) and (5), we have

$$C^{\alpha_1 \ldots \alpha_N \alpha}_{n_1 \ldots n_N n}(k; x_1, \ldots, x_N; x) = x^{-k} C^{\alpha_1 \ldots \alpha_N \alpha}_{n_1 \ldots n_N n}\left(k; \frac{x_1}{x}, \ldots, \frac{x_N}{x}\right)$$

where

$$t^k L^{\alpha_1}_{n_1}(x_1 t) \ldots L^{\alpha_N}_{n_N}(x_N t) = \sum_n C^{\alpha_1 \ldots \alpha_N \alpha}_{n_1 \ldots n_N n}(k; x_1, \ldots, x_n) L^{\alpha}_n(t).$$

Transforming the integral representation

$$C^{\alpha_1 \ldots \alpha_N \alpha}_{n_1 \ldots n_N n}(k; x_1, \ldots, x_N) = \frac{n!}{\Gamma(\alpha+1+n)} \int_0^{\infty} \mathrm{d}t\, t^{\alpha+k} \exp(-t) L^{\alpha_1}_{n_1}(x_1 t) \ldots L^{\alpha_N}_{n_N}(x_N t) L^{\alpha}_n(t) \tag{36}$$

to a form similar to equation (10), and for the case $x_s = 1$ to a form similar to equation (12), we obtain the following selection rule:

$$\max[0, n_s - n_1 - \ldots - n_{s-1} - n_{s+1} - \ldots - n_N - \alpha + \alpha_s - k] \leqslant n \leqslant k + n_1 + \ldots + n_N.$$

Using exactly the same reasoning as in § 3, we arrive at the following two expressions for coefficients C in terms of the functions ${}^N F$ (Niukkanen 1983), which are similar to equations (18) and (20), respectively†

$$C^{\alpha_1 \ldots \alpha_N \alpha}_{n_1 \ldots n_N n}(k; x_1, \ldots, x_N) = \prod_{s=1}^{N} \frac{(\alpha_s + 1)_{n_s}}{n_s!} \frac{(\alpha+1)_k (-k)_n}{(\alpha+1)_n} \times {}^N F^{2,1}_{1,1}\left[\begin{matrix} \alpha+k+1, k+1; -n_1, \ldots, -n_N; x_1, \ldots, x_N \\ k-n+1; \alpha_1+1, \ldots, \alpha_N+1 \end{matrix}\right] \tag{37}$$

$$C^{\alpha_1 \ldots \alpha_N \alpha}_{n_1 \ldots n_N n}(k; x_1, \ldots, x_N) = \prod_{s=1}^{N} \frac{(-x_s)^{n_s}}{n_s!} (\alpha+n+1)_{n_1+\ldots+n_N+k-n} (-k-n_1-\ldots-n_N)_n \times {}^N F^{1,2}_{2,0}\left[\begin{matrix} n-n_1-\ldots-n_N-k; -n_1, -\alpha_1-n_1, \ldots, -n_N, -\alpha_N-n_N; x_1^{-1}, \ldots, x_N^{-1} \\ -\alpha-n_1-\ldots-n_N-k, -n_1-\ldots-n_N-k; \varnothing \ldots \varnothing \end{matrix}\right]. \tag{38}$$

Generally, to calculate the coefficients C, recurrence relations and explicit expressions for the functions ${}^N F$ given in Niukkanen (1983) may be used. In the special case of the coefficients C in equation (35), in which the quantities k, α_s and α are interrelated by a linear relation, it is expedient to use such a recurrence equation that would not violate this relation, i.e. that would not involve in the recursion some coefficients other than R. For this purpose we use for coefficients R the integral representation of the

† Expressing polynomials L in equation (36) as a Kummer function Φ one can easily represent the coefficient C through the Lauricella function F_A depending on $N+1$ variables. In the case of $k=0$ this is equivalent to an earlier (Erdélyi 1936a) result. The possibility of expressing coefficients C through functions ${}^N F^{2,1}_{1,1}$ and ${}^N F^{1,2}_{2,0}$ depending on lesser number of variables is an evident advantage of our approach.

type (8)

$$R^{l_1 l_2 l}_{n_1 n_2 n}(\omega_1, \omega_2) = \frac{(n-l-1)!}{(n+l)!(2\omega_1+2\omega_2)^{l_1+l_2-l}} I^{l_1, l_2, l}_{n_1-l_1-1, n_2-l_2-1, n-l-1}(\omega_1', \omega_2')$$

$$I^{l_1 l_2 l}_{\nu_1 \nu_2 \nu}(\omega_1', \omega_2') = \int_0^\infty \mathrm{d}r\, r^{l_1+l_2+l+1} \exp(-r) L^{2l_1+1}_{\nu_1}(2\omega_1' r) L^{2l_2+1}_{\nu_2}(2\omega_2' r) L^{2l+1}_{\nu}(r)$$

where $\omega_1' = \omega_1(\omega_1+\omega_2)^{-1}$, $\omega_2' = \omega_2(\omega_1+\omega_2)^{-1}$.

Then, taking into account the recurrence relation for $L_n(x)$

$$nL^\alpha_n(x) = (n+\alpha)L^\alpha_{n-1}(x) - \alpha L^{\alpha+2}_{n-1}(x) + xL^{\alpha+2}_{n-2}(x)$$

which is a consequence of two standard relations for the Laguerre polynomials (Erdélyi 1953, equations 10.12 (23) and (24)), we obtain the necessary recurrence equation

$$\nu_1 I^{l_1 l_2 l}_{\nu_1 \nu_2 \nu}(\omega_1', \omega_2') = (\nu_1 + 2l_1 + 1) I^{l_1 l_2 l}_{\nu_1-1, \nu_2 \nu}(\omega_1', \omega_2') - \omega_1' I^{l_1-1, l_2 l}_{\nu_1-1, \nu_2 \nu}(\omega_1', \omega_2')$$
$$+ \omega_1' I^{l_1+1, l_2 l}_{\nu_1-2, \nu_2 \nu}(\omega_1', \omega_2')$$

as well as two similar relations for the indexes l_2, ν_2 and l, ν. Initial values for such a system of equations are either the Appell functions F_2, if the recursion over only one of ν_1, ν_2, ν indexes is used, or the Gauss functions, F^2_1, if the recursion over two indexes is utilised.

6. Expansion of the product $L^{\alpha_1}_{n_1}(u_1x)L^{\alpha_2}_{n_2}(u_2x)$ in terms of $L^{\alpha_1+\alpha_2}_n[(u_1+u_2)x]$

In some special cases there is no need in using general formulae for the coefficients C. Let us consider, for example, an alternative formulation of the linearisation theorem for the particular case of practical interest

$$N=2, \qquad k=0, \qquad \alpha=\alpha_1+\alpha_2, \qquad x=x_1+x_2$$

in equation (34), that leads to an especially simple expression for the coefficients C and thus yields a non-trivial reduction rule for the functions ${}^N F$ in equations (37) and (38).

Using in the Rodriguez formula for the Laguerre polynomials the differential identity

$$\frac{\mathrm{d}^n}{\mathrm{d}x^n} f(x) = x^{-n} \frac{\mathrm{d}^n}{\mathrm{d}\lambda^n} f(\lambda x)\bigg|_{\lambda=1}$$

we obtain the following 'parametric' representation for $L^\alpha_n(x)$:

$$L^\alpha_n(x) = \frac{1}{n!} \mathrm{e}^x\, \mathrm{d}^n(\lambda) \lambda^{n+\alpha}\, \mathrm{e}^{-\lambda x}\bigg|_{\lambda=1} \tag{39}$$

where $\mathrm{d}(\lambda) \equiv \mathrm{d}/\mathrm{d}\lambda$. Then

$$L^{\alpha_1}_{n_1}(u_1x)L^{\alpha_2}_{n_2}(u_2x) = \frac{1}{n_1!\,n_2!} \exp(-ux)\, \mathrm{d}^{n_1}(\lambda_1)\, \mathrm{d}^{n_2}(\lambda_2)\, \lambda_1^{n_1+\alpha_1} \lambda_2^{n_2+\alpha_2}$$
$$\times \exp[-(u_1'\lambda_1 + u_2'\lambda_2)ux]\bigg|_{\lambda_1=\lambda_2=1}$$

where

$$u = u_1 + u_2 \qquad u_1' = u_1/u \qquad u_2' = u_2/u.$$

Changing the variables λ_1, λ_2 to new variables

$$\lambda = u_1'\lambda_1 + u_2'\lambda_2 \qquad \mu = \lambda_1 - \lambda_2$$

and taking into account that

$$\lambda_1 = \lambda + u_2'\mu \qquad \lambda_2 = \lambda - u_1'\mu$$

$$\mathrm{d}(\lambda_1) = u_1'\,\mathrm{d}(\lambda) + \mathrm{d}(\mu) \qquad \mathrm{d}(\lambda_2) = u_2'\,\mathrm{d}(\lambda) - \mathrm{d}(\mu)$$

we have

$$\begin{aligned} L_{n_1}^{\alpha_1}(u_1x)L_{n_2}^{\alpha_2}(u_2x) &= \frac{1}{n_1!\,n_2!}(-1)^{\alpha_2}\exp(-ux)u_1'^{\,n_2+\alpha_2}u_2'^{\,n_1+\alpha_1}(\mathrm{d}(\mu)+u_1'\,\mathrm{d}(\lambda))^{n_1}(\mathrm{d}(\mu)-u_2'\,\mathrm{d}(\lambda))^{n_2} \\ &\quad \times(\mu+u_2'^{-1}\lambda)^{n_1+\alpha_1}(\mu-u_1'^{-1}\lambda)^{n_2+\alpha_2}\exp(-\lambda ux)\Big|_{\lambda=1,\mu=0}. \end{aligned} \tag{40}$$

Applying equation (34) from Niukkanen (1983) for the case $N = 2$, taking into account that the Lauricella functions, F_D, arising in such an expansion are transformed into the Gauss functions, F_1^2, and writing down the functions F_1^2 through the Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$, we have

$$(M+U_1\Lambda)^{\nu_1}(M+U_2\Lambda)^{\nu_2} = U_1^{\nu_1}U_2^{\nu_2}\sum_i \Lambda^{\nu_1+\nu_2-i}M^i\left(\frac{U_2-U_1}{U_2U_1}\right)^i P_i^{(\nu_1-i,\nu_2-i)}\left(\frac{U_2+U_1}{U_2-U_1}\right). \tag{41}$$

Using expansion (41) both for the product of operator binomials, and for the product of non-operator binomials in equation (40), taking into account that $u_1'+u_2'=1$, making appropriate differentiations, expressing the derivative with respect to λ via relation (39) and taking into account that, by virtue of $\mu=0$, the resulting double sum is reduced to a simple one, we can assert finally that the coefficients C in the expansion

$$L_{n_1}^{\alpha_1}(u_1x)L_{n_2}^{\alpha_2}(u_2x) = \sum_n C_{n_1,n_2,n}^{\alpha_1,\alpha_2,\alpha}(0;u_1,u_2)L_n^{\alpha}(x) \tag{42}$$

have the following simple form:

$$\begin{aligned} C_{n_1,n_2,n}^{\alpha_1,\alpha_2,\alpha_1+\alpha_2}(0;u_1,u_2) &= \frac{n!\,(n_1+n_2-n)!}{n_1!\,n_2!}u_1^{n-n_2}u_2^{n-n_1} \\ &\quad \times P_{n_1+n_2-n}^{(n-n_2,n-n_1)}(u_2-u_1)P_{n_1+n_2-n}^{(\alpha_1+n-n_2,\alpha_2+n-n_1)}(u_2-u_1) \end{aligned} \tag{43}$$

provided that $u_1+u_2=1$ and $\alpha_1+\alpha_2=\alpha$.

Note that the expansion (42) is a series of Clebsch-Gordan type with the constant weight $\alpha=\alpha_1+\alpha_2$ of Laguerre polynomials in the right-hand side, whereas Bailey and Howell expansions, for example, are modified series of Clebsch-Gordan type (for particular values of parameters) with the weight indexes depending on the summation variable n (see § 1).

Using definitions (27) and (28), equation (41) can be easily reformulated for hydrogen-like functions or their radial parts. Using expansion (42) in equations (31) and (36) for $N=2$, one may obtain alternative expansions over the Jacobi polynomials for both the transition probability integral I_l^{12} and the coefficient $C(k;u_1,u_2;u)$ of general type. In the cases $n_2=0$ or $\alpha_2=-n_2$ expansion (42) is equivalent to particular types of expansions discussed in § 3. If $n_1=n_2$, or $\alpha_1+n_1=\alpha_2+n_2$ or $n_1=n_2$ and $\alpha_1=\alpha_2$, then in the product of the Jacobi polynomials on the right-hand side of equation (43) the first multiplier or the second one, or both of them, respectively, turn out to be the Gegenbauer polynomials, C_m^λ (Erdélyi 1953, equation 10.9 (4)). Since the quantity $C_m^\lambda(0)$ has a form of Γ product (Erdélyi 1953, equation 10.9 (19)), this means that in the case $n_1=n_2$, $\alpha_1=\alpha_2$, $u_1=u_2$, the coefficient C in equation (43) has a simple form of Pochhammer symbols product.

Equation (43) can be obtained with the help of another method which can also be used to prove one of Koornwinder's positivity theorems (see § 1) in a more appropriate and compact way. Using the integral representation (8) for C in equation (42), transforming $L_n^\alpha(x)$ with the help of the Rodriguez formula, integrating by parts n times, applying the Leibnitz rule for the product derivative and expressing the derivatives of the Laguerre polynomials with the help of the standard formula (Erdélyi 1953, equation 10.12 (15)), we have

$$C_{n_1 n_2 n}^{\alpha_1\alpha_2\alpha}(0; u_1, u_2)=\frac{n!}{\Gamma(\alpha+1+n)}\sum_{[i_1 i_2|n]}\frac{u_1^{i_1}u_2^{i_2}}{i_1!\,i_2!}$$
$$\times\int_0^\infty \mathrm{d}x\, x^{\alpha+i_1+i_2}\exp(-x)L_{n_1-i_1}^{\alpha_1+i_1}(u_1x)L_{n_2-i_2}^{\alpha_2+i_2}(u_2x) \tag{44}$$

where $[i_1i_2|n]$ denotes the set of conditions $i_1\geqslant 0$, $i_2\geqslant 0$, $i_1+i_2=n$. Provided that $u_1=u_2=1$ and $\alpha=\alpha_1+\alpha_2$ (see equation (1)), one can use the following known formula†

$$\int_0^\infty \mathrm{d}x\, x^{\alpha_1+\alpha_2}\exp(-x)L_{n_1}^{\alpha_1}(x)L_{n_2}^{\alpha_2}(x)=\Gamma(\alpha_1+\alpha_2+1)\frac{(-\alpha_2-n_2)_{n_1}(-\alpha_1-n_1)_{n_2}}{n_1!\,n_2!} \tag{45}$$

which is another particular case of the coefficients $C(k,\tau)$ (see equations (8) and (20)). In the case of non-negative integral α_1 and α_2 this gives a representation of C in equation (44) as the product of of an explicitly positive expression and the factor $(-1)^{n_1+n_2-n}$. In other words, this method not only gives us a positivity proof for C_i in equation (1) but also leads to an explicitly positive, i.e. containing only non-negative contributions, expression for Koornwinder's coefficients.

One can transform equation (44) to the form of equation (43) with the aid of the following argument. If use is made of the Rodriguez formula for both the L in equation (44), then putting $u_1+u_2=1$ and $\alpha=\alpha_1+\alpha_2$ (see the note following equation (43)), one can verify that cancellation of both the exponential and the power factors takes place in the integrand of equation (44). This makes it easy to proceed with integration by parts which leads, eventually, to equation (43). Note that an equivalent approach is applicable to the product of Jacobi polynomials. This gives an alternative method of expanding the product $P_{n_1}^{(\alpha_1,\beta_1)}(x)P_{n_2}^{(\alpha_2,\beta_2)}(x)$ in terms of $P_n^{(\alpha_1+\alpha_2,\beta_1+\beta_2)}(x)$ (cf Vilenkin 1965).

Equation (42) can also be applied to give a new simple proof of the second Koornwinder positivity theorem (see equation (2)). Really, multiplying both sides of equation (42) by $S_1^{n_1}S_2^{n_2}$ we can carry out the summation over all integral n_1, n_2 with the help of the generating function for Laguerre polynomials (Erdélyi 1953, equation 10.12 (17)). Writing down the resulting exponential function and the polynomial $L_n^\alpha(x)$

† This formula is given by equation 7.414 (9) in Gradstein and Ryzhik (1971) with some misprints. The correct form is given by equation (45).

as ${}_0F_0$ and ${}_1F_1$, respectively, and applying the operator ${}_1F_0[\alpha+1;\, z\,\partial/\partial x]_{x=0}$ (Niukkanen 1983) to both sides of the equation, one can obtain a simple generating function for the coefficients C in equation (42). In the case $\alpha_1=\alpha_2=\alpha$ and $u_1+u_2=1$ (see equation (2)) such a function proves to be a product of the generating function f_0, corresponding to $\alpha=0$, and a simple function f_1 which can readily be represented by the Taylor series in $S_1^{n_1}S_2^{n_2}$ with the positive coefficients C_1. Note that equation (43) gives an explicitly positive expression for the coefficients C_0 of the second Koornwinder expansion equation (2) for the important particular case $\alpha=0$.

By definition the quantities C_0 represent the coefficients in the Taylor expansion of f_0. Since the product of two Taylor series with positive coefficients is again a series with positive coefficients, this argument should give, apparently, a simple positivity proof for the coefficients of the second Koornwinder expansion equation (2)†.

7. Modified series of Clebsch–Gordan type for the product of the Laguerre polynomials

An alternative type of linearisation theorem for the $L_{n_1}^{\alpha_1}(u_1x)L_{n_2}^{\alpha_2}(u_2x)$ product arises when the integral representation of L_n^α polynomials via the Bessel function, J_α, is used:

$$L_n^\alpha(x)=\frac{2}{n!}x^{-\alpha/2}\,e^x\int_0^\infty \mathrm{d}\tau\, t^{\alpha+1+2n}\,\mathrm{e}^{-\tau^2}J_\alpha(2\tau\sqrt{x}) \qquad \alpha+n+1>0 \tag{46}$$

which is obtained by a square substitution of the integration variable in the standard integral representation for L_n^α (Erdélyi 1953, equation 10.12 (21)). We transform each of the two multipliers L by means of equation (46), denote the corresponding integration variables by τ_1, τ_2 and introduce polar coordinates τ, φ in the τ_1, τ_2 plane ($\tau_1=\tau\cos\varphi$, $\tau_2=\tau\sin\varphi$). Introducing an arbitrary parameter, u, we use the Bailey (1935b) linearisation theorem (see also equation 7.15 (7) in Erdélyi (1953) and § 7 in Niukkanen (1983))‡

$$\begin{aligned}J_{\alpha_1}(w_1z)J_{\alpha_2}(w_2z)&=\frac{w_1^{\alpha_1}w_2^{\alpha_2}}{\Gamma(\alpha_1+1)\Gamma(\alpha_2+1)}\sum_{k=0}^{\infty}\frac{(\gamma+2k)\Gamma(\gamma+k)}{k!}\\&\quad\times{}^2F_{0,1}^{2,0}\left[\begin{matrix}-k,\ \gamma+k;\varnothing,\varnothing;\ w_1^2,\ w_1^2\\ \varnothing;\ \alpha_1+1,\ \alpha_2+1\end{matrix}\right]J_{\gamma+2k}(z)\end{aligned} \tag{47}$$

for the following values of parameters:

$$w_1=(u_1/u)^{1/2}\cos\varphi \qquad w_2=(u_2/u)^{1/2}\sin\varphi \qquad z=2\tau(ux)^{1/2}$$

The quantity γ, for the time being, is arbitrary, and this gives us an opportunity to simplify the resulting expansion at a final stage. If the quantity $\mu=\alpha_1+\alpha_2+1-\gamma$ assumes an integral value and if $k\leqslant n_1+n_2+\mu$ then according to equation (46), the integral over variable τ is expressed in terms of the Laguerre polynomial. As a result,

† This reasoning resulted from the discussion which took place in course of communication with the referee. The details of the approach will be published in a separate paper.

‡ Hypergeometric series, ${}^2F$, in equation (47) is just the Appell function, F_4, in the notation of Niukkanen (1983).

we obtain

$$L_{n_1}^{\alpha_1}(u_1x)L_{n_2}^{\alpha_2}(u_2x)$$
$$=2[n_1!\,n_2!\,\Gamma(\alpha_1+1)\Gamma(\alpha_2+1)]^{-1}\exp[-(u-u_1-u_2)x]$$
$$\times\sum_k\frac{\gamma+2k}{k!}\Gamma(\gamma+k)(n_1+n_2+\mu-k)!\,G_{n_1,n_2}^{\alpha_1,\alpha_2}\left(k,\gamma;\frac{u_1}{u},\frac{u_2}{u}\right)L_{n_1+n_2+\mu-k}^{\gamma+2k}(ux) \tag{48}$$

where

$$G_{n_1,n_2}^{\alpha_1,\alpha_2}\left(k,\gamma;\frac{u_1}{u},\frac{u_2}{u}\right)$$
$$=\int_0^{\pi/2}d\varphi(\cos\varphi)^{2\alpha_1+2n_1+1}(\sin\varphi)^{2\alpha_2+2n_2+1}$$
$$\times{}^2F_{0,1}^{2,0}\left[\begin{matrix}-k,\gamma+k;\varnothing,\varnothing;\frac{u_1}{u}\cos^2\varphi,\frac{u_2}{u}\sin^2\varphi\\ \varnothing;\alpha_1+1,\alpha_2+1\end{matrix}\right]. \tag{49}$$

By term-by-term integration of the series on the right-hand side of equation (49), one can easily show that the function G is expressed as a hypergeometric series of higher rank

$$G_{n_1,n_2}^{\alpha_1,\alpha_2}\left(k,\gamma;\frac{u_1}{u},\frac{u_2}{u}\right)$$
$$=\frac{1}{2}\frac{\Gamma(\alpha_1+n_1+1)\Gamma(\alpha_2+n_2+1)}{\Gamma(\alpha_1+\alpha_2+n_1+n_2+2)}$$
$$\times{}^2F_{1,1}^{2,1}\left[\begin{matrix}-k,\gamma+k;\alpha_1+n_1+1,\alpha_2+n_2+1;u_1/u,u_2/u\\ \alpha_1+\alpha_2+n_1+n_2+2;\alpha_1+1,\alpha_2+1\end{matrix}\right].$$

Expansion (48) still has a formal character since, though the quantity $\mu=\alpha_1+\alpha_2+1-\gamma$ can be made an integer by choosing γ, the inequality $k\leqslant n_1+n_2+\mu$, under which the right-hand side of equation (48) has meaning, is an outside condition and does not follow so far from the properties of coefficients. As a result of the condition $u_1+u_2=u$, not only does the exponential term in equation (48) vanish, but we also arrive at the desired selection rule, $k\leqslant n_1+n_2+\mu$, for the function G. Indeed, if $u=u_1+u_2$, then the arguments of the function ${}^2F_{0,1}^{2,0}$ on the right-hand side of equation (49) can be written as

$$(u_1/u)\cos^2\varphi=x(1-y)\qquad(u_2/u)\sin^2\varphi=y(1-x)$$

where $x=\cos^2\varphi$, $y=u_2/u$. This makes it possible to use the expansion (Burchnall and Chaundy 1940, equation (54)):

$${}^2F_{0,1}^{2,0}\left[\begin{matrix}a,b;\varnothing;x(1-y),y(1-x)\\ \varnothing;c,d\end{matrix}\right]$$
$$=\sum_r\frac{(a)_r(b)_r(a+b-c-d+1)_r}{(c)_r(d)_r r!}x^rF_1^2\left[\begin{matrix}a+r,b+r;x\\ c+r\end{matrix}\right]y^rF_1^2\left[\begin{matrix}a+r,b+r;y\\ c+r\end{matrix}\right]$$

for the function ${}^2F$ in equation (49). Writing down the Gauss functions, F_1^2, in the form of Jacobi polynomials, we obtain:

$$G^{\alpha_1,\alpha_2}_{n_1,n_2}\left(k,\gamma;\frac{u_1}{u},\frac{u_2}{u}\right)=\sum_r(-1)^r\frac{k!(k-r)!(\gamma+k)_r(-\mu)_r}{(\alpha_1+1)_k(\alpha_2+1)_k r!}$$
$$\times Z(r)\left(\frac{u_2}{u}\right)^r P^{(\gamma-\alpha_2-1+r,\alpha_2+r)}_{k-r}\left(\frac{u_2-u_1}{u_2+u_1}\right) \tag{50}$$

where

$$Z(r)=\int_0^{\pi/2}\mathrm{d}\varphi(\cos\varphi)^{2\alpha_1+2n_1+2r+1}(\sin\varphi)^{2\alpha_2+2n_2+1}P^{(\gamma+r-\alpha_1-1,\alpha_1+r)}_{k-r}(\cos 2\varphi). \tag{51}$$

On the right-hand side of equation (50) we have $0\leqslant r\leqslant k$ and $r\leqslant\mu$ if $\mu=0,1,2,\ldots$. Introducing the integration variable, $t=\cos 2\varphi$, into equation (51), the function $Z(r)$ may be written, by analogy with equation (10), as a scalar product of the Jacobi polynomial (with the proper weight function) by some 'residual' expression, which turns out to be polynomial if $\mu+n_2-r=0,1,2,\ldots$. This condition will be satisfied for any values of n_2, if $r\leqslant\mu$. Since the condition $r\leqslant\mu$ is satisfied for integral μ by virtue of the Pochhammer symbol $(-\mu)_r$ on the right-hand side of equation (50), we obtain, by analogy with the relation (9), the necessary selection rule $k\leqslant n_1+n_2+r$ according to which the value Z and, respectively, the function G are non-zero. The algebraic expression for the function $Z(r)$ is given by the standard relation (Gradstein and Ryzhik 1971, equation 7.391 (2)) (we introduce the missing multiplier $(\alpha+1)_n/n!$ into the right-hand side of this formula)

$$\int_{-1}^{1}\mathrm{d}t(1-t)^\rho(1+t)^\sigma P^{(\alpha,\beta)}_n(t)$$
$$=2^{\rho+\sigma+1}\frac{\Gamma(\rho+1)\Gamma(\sigma+1)}{\Gamma(\rho+\sigma+2)}\frac{(\alpha+1)_n}{n!}F^3_2\left[\begin{matrix}-n,n+\alpha+\beta+1,\rho+1;1\\ \alpha+1,\rho+\sigma+2\end{matrix}\right].$$

Combining the obtained transformations and selection rules, we come to the following result. Let γ be chosen so that the quantity $\mu\equiv\alpha_1+\alpha_2+1-\gamma$ assumes a non-negative integer value. Then the following linearisation theorem takes place:

$$L^{\alpha_1}_{n_1}(u_1x)L^{\alpha_2}_{n_2}(u_2x)$$
$$=\frac{\Gamma(\alpha_2+n_2+1)}{n_1!\,n_2!}\sum_k\frac{(\gamma+2k)(n_1+n_2+\mu-k)!}{\Gamma(\alpha_1+k+1)\Gamma(\alpha_2+k+1)}$$
$$\times R^{\alpha_1,\alpha_2}_{n_1,n_2}(\gamma,k;u_1,u_2)[(u_1+u_2)x]^k L^{\gamma+2k}_{n_1+n_2+\mu-k}[(u_1+u_2)x] \tag{52}$$

where $0\leqslant k\leqslant n_1+n_2+\mu$ and

$$R^{\alpha_1,\alpha_2}_{n_1,n_2}(\gamma,k;u_1,u_2)=\sum_r(-1)^r\frac{(\gamma-\alpha_1+r)_{k-r}\Gamma(\gamma+k+r)(-\mu)_r}{r!\,\Gamma(\alpha_1+\alpha_2+n_1+n_2+r+2)}$$
$$\times F^3_2\left[\begin{matrix}-k+r,k+\gamma+r,\alpha_2+n_2+1;1\\ \gamma-\alpha_1+r,\alpha_1+\alpha_2+n_1+n_2+r+2\end{matrix}\right]$$
$$\times\left(\frac{u_2}{u_1+u_2}\right)^2 P^{(\gamma-\alpha_2-1+r,\alpha_2+r)}_{k-r}\left(\frac{u_2-u_1}{u_2+u_1}\right) \tag{53}$$

where $0\leqslant r\leqslant\min(k,\mu)$.

In the case $\gamma=\alpha_1+\alpha_2+1$ only a single term with $r=0$ survives on the right-hand side of equation (53), and the linearisation theorem, equation (52), assumes a simpler form:

$$
\begin{aligned}
&L_{n_1}^{\alpha_1}(u_1x)L_{n_2}^{\alpha_2}(u_2x)\\
&\quad=\frac{\Gamma(\alpha_2+n_2+1)\Gamma(\alpha_1+n_1+1)}{n_1!\,n_2!\,\Gamma(\alpha_1+\alpha_2+n_1+n_2+2)}\sum_{k=0}^{n_1+n_2}\frac{(\alpha_1+\alpha_2+2k+1)\Gamma(\alpha_1+\alpha_2+k+1)}{k!\,\Gamma(\alpha_1+k+1)}\\
&\quad\quad\times(n_1+n_2-k)!\,F_2^3\left[\begin{matrix}-k,\ \alpha_1+\alpha_2+k+1,\ \alpha_2+n_2+1;\ 1\\ \alpha_2+1,\ \alpha_1+\alpha_2+n_1+n_2+2\end{matrix}\right]P_k^{(\alpha_1,\alpha_2)}\left(\frac{u_2-u_1}{u_2+u_1}\right)\\
&\quad\quad\times[(u_1+u_2)x]^k L_{n_1+n_2-k}^{\alpha_1+\alpha_2+1+2k}[(u_1+u_2)x] \qquad (54)
\end{aligned}
$$

which is equivalent to an earlier (Carlitz 1957) result. This result was rediscovered later in nuclear physics with the help of the group theoretical approach†. By taking various normalisations into account, the coefficient F_2^3 appears as a Clebsch-Gordan coefficient of SU_2, if α_1 and α_2 are integers. Half-integral values of α_1 and α_2 have been considered by Knyr *et al* (1976). Seven different formulae and recurrence relations have been given by Raynal (1976), all these formulae being equivalent and valid for arbitrary values of α_1 and α_2. The case of arbitrary values of α_1 and α_2 has also been considered more recently by Chacon *et al* (1979). It is worth noting that there are 8 symbols F_2^3 with two negative integers, and 20 with one negative integer as a consequence of Whipple relations (Raynal 1978). Note also that such symbols as F_2^3 are closely connected with the well known 'Regge symbols'.

So equations (52) and (54) give a good way of comparing classical and group theoretical methods. It seems that the latter are more elegant and efficient in particular cases but the former have a wider field of application. Note that from the classical point of view the difference between the integral, half-integral and arbitrary values of α_1 and α_2 seems to be artificial and, therefore, many difficulties can be avoided. On the other hand, we have a more general equation (52) that is more useful in applications since it allows us a possibility of shifting the weight index in the Laguerre polynomials. This expansion seems to be a 'hard nut' for the group theoretical methods.

In some particular cases expansion (54) can be transformed to a simpler form.

In the case $n_1=n_2$ and $\alpha_1=\alpha_2$ the series F_2^3 (1) in equation (54) may be summed up with the help of the Watson theorem (Erdélyi 1953, equation 4.4 (6)). As a result, the coefficients in equation (54) assume a simple form of Γ products. If $\alpha_1=\alpha_2$ and $u_1=u_2$, then, as in the case considered in § 6, the Jacobi polynomial assumes a simple form of Γ product. Note that these two cases give analogues of the Bailey and Howell theorems (see § 1) with the difference that the Laguerre polynomial on the right-hand sides of our expansions has the multiplier, x^k, rather than x^{2k}. It is worth noting also that in the case $n_2=0$ the series F_2^3 (1) in equation (54) reduces to the function F_1^2 (1) which is summed up by means of the Gauss theorem. In this case expansion (54) transforms into the Erdélyi (1936b) multiplication theorem (see also equation 6.14 (7) in Erdélyi (1953)).

8. Conclusions

It is shown that the product $x^kL_{n_1}^{\alpha_1}(u_1x)\ldots L_{n_N}^{\alpha_N}(u_Nx)$ is expressed as a linear combination of polynomials $L_n^{\alpha}(ux)$ with coefficients C having a form of generalised hypergeometric series, ${}^NF$ (Niukkanen 1983). In some particular cases the coefficients C

† Technically, this approach is closely related to hyperspherical harmonics formalism (see, for example, Raynal 1976). The author is indebted to Professor J Raynal for useful discusion of the group theoretical topics.

assume an especially simple form: for $N=1$ they are expressed via the Clausen function, $F^3_2\,(1/u_1)$, and for $k=0$ and $N=2$ either as a product of two Jacobi polynomials (for the case of a series of Clebsch-Gordan type), or as a product of the Clausen function, $F^3_2\,(1)$, by the Jacobi polynomial (in the case of a series of modified type). On the one hand, these special forms of linearisation theorems give reduction rules for the series ${}^NF$ of a particular type and, besides, allow us to represent the corresponding series ${}^NF$ of a more general type as expansions in terms of simpler functions. On the other hand, particular types of linearisation theorems are general enough for many physical applications. In particular, these linearisation relations can be easily reformulated for the hydrogen-like functions, which considerably facilitates the analytical formulation of the multicentre integral problem in variational calculations of molecular electron wavefunctions.

Many types of expansions known from literature turn out to be particular cases of expansions presented in this paper that result in unifying numerous relations involving Laguerre polynomials.

Acknowledgments

I express my gratitude to Professor L A Gribov whose kind attention to the present work greatly contributed to its development and completion.

I am very indebted to Professor J Raynal for useful discussion of the SU_2 formalism. I highly appreciate the referee's suggestions which inspired some new proofs and relations. I am very obliged to Professor N Ya Vilenkin for general discussion of the results presented in this paper.

Note added in proof. Useful additional comments on *operator factorisation relations*, like that mentioned at the end of § 6 in connection with positivity proofs, are given in Niukkanen (1984b).

References

Askey R, Koornwinder T and Ismail M 1978 *J. Combinatorial Theory* A **25** 277-87
Bailey W N 1935a *Generalized Hypergeometric Series* (Cambridge: Cambridge University Press)
—— 1935b *Q. J. Math.* **6** 233-8
—— 1936 *Proc. London Math. Soc.* **41** 215-20
Burchnall J L and Chaundy T W 1940 *Oxford J. Math.* **11** 249-270
—— 1941 *Oxford J. Math.* **12** 112-28
Carlitz L 1957 *Boll. Unione Mat. Ital. Ser. III* **12** 34-40
Chacon E, Moshinsky M and Winternitz P 1979 *Kinam* **1** 259-68
Condon E U and Shortley G H 1935 *The Theory of Atomic Spectra* (Cambridge: Cambridge University Press)
Durand L 1977 *SIAM J. Math. Anl.* **8** 541-6
Ephremov Yu S 1977 *Opt. Spectrosk.* **43** 1174-6
—— 1978 *Opt. Spectrosk.* **44** 198-201
Erdélyi A 1936a *Math. Z.* **40** 693-702, **42** 125-43
—— 1936b *Monatsh. Math. Phys.* **45** 31-52
Erdélyi A (ed) 1953 *Higher Transcendental Functions* vol 1 and 2 (New York: McGraw-Hill)
Gradstein I S and Ryzhik I M 1971 *Tables of integrals, sums, series and products* (Moscow: Nauka) (in Russian)
Howell W T 1937 *Phil. Mag.* **24** 396-405
Koornwinder T 1977 *SIAM J. Math. Anal.* **8** 535-40
—— 1978 *J. London Math. Soc.* **18** 101-14
Knyr V A, Pipirajte P P and Smirnov Yu F 1976 *Sov. J. Nucl. Phys.* **22** 554-60

Niukkanen A W 1983 *J. Phys. A: Math. Gen.* **16** 1813-25

—— 1984a *Int. J. Quantum Chem.* **25** 941-55

—— 1984b *J. Phys. A: Math. Gen.* **17** L731-6

Raynal J 1976 *Nucl. Phys.* A **259** 272-300

—— 1978 *J. Math. Phys.* **19** 467-76

Smorodinsky Ya A and Shelepin L A 1972 *Usp. Fiz. Nauk.* **106** 3-45

Varshalovich D A, Moskalev A N and Khersonsky V K 1975 *Quantum theory of angular momentum* (Leningrad: Nauka) (in Russian)

Vilenkin N Ya 1965 *Special functions and group representation theory* (Moscow: Nauka) (in Russian)

Wallace R 1976 *Chem. Phys. Lett.* **37** 115-8