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A new method for calculating the hyperspherical functions for the quantum mechanics of three bodies

S Marsh†‡ and B Buck

Department of Theoretical Physics, 1 Keble Road, Oxford, England

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Abstract. Using the shift operators of Hughes for the group SU(3) in an O(3) basis, a simple method is developed to obtain the three-body hyperspherical functions of a definite symmetry for any angular momentum in a given SU(3) representation.

1. Introduction

The method of solution of the quantum mechanical three-body problem based on the expansion of the wavefunction in terms of hyperspherical functions has been used in recent years in a variety of problems in nuclear, molecular and elementary particle physics (e.g. Ballot and Fabre de la Ripelle 1969, Erens 1971, Fray 1980, Mandelzweig 1980, Richard 1979, Zickendraht 1972), but its wider acceptance seems to have been hindered by the practical difficulties in defining functions of a given symmetry with angular momentum greater than two.

The problem is that the hyperspherical functions are representations of the group SU(3), but for physical reasons we wish them to be classified according to the total angular momentum and symmetry under particle interchange. As is well known (Racah 1949), the representations $D(L)$ of O(3) may occur several times in a representation (λ, μ) of SU(3). No physically relevant operator has been found to resolve this degeneracy (Pustovalov and Simonov 1967, Pustavalov and Smorodinsky 1970), and it considerably complicates the solution of the differential equations defining the hyperspherical functions.

The group theoretical aspects of the problem have been studied extensively by, for example, Racah (1949, 1962), Bargmann and Moshinsky (1960, 1961), Levy-Leblond (1965, 1966, Levy-Leblond and Levy-Nahas 1965), Dragt (1965) and Simonov (1966). The latter authors developed a group theoretical approach to calculating the hyperspherical functions forming a complete normalised orthogonal set on the six-dimensional unit sphere. However, this method becomes difficult in practice even for small values of L. Nyiri and Smorodinsky (1969, 1971, 1979) used a generalised Fourier transform method to produce general expressions for functions

† Present address: Department of Physics, University of Wisconsin-Madison, 1150 University Avenue, Madison, Wisconsin, 53706, USA

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classified by the internal angular momenta, but they did not proceed to an orthogonal specification of these functions. Hughes (1973a, b) introduced the shift operators and showed that the SU(3) state labelling problem could be solved, in principle, and an orthogonal basis derived. Most recently, del Aguila and Doncel (1980) reverted to Dragt's method of calculating the functions by factorising the angular part of a set of harmonic oscillator states. They tabulated these functions for some representations with some states up to $L=4$.

The alternative approach of trying to solve the Schrödinger equation directly was first attempted by Zickendraht (1965), who obtained expressions for states with $L=0, 1, 2$ in terms of hypergeometric functions. Whitten and Smith (1968) also developed a general method of solution but this is very cumbersome. They did, however, suggest the general form of the solutions as derived by Nyiri and Smorodinsky (1971), though they were unable to evaluate the numerical coefficients. Mayer (1975) introduced an algebraic approach with a different form for the general solution, but again only calculated up to $L=2$.

In this paper, we combine the group theoretical and coordinate space approaches and derive the shift operators of Hughes in a coordinate representation. We then adopt the general expression for the hyperspherical harmonics and use the expressions for the shift operators to derive simple relations between the numerical coefficients in the general expression. These may be rapidly evaluated by computer to provide not only the hyperspherical functions but also the SU(3) Clebsch–Gordan coefficients.

The layout of the paper is as follows. In § 2 we introduce the notation and define the hyperspherical coordinates and the general form of the functions. In § 3 we review the work of Hughes and in § 4 derive the coordinate representation of the shift operators. These are applied in § 5 to rederive some of the general formulae for small values of L. In § 6 we describe the calculation of the numerical coefficients in the general expression, and supply tables for the SU(3) representations of definite symmetry up to a global angular momentum value of $2N=6$, where we have introduced N for future convenience.

2. The hyperspherical coordinates

We specialise the many-body theory of Buck *et al* (1979) to the three-particle case.

Let the position vectors of the particles be $\boldsymbol{x}_n$ ($n=1, 2, 3$) and assume that the particles are of equal mass (the generalisation to unequal masses is simple: see Buck *et al* (1979)). Then define the centre-of-mass coordinates $3\boldsymbol{R}=\Sigma\, \boldsymbol{x}_n$ and the relative position vectors $\boldsymbol{r}_n=\boldsymbol{x}_n-\boldsymbol{R}$ so that

$$\sum \boldsymbol{r}_n=0 \tag{1}$$

We now write $\boldsymbol{r}_n=\mu_1 v_{1n}\boldsymbol{s}_1+\mu_2 v_{2n}\boldsymbol{s}_2$ where μ_1 and μ_2 are the square roots of the quadrupole eigenvectors in the principal axis frame defined by the orthonormal vectors $\boldsymbol{s}_1$, $\boldsymbol{s}_2$ and $\boldsymbol{s}_3=\boldsymbol{s}_1\times\boldsymbol{s}_2$. The vectors $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$ are unit orthonormal vectors in the particle label space, satisfying

$$\boldsymbol{v}_1^2=\boldsymbol{v}_2^2=1, \qquad \boldsymbol{v}_1\cdot\boldsymbol{v}_2=\boldsymbol{v}_1\cdot\boldsymbol{v}_0=\boldsymbol{v}_2\cdot\boldsymbol{v}_0=0, \qquad \text{where } \boldsymbol{v}_0=[1, 1, 1]/\sqrt{3}.$$

The last two conditions are equivalent to the centre-of-mass constraint (1).

We introduce the hyper-radius $\rho=(\Sigma_n \boldsymbol{r}_n^2)^{1/2}$ and two internal angles θ and ϕ to parametrise $\boldsymbol{\mu}_1$, $\boldsymbol{\mu}_2$, $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$ giving

$$\boldsymbol{r}_n=\left(\frac{2}{3}\right)^{1/2}\rho\left(\sin\left(\frac{\theta+\pi}{4}\right)\sin\left(\frac{\phi}{2}+\frac{2\pi n}{3}\right)\boldsymbol{s}_1+\cos\left(\frac{\theta+\pi}{4}\right)\cos\left(\frac{\phi}{2}+\frac{2\pi n}{3}\right)\boldsymbol{s}_2\right)$$

with $0\leqslant\theta\leqslant\pi$ and $0\leqslant\phi\leqslant 2\pi$.

Let $P(ij)$ interchange particles i and j: then it can be seen that

$$\begin{array}{lll} \text{under } P(12) & \theta\to 2\pi-\theta, & \phi\to 2\pi-\phi, \\ \text{under } P(23) & \theta\to 2\pi-\theta, & \phi\to -\tfrac{2}{3}\pi-\phi, \\ \text{under } P(31) & \theta\to 2\pi-\theta, & \phi\to \tfrac{2}{3}\pi-\phi. \end{array}$$

We may further parametrise the principal axes $\boldsymbol{s}_1$, $\boldsymbol{s}_2$ in terms of Euler angles $\Omega=(\alpha,\beta,\gamma)$, giving the orientation with respect to a space fixed frame $\boldsymbol{e}_1$, $\boldsymbol{e}_2$, $\boldsymbol{e}_3$ as follows.

Define

$$k_{\pm1}=\mp(\boldsymbol{e}_1\pm\mathrm{i}\boldsymbol{e}_2)/\sqrt{2}, \qquad k_0=\boldsymbol{e}_3,$$
$$t_{\pm1}=\mp(\boldsymbol{s}_1\pm\mathrm{i}\boldsymbol{s}_2)/\sqrt{2}, \qquad t_0=\boldsymbol{s}_3.$$

Then

$$k_m=\sum_{m'} D^1_{mm'}(\Omega)t_{m'}$$

giving, on inversion,

$$s_{1x}=-\sin\alpha\sin\gamma+\cos\alpha\cos\beta\cos\gamma \qquad \text{etc.}$$

Note that we use a convention for the D function which is the complex conjugate of that used by Brink and Satchler (1979).

As in Zickendraht (1965), we may derive an expression for the six-dimensional Laplacian, and writing the hyperspherical harmonic as

$$F^{Nn\omega}_{LM}(\theta\phi\Omega)=\left(\frac{2L+1}{16\pi^3}\right)^{1/2}\sum_K D^L_{MK}(\Omega)g^{Nn\omega}_{LK}(\theta)\,\mathrm{e}^{\mathrm{i}n\phi}$$

we obtain the defining equation for the functions $g^{Nn\omega}_{LK}(\theta)$:

$$\begin{aligned}\bigg[\frac{4}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)&-\frac{L(L+1)}{2\cos^2\theta/2}-\frac{(3\cos\theta-1)K^2}{2\sin^2\theta}\\ &-\frac{n^2}{\sin^2\theta/2}-\frac{Kn\cos\theta/2}{\sin^2\theta/2}+N(N+2)\bigg]g^{Nn\omega}_{LK}(\theta)\\ &=\frac{\sin\theta/2}{4\cos^2\theta/2}\{[(L+K+2)(L+K+1)(L-K-1)(L-K)]^{1/2}g^{Nn\omega}_{LK+2}(\theta)\\ &\quad+[(L-K+2)(L-K+1)(L+K)(L+K-1)]^{1/2}g^{Nn\omega}_{LK-2}(\theta)\}\end{aligned} \tag{2}$$

where $2N$ is the global (grand) angular momentum, n is a quantum number related to the symmetry of the states, L is the angular momentum of the system with projection K in the body fixed frame, and ω is the fifth quantum number needed to resolve the remaining degeneracy of the states. N and n define an SU(3) representation given in terms of the normal (λ, μ) form by

$$\lambda = N+n, \qquad \mu = N-n.$$

For states of positive parity $N=0, 1, 2 \ldots$. For states of negative parity $N=\frac{1}{2}, \frac{3}{2}, \frac{5}{2} \ldots$ while $n=-N, -N+1, \ldots, N-1, N$.

States which are totally symmetric or antisymmetric under particle interchange correspond to $n=0, 3, 6 \ldots$ or to $n=\frac{3}{2}, \frac{9}{2}, \ldots$ for positive and negative parity states respectively. Other values of n give states of mixed symmetry.

3. The shift operators of Hughes

In considering the decomposition of the group $SU(3) \supset O(3)$ it is useful to consider the generators l_i, $i=-1, 0, 1$ and q_μ, $\mu=-2, \ldots, +2$ satisfying the commutation relations

$$[l_0, l_{\pm 1}] = \pm l_{\pm 1}, \qquad [l_{+1}, l_{-1}] = 2l_0, \qquad [l_0, q_\mu] = \mu q_\mu,$$

$$[l_{\pm 1}, q_\mu] = \pm(-1)^\mu [6-\mu(\mu \pm 1)]^{1/2} q_{\mu \pm 1}, \qquad [q_0, q_{\pm 1}] = \mp 3\sqrt{\tfrac{3}{2}} l_{\pm 1}, \qquad [q_0, q_{\pm 2}] = 0,$$

$$[q_{+1}, q_{-1}] = 3l_0, \qquad [q_{+2}, q_{-2}] = 6l_0, \qquad [q_{\pm 2} q_{\mp 1}] = \mp 3l_{\pm 1}, \qquad [q_{\pm 2}, q_{\pm 1}] = 0.$$

The l_i are in fact the generators of the O(3) subgroup with respect to which the q_μ form a five-dimensional irreducible tensor.

Hughes (1973a) now takes a combination, O_L, of these generators which contains the q_μ to first order only, and requires this operator to satisfy the following commutation relations:

$$[O_L, l_0] = 0, \qquad [L^2, O_L] = 2xO_L,$$

where x remains to be determined and of course

$$l_0 F_{LM}^{Nn\omega}(\theta\phi\Omega) = MF_{LM}^{Nn\omega}(\theta\phi\Omega), \qquad L^2 F_{LM}^{Nn\omega}(\theta\phi\Omega) = L(L+1)F_{LM}^{Nn\omega}(\theta\phi\Omega).$$

Writing O_L as

$$O_L = \sqrt{6}aq_0 + bl_{+1}q_{-1} + cl_{-1}q_{+1} + dl_{+1}^2 q_{-2} + el_{-1}^2 q_{+2}$$

gives a fifth-order secular equation with solution $x_k = k(2L+k+1)$, where $k=0, \pm 1, +2$, which yields five operators O_L^k with the property that

$$O_L^k F_{LM}^{Nn\omega}(\theta\phi\Omega) \propto F_{L+k,M}^{Nn\omega'}(\theta\phi\Omega).$$

Now O_L^0 is just the cubic Racah operator, LQL, while the other operators shift the angular momentum eigenvalue while leaving the SU(3) quantum numbers unchanged. Note that in general O_L^k does not commute with either the cubic or quartic Racah operators. This means that the new state of angular momentum $L+k$ produced by the action of the operator O_L^k on a state of angular momentum L is in general a linear combination of the degenerate states. The degeneracy of the functions with the same L, M in a given SU(3) representation can be seen to arise since for example $O_{L+1}^1 O_L^1 \neq O_L^2$.

Hughes (1973b) gives an algorithm for constructing an orthonormal set of states, using products of these operators which leave L unchanged. We wish, instead, to use them to calculate the functions $g_{LK}^{Nn\omega}(\theta)$. To this end we may take $M=0$ without loss or generality (since $g_{LK}^{Nn\omega}(\theta)$ is independent of M) and we commute the l_i's with the

q_μ's, giving the final expression for the operators as

$$O_L^k = \sqrt{\tfrac{2}{3}}(L+x_k)(L+1-x_k)q_0 + (1+x_k)(q_{-1}l_{+1} + (-1)^k q_{+1}l_{-1}) + (q_{-2}l_{+1}^2 - (-1)^k q_{+2}l_{-1}^2).$$

4. Coordinate representation of the shift operators

We write the generators l_i, q_μ in terms of the usual SU(3) generators as follows:

$$l_{\pm 1} = [\mathrm{i}(G_{zy} - G_{yz}) \pm (G_{zx} - G_{xz})], \qquad l_0 = \mathrm{i}(G_{yx} - G_{xy}),$$
$$q_{\pm 2} = -\sqrt{\tfrac{3}{2}}[(G_{xx} - G_{yy}) \pm \mathrm{i}(G_{xy} + G_{yx})],$$
$$q_{\pm 1} = -\sqrt{\tfrac{3}{2}}[(G_{zx} + G_{xz}) \pm \mathrm{i}(G_{xz} + G_{zy})],$$
$$q_0 = (2G_{zz} - G_{xx} - G_{yy}),$$

where

$$G_{\alpha\beta} = 4\mathrm{i}b_{12}^{\alpha\beta}\frac{\partial}{\partial\theta} - \mathrm{i}\left(\frac{(1+\sin\theta/2}{\sin\theta/2}b_{11}^{\alpha\beta} - \frac{(1-\sin\theta/2)}{\sin\theta/2}b_{22}^{\alpha\beta}\right)\frac{\partial}{\partial\phi} + \left(\frac{-\mathrm{i}(1+\sin\theta/2)}{\cos\theta/2}b_{13}^{\alpha\beta} + a_{13}^{\alpha\beta}\right)\frac{\partial}{\partial\Omega_1} + \left(\frac{-\mathrm{i}(1-\sin\theta/2)}{\cos\theta/2}b_{23}^{\alpha\beta} - a_{13}^{\alpha\beta}\right)\frac{\partial}{\partial\Omega_2} + \left(\frac{-\mathrm{i}\cos\theta/2(b_{11}^{\alpha\beta} - b_{22}^{\alpha\beta})}{2\sin\theta/2} + a_{12}^{\alpha\beta}\right)\frac{\partial}{\partial\Omega_3},$$

with

$$a_{ij}^{\alpha\beta} = \tfrac{1}{2}(s_{i\alpha}s_{j\beta} - s_{i\beta}s_{j\alpha}), \qquad b_{ij}^{\alpha\beta} = \tfrac{1}{2}(s_{i\alpha}s_{j\beta} + s_{i\beta}s_{j\alpha}), \qquad (\alpha, \beta \to x, y, z)$$

where the $s_{i\alpha}$ are given in terms of the Euler angles in §2. This formula may be calculated from the expression (Nyiri and Smorodinsky (1971))

$$G_{\alpha\beta} = z_\alpha\, \partial/\partial z_\beta - z_\beta^*\, \partial/\partial z_\alpha^*$$

where

$$z = \rho\, \mathrm{e}^{\mathrm{i}\phi/2}\left[\sin\left(\frac{\theta+\pi}{4}\right)s_1 + \mathrm{i}\cos\left(\frac{\theta+\pi}{4}\right)s_2\right].$$

After tedious algebra the operators O_L^k can then be obtained in terms of θ, ϕ, α, β and γ. We wish to obtain operators as functions of θ only, so using the expression for $F_{LM}^{Nn\omega}(\theta\phi\Omega)$ we let the operators act on $\Sigma_K[(2L+1)/16\pi^3]^{1/2}D_{0K}^L(\Omega|\mathrm{e}^{\mathrm{i}n\phi}g_{LK}^{Nn\omega}(\theta)$ then multiply on the left by $[(2L'+1)/16\pi^3]^{1/2}D_{0K'}^{L'*}(\Omega)\,\mathrm{e}^{-\mathrm{i}n'\phi}$ and integrate. The integrations over α, γ and ϕ are trivial, but the integration over β requires the use of the differential relations for the d functions (Talman 1968):

$$\left(\frac{\partial}{\partial\beta} + m'\operatorname{cosec}\beta - m\cot\beta\right)d_{m'm}^j(\beta) = -[(j-m)(j+m+1)]^{1/2}d_{m'm+1}^j(\beta),$$

$$\left(\frac{\partial}{\partial\beta} - m'\operatorname{cosec}\beta + m\cot\beta\right)d_{m'm}^j(\beta) = [(j+m)(j-m+1)]^{1/2}d_{m'm-1}^j(\beta).$$

On substituting d-function representations for some simple trignometric forms the integrands are all products of three d-functions, which may then be integrated to yield a product of $3-j$ coefficients.

We define

$$h_{LK}^{Nn\omega}(\theta)=[(L-K)!(L+K)!]^{1/2}g_{LK}^{Nn\omega}(\theta)$$

and then, evaluating the $3-j$ coefficients for each operator (Brink and Satchler 1979), we obtain the following relation between the functions $h_{LK}^{Nn\omega}(\theta)$:

$$\begin{aligned} h_{L+k,K}^{Nn\omega'}(\theta) \propto & \left[A_k^{LK}\left(n+\frac{K}{\cos\theta/2}\right)+\frac{B_k^{LK}}{\cos\theta/2}\right] h_{LK}^{Nn\omega}(\theta) \\ & + C_k^{LK}\left[\frac{\partial}{\partial\theta}-\frac{n}{2\sin\theta/2}-\frac{K-2}{4}\cot\frac{\theta}{2}+\frac{1-2K+x_k}{4}\tan\frac{\theta}{2}\right] h_{LK-2}^{Nn\omega}(\theta) \\ & -(-1)^k C_k^{L,-K}\left(\frac{\partial}{\partial\theta}+\frac{n}{2\sin\theta/2}+\frac{K+2}{4}\cot\frac{\theta}{2}+\frac{1+2K+x_k}{4}\tan\frac{\theta}{2}\right) h_{LK+2}^{Nn\omega}(\theta) \end{aligned}$$

where

$$A_k^{LK}=A_{-k}^{-(L+1)K}, \qquad B_k^{LK}=B_{-k}^{-(L+1)K}, \qquad C_k^{LK}=C_{-k}^{-(L+1)K},$$

and

$$A_0^{LK}=\tfrac{2}{3}L(L+1)-K^2, \qquad A_1^{LK}=2K, \qquad A_2^{LK}=1,$$

$$B_0^{LK}=\tfrac{1}{3}K(2L-1)(2L+3), \qquad B_1^{LK}=-L(L+2), \qquad B_2^{LK}=0,$$

$$C_0^{LK}=-2(L-K+2)(L-K+1), \qquad C_1^{LK}=2(L-K+2), \qquad C_2^{LK}=1.$$

5. Analytic expressions for small L values

For some simple cases the defining equation (2) may be solved directly. We define the following symbols for convenience:

$A(N,n)=d^{N/2}_{-n/2n/2}(\theta)$ for N, n integer, $N+n$ even,

$B(N,n)=d^{N/2}_{(1+n)/2(1-n)/2}(\theta)$ for N, n integer, $N+n$ odd,

$C(N,n)=d^{N/2-1/4}_{n/2+1/4,-(n/2+1/4)}(\theta)$ for N, n half-integral,

$D(N,n)=d^{N/2-1/4}_{n/2+1/4,3/4-n/2}(\theta)$ for N, n half-integral.

$L=0, K=0, N+n$ even $\quad g_{00}^{Nn}(\theta)\propto A(N,n)$ (Zickendraht 1965),

$L=1, K=0, N+n$ odd $\quad g_{10}^{Nn}(\theta)\propto B(N,n)$.

Then considering the operator O_0^1 gives

$$L=1, K=0, N+n \text{ even} \qquad g_{10}^{Nn}(\theta)=0$$

as required from Racah's formula giving the number of occurrences of D^L in $(\lambda\mu)$.

The odd-parity states may be obtained from Zickendraht (1965) as

$L=1, K=1, N+n$ even

$$g_{1,1}^{Nn}(\theta)\propto(N+n)^{1/2}\sin\frac{\theta}{4}C(N,n)-(N-n+1)^{1/2}\cos\frac{\theta}{4}D(N,n),$$

$L=1, K=-1, N+n$ even

$$g^{Nn}_{1,-1}(\theta) \propto (N+n)^{1/2} \cos\frac{\theta}{4}\, C(N,n) + (N-n+1)^{1/2} \sin\frac{\theta}{4}\, D(N,n),$$

$L=1, K=1, N+n$ odd

$$g^{Nn}_{11}(\theta) \propto (N-n)^{1/2} \cos\frac{\theta}{4}\, C(N,-n) + (N+n+1)^{1/2} \sin\frac{\theta}{4}\, D(N,-n),$$

$L=1, K=-1, N+n$ odd

$$g^{Nn}_{1,-1}(\theta) \propto (N-n)^{1/2} \sin\frac{\theta}{4}\, C(N,-n) - (N+n+1)^{1/2} \cos\frac{\theta}{4}\, D(N,-n).$$

Note that these functions obey the symmetry relation

$$g^{Nn\omega}_{LK} = g^{N,-n\omega}_{L,-K}(\theta).$$

Considering O^2_0 gives

$L=2, K=0, N+n$ even $\qquad g^{Nn\,1}_{20}(\theta) \propto A(N,n),$

$L=2, K=\pm 2, N+n$ even $\qquad g^{Nn\,1}_{2\pm 2}(\theta)\ \sqrt{6}\left(\frac{-n}{2\sin\theta/2} \pm \frac{\partial}{\partial\theta}\right) A(N,n).$

Considering O^1_1 gives

$L=2, K=0, N+n$ odd $\qquad g^{Nn}_{20}(\theta) \propto (\cos\theta/2)^{-1}\, B(N,n),$

$L=2, K=\pm 2, N+n$ odd $\qquad g^{Nn}_{2\pm 2}(\theta) \propto \frac{1}{\sqrt{6}}\left(-\tan\frac{\theta}{a} \mp \frac{2n}{\sin\theta/2} + 4\frac{\partial}{\partial\theta}\right) B(N,n).$

The $L=2$, $N+n$ even state is, in fact, doubly degenerate and since $g^{Nn}_{10}(\theta)=0$ we cannot obtain the second solution using O^1_1 as would usually be done. This is the only case where this difficulty occurs, as may be seen, for example, from the SU(3) multiplet diagrams in Hughes (1973b). We may get around the problem, in this case, since we can use O^0_2 and extract a linearly independent part yielding

$L=2, K=0, N+n$ even $\qquad g^{Nn\,2}_{20}(\theta) \propto \left(1 + \frac{3\tan\theta/2}{n^2-N(N+2)}\frac{\partial}{\partial\theta}\right) A(N,n),$

L = 2, K = ±2, N + n even

$$g^{Nn\,2}_{2\pm 2}(\theta) \propto \frac{\sqrt{6}}{4}\left(\mp \frac{n\cot\theta/2}{n^2-N(N+2)} + \frac{2\sec\theta/2}{n^2-N(N+2)}\frac{\partial}{\partial\theta}\right) A(N,n).$$

These functions may then be orthogonalised using the Schmidt procedure. The operators may then, of course, be reapplied to give the $L=3$ and $L=4$ states, and so on.

6. Numerical calculation of hyperspherical functions

Although derivation of the analytical expressions is not difficult, the process is still fairly tedious for L much greater than 4, so we look instead for an alternative procedure which is more amenable to mechanisation.

To achieve this we use the general ansatz suggested by Whitten and Smith (1968) in the form

$$g_{LK}^{Nn\omega}(\theta)=[(L-K)!\,(L+K)!]^{-1/2}\sum_{j}^{N}\alpha^{j}_{Nn\omega LK}d^{j}_{-n,K/2}(\theta/2).$$

Then using

$$\left(\frac{\partial}{\partial\theta}-\frac{n}{2\sin\theta/2}-\frac{K-2}{4}\cot\frac{\theta}{2}\right)d^{j}_{-n,K/2-1}\left(\frac{\theta}{2}\right)=-\frac{1}{2}\left[\left(j-\frac{K}{2}+1\right)\left(j+\frac{K}{2}\right)\right]^{1/2}d^{j}_{-nK/2}\left(\frac{\theta}{2}\right)$$

and

$$\left(\frac{\partial}{\partial\theta}+\frac{n}{2\sin\theta/2}+\frac{K+2}{4}\cot\frac{\theta}{2}\right)d^{j}_{-nK/2+1}(\theta)=\frac{1}{2}\left[\left(j+\frac{K}{2}+1\right)\left(j-\frac{K}{2}\right)\right]^{1/2}d^{j}_{-nK/2}\left(\frac{\theta}{2}\right)$$

and writing $\cos\theta/2=d^{1}_{00}(\theta/2)$, $\sin\theta/2=\sqrt{2}d^{1}_{01}(\theta/2)=-\sqrt{2}d^{1}_{0-1}(\theta/2)$, multiplying on the left by $\cos(\theta/2)d^{j'}_{-nK/2}(\theta/2)$ and integrating over $\cos\theta/2$, we obtain from O_L^{-2}

$$\begin{aligned}\mathbf{A}_{nK}\cdot\boldsymbol{\alpha}_{L-1K}\propto\{n\mathbf{A}_{nK}+K\mathbf{D}_{nK}\}\cdot\boldsymbol{\alpha}_{LK}&-\tfrac{1}{2}[\mathbf{A}^{-}_{nK}+\sqrt{2}(L+K-1)\mathbf{B}_{nK}]\cdot\boldsymbol{\alpha}_{LK-2}\\&-\tfrac{1}{2}[\mathbf{A}^{+}_{nK}+\sqrt{2}(L-K-1)\mathbf{C}_{nK}]\cdot\boldsymbol{\alpha}_{LK+2}\end{aligned}$$

and from O_L^{-1}

$$\begin{aligned}\mathbf{A}_{nK}\cdot\boldsymbol{\alpha}_{L-2,K}\propto&[2nK\mathbf{A}_{nK}+[2K^{2}-(L-1)(L+1)]\mathbf{D}_{nK}\}\cdot\boldsymbol{\alpha}_{LK}\\&-(L+K-1)[\mathbf{A}^{-}_{nK}+(1/\sqrt{2})(L+2K-1)\mathbf{B}_{nK}]\cdot\boldsymbol{\alpha}_{LK-2}\\&+(L-K-1)[\mathbf{A}^{+}_{nK}+(1/\sqrt{2})(L-2K-1)\mathbf{C}_{nK}]\cdot\boldsymbol{\alpha}_{LK+2}\end{aligned}$$

where

$$(\mathbf{A}_{nK})_{j'j}=\begin{pmatrix}j'&j&1\\n&-n&0\end{pmatrix}\begin{pmatrix}j'&j&1\\-K/2&K/2&0\end{pmatrix}$$

$$(\mathbf{A}^{\pm}_{nK})_{j'j}=[(j\pm\tfrac{1}{2}K+1)(j\mp\tfrac{1}{2}K)]^{1/2}(\mathbf{A}_{nK})_{j'j},$$

$$(\mathbf{B}_{nK})_{j'j}=\begin{pmatrix}j'&j&1\\n&-n&0\end{pmatrix}\begin{pmatrix}j'&j&1\\-K/2&K/2-1&1\end{pmatrix},$$

$$(\mathbf{C}_{nK})_{j'j}=\begin{pmatrix}j'&j&1\\n&-n&0\end{pmatrix}\begin{pmatrix}j'&j&1\\-K/2&K/2+1&-1\end{pmatrix},$$

$$(\mathbf{D}_{nK})_{j'j}=(-1)^{n+K/2}\frac{\delta_{jj'}}{2j+1},\qquad(\boldsymbol{\alpha}_{LK})_{j}=\alpha^{j}_{Nn\omega LK},$$

which, given the simple expressions for the $3-j$ coefficients with one index equal to 1, are two sets of simple simultaneous equations relating the $\alpha^{j}_{L-1,K}$ and $\alpha^{j}_{L-2,K}$ to the $\alpha^{j}_{L,K}$.

The function $g_{LK}^{Nn\omega}(\theta)$ for the state of maximum $L(=2N)$ is non-degenerate and was calculated by Zickendraht (1965) as

$$\begin{aligned}g_{LK}^{Nn}(\theta)=&\frac{[(2N-K)!\,(2N+K)!]^{1/2}}{(N-\frac{1}{2}K)!\,\Gamma(\frac{1}{2}K+n+1)}(1+\cos\theta/2)^{N}(\tan\theta/4)^{K/2+n}\\&\times{}_2F_1(-(N-n),-(N-K/2);1+K/2+n;\tan^{2}\theta/4)\end{aligned}$$

and using the standard expression for the hypergeometric function, we may write this in the general form with

$$\alpha^j_K = \frac{(2j+1)2^N[(2N-K)!(2N+K)!][(j-n)!(j+n)!(j-K/2)!(j+K/2)!]^{1/2}(N-n)!}{\Gamma(N+j+2)}$$

$$\times\sum_m\sum_t \frac{(-1)^t\Gamma(m+t+K/2+n+1)\Gamma[N+j+1-(m+t+K/2+n)]}{m!t!(N-n-m)!(N-K/2-m)!\Gamma(m+1+K/2+n)(j-n-t)!}$$

$$\times\frac{1}{(j-K/2-t)!(t+K/2+n)!}$$

where the sum is over m and t such that there are no negative factorials.

To summarise: given the coefficients for the state of maximum L, the states of smaller L in a given representation may be generated by successive solution of the sets of simultaneous equations derived from the operators O_L^{-1} and O_L^{-2}. At each stage a set of linearly independent non-zero solutions is extracted and orthonormalised using the Schmidt procedure.

Analyses of the SU(3) representations admitting completely symmetric or antisymmetric solutions up to $N=3$ are presented in table 1.

Table 1. Values of the α coefficients in the general expansion formula of § 6.

N	n	Index	L	K	j	Alpha
0	0	1	0	0	0	0.707 106 78
1	0	1	1	0	1	−1.000 000 0
1	0	1	2	2	1	−3.794 733 2
1	0	1	2	0	0	0.894 427 19
3/2	3/2	1	1	1	3/2	1.632 993 2
3/2	3/2	1	3	3	3/2	−22.677 868
3/2	3/2	1	3	1	3/2	2.613 614 7
2	0	1	0	0	0	−0.408 248 29
2	0	1	0	0	2	1.632 993 2
2	0	1	2	2	1	2.484 236 0
2	0	1	2	0	0	0.390 360 03
2	0	1	2	0	2	1.951 800 1
2	0	1	3	2	2	6.546 536 7
2	0	1	3	0	1	−4.810 702 4
2	0	1	4	4	2	183.303 03
2	0	1	4	2	1	−22.677 868
2	0	1	4	0	0	3.552 359 7
2	0	1	4	0	2	−2.138 089 9
2	0	2	2	2	2	−4.898 979 5
5/2	3/2	1	1	1	3/2	0.461 380 22
5/2	3/2	1	1	1	5/2	1.697 056 3
5/2	3/2	1	2	1	3/2	−0.979 795 90
5/2	3/2	1	2	1	5/2	2.400 000 0
5/2	3/2	1	3	3	3/2	4.898 979 5
5/2	3/2	1	3	3	5/2	29.393 877
5/2	3/2	1	3	1	3/2	−5.091 168 8
5/2	3/2	1	3	1	5/2	−1.385 640 6
5/2	3/2	1	4	3	3/2	−46.008 695
5/2	3/2	1	4	3	5/2	30.672 463

Table 1 (continued)

N	n	Index	L	K	j	Alpha
5/2	3/2	1	4	1	3/2	3.794 733 2
5/2	3/2	1	4	1	5/2	−9.295 160 0
5/2	3/2	1	5	5	5/2	1861.143 3
5/2	3/2	1	5	3	3/2	−147.969 53
5/2	3/2	1	5	3	5/2	−55.488 574
5/2	3/2	1	5	1	3/2	54.919 445
5/2	3/2	1	5	1	5/2	56.051 924
3	0	1	1	0	1	−0.282 842 71
3	0	1	1	0	3	1.697 056 3
3	0	1	2	2	1	−1.571 168 8
3	0	1	2	2	3	5.986 651 8
3	0	1	2	0	0	0.617 213 40
3	0	1	2	0	2	−1.234 426 8
3	0	1	3	2	2	−7.559 289 5
3	0	1	3	0	1	2.221 968 2
3	0	1	3	0	3	−5.184 592 6
3	0	1	4	4	2	−127.635 85
3	0	1	4	2	1	4.737 252 2
3	0	1	4	2	3	−18.050 434
3	0	1	4	0	0	4.466 324 2
3	0	1	4	0	2	22.331 621
3	0	1	5	4	3	−303.923 44
3	0	1	5	2	2	113.265 58
3	0	1	5	0	1	−79.269 391
3	0	1	5	0	3	13.211 565
3	0	1	6	6	3	−22 712.285
3	0	1	6	4	2	1884.853 1
3	0	1	6	2	1	−522.345 82
3	0	1	6	2	3	35.541 131
3	0	1	6	0	0	219.853 73
3	0	1	6	0	2	−109.926 87
3	0	2	3	2	1	5.366 563 1
3	0	2	3	2	3	8.763 560 9
3	0	2	4	4	3	224.000 00
3	0	2	4	2	2	−17.888 544
3	3	1	0	0	3	−2.529 822 1
3	3	1	2	2	3	7.155 417 5
3	3	1	2	0	3	−2.065 591 1
3	3	1	4	4	3	−238.784 80
3	3	1	4	2	3	21.574 396
3	3	1	4	0	3	−11.210 385
3	3	1	6	6	3	22 712.285
3	3	1	6	4	3	−842.931 95
3	3	1	6	2	3	177.705 66
3	3	1	6	0	3	−109.926 87

Note to table.

The alphas are only tabulated for n, K non-negative; the alphas for negative n, K may be obtained from the relations $g_{LK}^{Nn\omega}(\theta) = g_{L-K}^{N-n\omega}(\theta)$ and $\alpha_{n,-K}^{j} = (-1)^{L-K+3j+n}\alpha_{n,K}^{j}$.

It was chosen to iterate downwards so that a check on the numerical evaluation could be made since the $L=0$ and $L=1$ expansions are known analytically. Alternatively, of course, one could start from the $L=1$ and $L=2$ expansions and iterate upwards just to the required L value—this would be more economical for large values of N. There should be no significant inaccuracy incurred using these procedures: the results in table 1 were the same as the analytical values to the eight significant figures printed (calculations were carried out in FORTRAN double precision on a VAX-11/780).

This method is also quite fast: the analysis of the $N=4$, $n=0$ representation took less than 30 secs CPU time on the VAX, and this could be substantially reduced, if necessary, by taking advantage of the symmetries of the coefficients and the tri-diagonal form of the stimultaneous equations.

Once the expansion coefficients are available it is, of course, easy to calculate the coupling coefficients (3-ν coefficients of del Aguila and Doncel 1980) analogous to the Wigner 3-j coefficients. This is done by expanding the products of d functions until the integrand is just a Legendre polynomial for which the integral is known.

7. Conclusion

In this paper we have derived a coordinate representation of the $SU(3) \supset O(3)$ shift operators of Hughes. We have used these to rederive some analytic expressions for the hyperspherical harmonics and also developed a method for calculating states of every L value in a given representation. Results are presented for some of the symmetric SU(3) representations.

Work is in progress applying these results to the cluster model of Carbon-12. It is hoped to model all the excited states up to and including the first 4^+ state.

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