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Construction of SO(5) ⊃ SO(3) spherical harmonics and Clebsch–Gordan coefficients ☆

M.A. Caprio [a,*], D.J. Rowe [b], T.A. Welsh [b]

[a] Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556-5670, USA
[b] Department of Physics, University of Toronto, Toronto, Ontario M5S 1A7, Canada

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ABSTRACT

The SO(5) ⊃ SO(3) spherical harmonics form a natural basis for expansion of nuclear collective model angular wave functions. They underlie the recently-proposed algebraic method for diagonalization of the nuclear collective model Hamiltonian in an SU(1, 1) × SO(5) basis. We present a computer code for explicit construction of the SO(5) ⊃ SO(3) spherical harmonics and use them to compute the Clebsch–Gordan coefficients needed for collective model calculations in an SO(3)-coupled basis. With these Clebsch–Gordan coefficients it becomes possible to compute the matrix elements of collective model observables by purely algebraic methods.

Program summary

Program title: GammaHarmonic
Catalogue identifier: AECY_v1_0
Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AECY_v1_0.html
Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland
Licensing provisions: Standard CPC licence, http://cpc.cs.qub.ac.uk/licence/licence.html
No. of lines in distributed program, including test data, etc.: 346 421
No. of bytes in distributed program, including test data, etc.: 16 037 234
Distribution format: tar.gz
Programming language: Mathematica 6
Computer: Any which supports Mathematica
Operating system: Any which supports Mathematica; tested under Microsoft Windows XP and Linux
Classification: 4.2
Nature of problem: Explicit construction of SO(5) ⊃ SO(3) spherical harmonics on S_4. Evaluation of SO(3)-reduced matrix elements and SO(5) ⊃ SO(3) Clebsch–Gordan coefficients (isoscalar factors).
Solution method: Construction of SO(5) ⊃ SO(3) spherical harmonics by orthonormalization, obtained from a generating set of functions, according to the method of Rowe, Turner, and Repka [1]. Matrix elements and Clebsch–Gordan coefficients follow by construction and integration of SO(3) scalar products.
Running time: Depends strongly on the maximum SO(5) and SO(3) representation labels involved. A few minutes for the calculation in the Mathematica notebook.
References:
[1] D.J. Rowe, P.S. Turner, J. Repka, J. Math. Phys. 45 (2004) 2761.

1. Introduction

The SO(5) ⊃ SO(3) spherical harmonics constitute the natural basis for the "angular" wave functions in the collective model of nuclear quadrupole motion [1]. The SO(5) ⊃ SO(3) spherical harmonics underlie the recently-proposed algebraic scheme [2–4] for the nuclear

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* Corresponding author.

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collective model. Direct products of the SO(5) ⊃ SO(3) spherical harmonics with appropriate optimal radial wave functions provide an SU(1, 1) × SO(5) algebraic basis [2–4] which allows for exceedingly efficient numerical diagonalization of nuclear collective model Hamiltonians.

For applications to transitional and deformed nuclei, the SU(1, 1) × SO(5) scheme reduces by orders of magnitude [3] the basis size needed for convergence as compared to conventional diagonalization in a five-dimensional oscillator [U(5) ⊃ SO(5)] basis [5–7]. Matrix elements of an essentially unlimited set of potential and kinetic energy operators, often in analytic form, can easily be constructed in an SU(1, 1) × SO(5) basis [3,4], in terms of SO(5) ⊃ SO(3) Clebsch–Gordan coefficients. The resulting calculational scheme, the so-called algebraic collective model (ACM), is described in Refs. [2–4,8]. Examples of physical applications may be found in Ref. [9].

In this article, we present a computer code for explicit construction of the SO(5) ⊃ SO(3) spherical harmonics and for using them to determine the Clebsch–Gordan coefficients for coupling of symmetric irreducible representations of SO(5) in an SO(3) basis. The construction of the SO(5) ⊃ SO(3) spherical harmonics is carried out by orthonormalization of monomials in a set of four generating functions, according to the method of Rowe, Turner, and Repka [10]. The purpose of this code is to make calculations using the ACM routinely possible, without the need to reconstruct the SO(5) machinery for each new application. The SO(5) ⊃ SO(3) Clebsch–Gordan coefficients yielded by the code are also relevant to the U(6) interacting boson model (IBM) [11,12] which, in U(6) ⊃ U(5) ⊃ SO(5) and U(6) ⊃ SO(6) ⊃ SO(5) bases, is in close correspondence with the collective model in appropriate SU(1, 1) × SO(5) bases [13]. They can, furthermore, be used as seed coefficients in the generation of Clebsch–Gordan coefficients for the coupling of more general (non-symmetric) representations of SO(5) or Sp(4) in an SO(3) basis [14].

The code accompanying this article is implemented in Mathematica 6 [15]. All calculations are carried out in exact symbolic arithmetic. A machine-readable tabulation of calculated Clebsch–Gordan coefficients is included along with the code in the CPC Program Library. This tabulation is of sufficient extent to support basic calculations using the algebraic collective model, without the necessity of re-running the code.

The basic algorithm used here is that presented in Ref. [10]. However, the computational techniques have been substantially developed. For example, integration via the Fourier representation of functions has been used to greatly increase the efficiency of the calculations and considerably extend the practical range of application of the algorithm.

The necessary mathematical definitions for the SO(5) ⊃ SO(3) spherical harmonics and the general method for construction of the basis and evaluation of Clebsch–Gordan coefficients are discussed in Section 2. The more technical details of the computer implementation are summarized in Section 3. Instructions for installation and use of the computer code are given in Section 4.

2. The basic algorithm

2.1. The SO(5) ⊃ SO(3) spherical harmonics

The SO(5) spherical harmonics are eigenfunctions of the Laplace–Beltrami operator $\hat{\Lambda}^2$ on the four-sphere S_4, that is, the angular part of the Laplacian in five dimensions. This operator $\hat{\Lambda}^2$ is also the second order Casimir invariant of SO(5). Thus, the spherical harmonics are functions of a set of coordinates on S_4. Standard (γ, Ω) coordinates for S_4 are reviewed below in Section 2.2. The SO(5) spherical harmonics constitute a complete orthonormal basis for the space $L^2(S_4)$ of square-integrable functions on S_4 and transform under SO(5) rotations as bases for the symmetric irreps $(\nu, 0)$, for $\nu = 0, 1, \ldots$, of SO(5).

For applications to the nuclear collective model, we seek spherical harmonics which have "good SO(3) angular momentum", that is, which also transform as bases for irreps, labelled by (L), of the SO(3) subalgebra of SO(5). The desired SO(5) ⊃ SO(3) spherical harmonics, which we denote by $\Psi_{\nu\alpha LM}(\gamma, \Omega)$, thus reduce the subalgebra chain

$$\begin{matrix} \mathrm{SO}(5) & \supset & \mathrm{SO}(3) & \supset & \mathrm{SO}(2), \\ \nu & & \alpha\ L & & M \end{matrix} \tag{1}$$

with the representation labels as shown. The label ν is conventionally termed the "boson seniority" quantum number, following Racah. It is the five-dimensional [SO(5)] analog of the angular momentum quantum number. The SO(5) spherical harmonics satisfy the eigenvalue equation

$$\hat{\Lambda}^2 \Psi_{\nu\alpha LM}(\gamma, \Omega) = \nu(\nu+3)\Psi_{\nu\alpha LM}(\gamma, \Omega). \tag{2}$$

They are also eigenfunctions of the Casimir operators of the other algebras in the chain (1). However, the labels νLM provided by these Casimir operators are insufficient to fully distinguish the spherical harmonics. In particular, multiple SO(3) representations of the same L may occur within a given SO(5) representation. The "missing label" is provided by a multiplicity index α. The branching rule for SO(3) irreps occurring within an SO(5) irrep is well known [16,17], and the multiplicity is given by (A.1).

The SO(5) ⊃ SO(3) spherical harmonics have physical significance as the angular, *i.e.*, (γ, Ω), wave functions for the nuclear collective model, for the case in which the collective potential is SO(5) invariant [18,19]. Recall the quantum mechanics of a particle in three-dimensional Euclidean space, subject to a central force, *i.e.*, in spherical coordinates, $V(r, \theta, \varphi) \to V(r)$. The Hamiltonian is then SO(3) invariant, and its eigenfunctions, with good angular momentum quantum numbers, factorize into products $f_{nl}(r)Y_{lm}(\theta, \varphi)$ of radial wave functions and SO(3) spherical harmonics. Similarly, for the Bohr Hamiltonian, which is given in terms of quadrupole deformation variables β, γ, and Ω (Section 2.2) by

$$-\frac{\hbar^2}{2B}\left[\frac{1}{\beta^4}\frac{\partial}{\partial\beta}\beta^4\frac{\partial}{\partial\beta} - \frac{\hat{\Lambda}^2}{\beta^2}\right] + V(\beta, \gamma), \tag{3}$$

if the potential is a function $V(\beta)$ of the radial coordinate only, then the five-dimensional analog of a central force problem arises. The Hamiltonian is SO(5) invariant, and its eigenfunctions, with good seniority and angular momentum quantum numbers, factorize into products $f_{n\nu}(\beta)\Psi_{\nu\alpha LM}(\gamma, \Omega)$ of radial, *i.e.*, β, wave functions and SO(5) spherical harmonics, as in Ref. [18]. An example of application of the present methods to such "γ-unstable" problems is found in Ref. [14].

A limited set of SO(5) ⊃ SO(3) spherical harmonics was computed many years ago by Bès [19], for values of the angular momentum $L \leqslant 6$. These were obtained by series solution of coupled differential equations in the coordinate γ, to find the eigenfunctions of the SO(5) Casimir invariant. However, this approach becomes prohibitively complicated for $L > 6$. The SO(5) ⊃ SO(3) spherical harmonics are the angular wave functions for the five-dimensional quadrupole harmonic oscillator [20,21]. Thus, alternative approaches based on the oscillator basis construction are possible, as summarized in Ref. [7]. A method based on the Cartan–Weyl reduction is given in Ref. [22].

Here we make use of the construction proposed in Ref. [10], in which the SO(5) ⊃ SO(3) spherical harmonics are developed as polynomials in a set of four basic generating functions defined on S_4. These functions were identified as generators of a complete linearly independent basis of SO(3)-coupled wave functions for $L^2(S_4)$ [23], based on a knowledge of $L^2(S_4)$ as a direct sum of irreducible SO(3) subspaces [obtained from the SO(5) → SO(3) branching rules]. The generating functions can be related to the "elementary permissible diagrams" of the well-known algorithm of Chacón et al. [20,21] for construction of a U(5) ⊃ SO(5) ⊃ SO(3) basis for the five-dimensional harmonic oscillator, implemented in the nuclear collective model code of Hess et al. [24,25]. The salient property of the generating functions for $L^2(S_4)$ [10] is that they yield a direct route to the construction of SO(5) ⊃ SO(3) spherical harmonics without reference to the full harmonic oscillator problem. The method is set forth more concretely in Section 2.3.

2.2. Representation of functions on S_4

The quadrupole moments q_m ($m = 0, \pm 1, \pm 2$) for the collective model transform as components of an $L = 2$ spherical tensor under SO(3) rotations, *i.e.*,

$$q_m \to \sum_k q_k \mathcal{D}^{(2)}_{km}(\Omega), \tag{4}$$

where Ω represents the Euler angles for the SO(3) rotation, and the Wigner $\mathcal{D}$ function [26] is the rotation matrix element. [The quantities q_m can alternatively be taken to represent the nuclear surface deformation parameters α_m ($m = 0, \pm 1, \pm 2$). The difference is only in physical interpretation and does not affect the following results for SO(5).]

These quadrupole moments are conveniently expressed in terms of Bohr's spherical polar coordinates (β, γ, Ω) [27], by the relation

$$q_m = \beta \cos\gamma \mathcal{D}^{(2)}_{0,m}(\Omega) + \frac{1}{\sqrt{2}} \beta \sin\gamma \left[\mathcal{D}^{(2)}_{2,m}(\Omega) + \mathcal{D}^{(2)}_{-2,m}(\Omega) \right]. \tag{5}$$

The squared length of a vector $q \in \mathbb{R}^5$ is given by $\sum_m |q_m|^2 = \beta^2$. Thus, β is the radial coordinate for $\mathbb{R}^5$, and (γ, Ω) are angular coordinates.

For consideration of the angular functions on the unit sphere S_4, we henceforth set $\beta = 1$ and restrict consideration to the unit length quadrupole moments $\mathcal{Q}_m$, defined as

$$\mathcal{Q}_m = \cos\gamma \mathcal{D}^{(2)}_{0,m}(\Omega) + \frac{1}{\sqrt{2}} \sin\gamma \left[\mathcal{D}^{(2)}_{2,m}(\Omega) + \mathcal{D}^{(2)}_{-2,m}(\Omega) \right]. \tag{6}$$

These unit-length quadrupole moments are then proportional to the basic $v = 1$ spherical harmonics on S_4.

Consider a function $\Psi^{(L)}_M(\gamma, \Omega)$ on S_4, of good SO(3) angular momentum L and SO(2) quantum number M. Any such function may be expanded [27] in the form

$$\Psi^{(L)}_M(\gamma, \Omega) = \sum_{\substack{K=0 \\ \text{even}}}^{L} F_K(\gamma) \xi^{(L)}_{KM}(\Omega), \tag{7}$$

where

$$\xi^{(L)}_{KM}(\Omega) \equiv \frac{1}{(1+\delta_K)^{1/2}} \left[\mathcal{D}^{(L)}_{KM}(\Omega) + (-)^L \mathcal{D}^{(L)}_{-KM}(\Omega) \right]. \tag{8}$$

Note that the $\mathcal{D}$ functions occur only in the symmetrized linear combinations $\mathcal{D}^{(L)}_{KM} + (-)^L \mathcal{D}^{(L)}_{-KM}$ with even values of K. Thus, because $\xi^{(L)}_{-KM} = (-)^L \xi^{(L)}_{KM}$, we can restrict to $K \geqslant 0$. Note also that the functions $\xi^{(L)}_{KM}$ vanish identically for $K = 0$ when L is odd. The normalization factor $(1+\delta_K)^{-1/2}$ (where $\delta_K \equiv \delta_{K,0}$) is included for later convenience.

The functions $\xi^{(L)}_{KM}(\Omega)$, with $K \geqslant 0$, provide an orthogonal basis for those functions of the SO(3) angles which respect the symmetry properties of collective model wave functions. From the inner product for the $\mathcal{D}$ functions [26],

$$\int \mathcal{D}^{(L')*}_{K'M'}(\Omega) \mathcal{D}^{(L)}_{KM}(\Omega)\, d\Omega = \frac{8\pi^2}{2L+1} \delta_{L'L} \delta_{K'K} \delta_{M'M}, \tag{9}$$

we obtain the inner product for the nonzero $\xi^{(L)}_{KM}(\Omega)$

$$\int \xi^{(L')*}_{K'M'}(\Omega) \xi^{(L)}_{KM}(\Omega)\, d\Omega = \frac{16\pi^2}{2L+1} \delta_{L'L} \delta_{K'K} \delta_{M'M}. \tag{10}$$

The volume element on S_4 is given by $dv = \sin 3\gamma\, d\gamma\, d\Omega$, where γ is integrated over the range $[0, \pi/3]$. Thus, the inner product $\langle \Psi_2 | \Psi_1 \rangle \equiv \int \Psi_2^* \Psi_1 \sin 3\gamma\, d\gamma\, d\Omega$ of two functions on S_4, when expanded according to (7), is given simply by

$$\langle \Psi^{(L)}_{2M} | \Psi^{(L)}_{1M} \rangle = \frac{16\pi^2}{2L+1} \int \left[\sum_{\substack{K=0 \\ \text{even}}}^{L} F_{1K}(\gamma) F_{2K}(\gamma) \right] \sin 3\gamma\, d\gamma. \tag{11}$$

Functions of distinct L or M are orthogonal.

2.3. SO(3)-coupled basis functions

The generating function method [10] for construction of the SO(5) ⊃ SO(3) spherical harmonics rests upon the observation that a complete set of normalizable SO(3) highest-weight (*i.e.*, those for which $M = L$) functions on S_4 is provided by the products

$$\Phi_{[n_1,n_2,n_3,n_4]}(\gamma,\Omega) = \left[\Phi_1(\gamma,\Omega)\right]^{n_1}\left[\Phi_2(\gamma,\Omega)\right]^{n_2}\left[\Phi_3(\gamma,\Omega)\right]^{n_3}\left[\Phi_4(\gamma,\Omega)\right]^{n_4}, \tag{12}$$

where the exponents n_1, n_2, and n_3 take on the values 0, 1, ..., and n_4 is restricted to 0 or 1. These $\Phi_{[n_1,n_2,n_3,n_4]}$ are monomials in four generating functions Φ_1, Φ_2, Φ_3, and Φ_4, which are simply the $M = L$ components

$$\begin{aligned}
&\Phi_1 \propto \mathcal{Q}_2,\\
&\Phi_2 \propto (\mathcal{Q}\times\mathcal{Q})^{(2)}_2,\\
&\Phi_3 \propto (\mathcal{Q}\times\mathcal{Q}\times\mathcal{Q})^{(0)}_0,\\
&\Phi_4 \propto (\mathcal{Q}\times\mathcal{Q}\times\mathcal{Q})^{(3)}_3,
\end{aligned} \tag{13}$$

of SO(3)-coupled products involving $\mathcal{Q}$. The coupled product of two tensors is defined by

$$\left[U^{(L_2)}\times T^{(L_1)}\right]^{(L)}_M \equiv \sum_{M_1M_2}\left(\begin{array}{cc|c} L_1 & L_2 & L\\ M_1 & M_2 & M\end{array}\right) U^{(L_2)}_{M_2} T^{(L_1)}_{M_1}. \tag{14}$$

Note the right-to-left coupling order in this definition of the SO(3) tensor product, used for consistency with Refs. [8,10] and to simplify the phases [28] arising in the Wigner–Eckart theorem. The norms of these generating functions are arbitrary and can be chosen for convenience. In the standard form (7), we take

$$\begin{aligned}
\Phi_1(\gamma,\Omega) &= \cos\gamma\,\xi^{(2)}_{02}(\Omega) + \sin\gamma\,\xi^{(2)}_{22}(\Omega),\\
\Phi_2(\gamma,\Omega) &= \cos 2\gamma\,\xi^{(2)}_{02}(\Omega) - \sin 2\gamma\,\xi^{(2)}_{22}(\Omega),\\
\Phi_3(\gamma,\Omega) &= \cos 3\gamma\,\xi^{(0)}_{00}(\Omega),\\
\Phi_4(\gamma,\Omega) &= \sin 3\gamma\,\xi^{(3)}_{23}(\Omega).
\end{aligned} \tag{15}$$

The multiplication of two highest-weight functions yields another highest-weight function (equivalent to the stretched coupling of two angular momentum functions). Hence, every $\Phi_{[n_1,n_2,n_3,n_4]}$ is a highest-weight function, with $L = M = 2n_1 + 2n_2 + 3n_4$ and "degree" $N = n_1 + 2n_2 + 3n_3 + 3n_4$ in the unit quadrupole moments $\mathcal{Q}$ [29]. The multiplication of the basis functions is carried out using the multiplication rule for the highest-weight functions $\xi^{(L)}_{KL}$. This rule, which follows from the multiplication rule [26] for $\mathcal{D}$ functions

$$\mathcal{D}^{(L_2)}_{K_2M_2}(\Omega)\mathcal{D}^{(L_1)}_{K_1M_1}(\Omega) = \sum_L \left(\begin{array}{cc|c} L_1 & L_2 & L\\ K_1 & K_2 & K\end{array}\right)\left(\begin{array}{cc|c} L_1 & L_2 & L\\ M_1 & M_2 & M\end{array}\right)\mathcal{D}^{(L)}_{KM}(\Omega), \tag{16}$$

where $K = K_1 + K_2$ and $M = M_1 + M_2$, is expressed by the equation

$$\xi^{(L_2)}_{K_2L_2}\xi^{(L_1)}_{K_1L_1} = \sum_{K\geqslant 0}\frac{(1+\delta_K)^{1/2}}{(1+\delta_{K_1})^{1/2}(1+\delta_{K_2})^{1/2}}\left[\left(\begin{array}{cc|c} L_1 & L_2 & L_1+L_2\\ K_1 & K_2 & K\end{array}\right) + (-)^{L_2}\left(\begin{array}{cc|c} L_1 & L_2 & L_1+L_2\\ K_1 & -K_2 & K\end{array}\right)\right]\xi^{L_1+L_2}_{K,L_1+L_2}. \tag{17}$$

The more general tensor-coupled product of the spherical tensors $\xi^{(L)}_K$, which have components $\xi^{(L)}_{KM}$, is considered in Section 2.4.

An equivalent but more descriptive labeling for the highest-weight monomials $\Phi_{[n_1,n_2,n_3,n_4]}(\gamma,\Omega)$ is given by regarding each of them as the $M = L$ component of the set of angular momentum L functions $\Phi_{NtLM}(\gamma,\Omega)$ to which they naturally extend. Here monomials of the same degree N and angular momentum L are distinguished by the label $t \equiv n_3$, which counts the number of zero-coupled triplets of the quadrupole coordinates. In addition, the Φ may be organized into quasibands of given bandhead angular momentum $K = 2n_2 + 2n_4$, as shown in Fig. 1. Together these functions $\Phi_{NtLM}(\gamma,\Omega)$ constitute a spherical tensor $\Phi_{NtL}(\gamma,\Omega)$. Once the highest weight function $\Phi_{NtLL}(\gamma,\Omega)$ has been defined, the remaining $\Phi_{NtLM}(\gamma,\Omega)$ follow immediately, since they share the same coefficients $F_K(\gamma)$ in the expansion (7).

An important characteristic of the generating function construction is that the set of L values appearing at a given degree N is identical to the set of L values arising for SO(3) irreps in an SO(5) irrep of seniority $v = N$. These are given by the known SO(5) ⊃ SO(3) branching rule [16,17]. Thus, Fig. 1 also enumerates the labels of all highest-weight spherical harmonics $\Psi_{v\alpha LL}$ up to the maximum seniority ($v = 6$) shown. The multiplicity d_{NL} of angular momentum L at degree N (also the multiplicity d_{vL} of angular momentum L at seniority v) is given by (A.1). A multiple occurrence of the same L at a given N first arises at $N = 6$, for $L = 6$ (Fig. 1).

Although the Φ_{NtLL} form a complete set of highest-weight functions and are angular momentum eigenfunctions, they are, in general, non-orthogonal (for a given L) and also not eigenfunctions of $\hat{\Lambda}^2$. Thus, they are not the desired SO(5) spherical harmonics. Construction of the spherical harmonics $\Psi_{v\alpha LM}(\gamma,\Omega)$ relies on the observation that the highest-weight spherical harmonics $\Psi_{v\alpha LL}$, like the Φ_{NtLL}, form a complete set of highest-weight functions and that they are polynomials of degree v in the unit quadrupole moments $\mathcal{Q}$. For any given $N_{\max}$, the sets $\{\Psi_{v\alpha LL} \mid v \leqslant N_{\max}\}$ and $\{\Phi_{NtLL} \mid N \leqslant N_{\max}\}$ both span the space of highest-weight polynomials of degree $\leqslant N_{\max}$ in $\mathcal{Q}$. Construction therefore proceeds inductively, by orthonormalization of the bases of successively higher $N_{\max}$. The $\Psi_{v\alpha LL}$, as polynomials of degree v in $\mathcal{Q}$, are linear combinations of the Φ_{NtLL} with $N \leqslant v$. Because they must be orthogonal to all $\Psi_{v'\alpha'LL}$ of lower seniority $v' < v$, they can therefore be obtained by Gram–Schmidt orthogonalizing the monomials of degree $N = v$ with respect to the space of lower degree.

The orthogonality of the spaces with differing L implies that orthogonalization can be performed separately in each space of given L. Within an L-space, the spherical harmonics up to seniority $v_{\max}$ are obtained as follows:

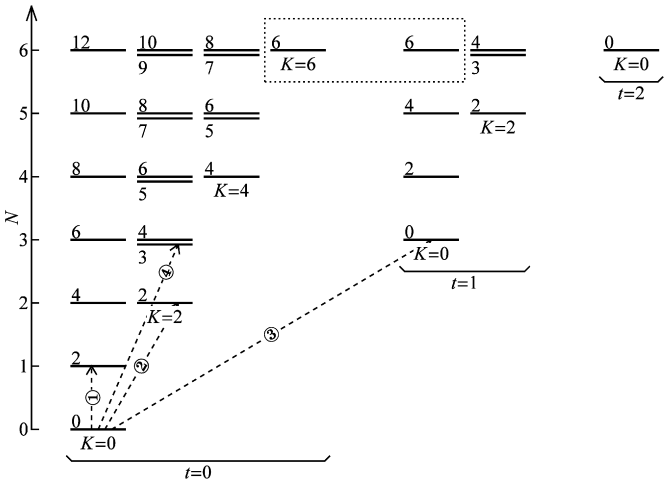

Fig. 1. The set of basis monomials Φ_{NtL} of degree $N \leqslant 6$, with labels N, L, t, and K indicated. The numbered arrows indicate the raising actions of multiplication by the generating functions Φ_1, Φ_2, Φ_3, and Φ_4. The angular momentum multiplicity at $N = 6$ is highlighted (dotted box). This same diagram enumerates the $\Psi_{v\alpha L}$ with $v \leqslant 6$, that is, it gives the branching of SO(5) irreps $(v, 0)$ into angular momenta L, if the axis label N is read as v.

Table 1
The SO(5) ⊃ SO(3) spherical harmonics $\Psi_{v\alpha L}$ for $v \leqslant 3$. For these lowest-seniority spherical harmonics, orthonormalization is trivial, and the spherical harmonics are simply proportional to the corresponding monomial basis members ($\Psi_{v\alpha L} = \mathcal{N}_{v\alpha L}^{-1/2}\Phi_{NtL}$). The relations between the $\Psi_{v\alpha L}$ (with $L = 0$ and 2) and commonly-encountered scalar and quadrupole operators are given in brackets.

v	L	$\mathcal{N}_{v\alpha L}/(8\pi^2)$	$(8\pi^2)^{1/2}\Psi_{v\alpha L}$
0	0	2/3	$\frac{\sqrt{3}}{2}\xi_0^{(0)}$ $\left[=\sqrt{\frac{3}{2}}\right]$
1	2	4/15	$\frac{\sqrt{15}}{2}\cos\gamma\,\xi_0^{(2)} + \frac{\sqrt{15}}{2}\sin\gamma\,\xi_2^{(2)}$ $\left[=\sqrt{\frac{15}{2}}\mathcal{Q}\right]$
2	4	16/105	$\frac{\sqrt{3}}{8}(7+5\cos 2\gamma)\xi_0^{(4)} + \frac{3\sqrt{5}}{4}\sin 2\gamma\,\xi_2^{(4)} + \frac{\sqrt{105}}{8}(1-\cos 2\gamma)\xi_4^{(4)}$
	2	4/15	$\frac{\sqrt{15}}{2}\cos 2\gamma\,\xi_0^{(2)} - \frac{\sqrt{15}}{2}\sin 2\gamma\,\xi_2^{(2)}$ $\left[=-\frac{\sqrt{105}}{2}(\mathcal{Q}\times\mathcal{Q})^{(2)}\right]$
3	6	32/315	$\frac{9}{16}\sqrt{\frac{5}{11}}(7\cos\gamma+\cos 3\gamma)\xi_0^{(6)} + \frac{3}{16}\sqrt{\frac{7}{22}}(15\sin\gamma+11\sin 3\gamma)\xi_2^{(6)}$ $+ \frac{9}{16}\sqrt{\frac{35}{11}}(\cos\gamma-\cos 3\gamma)\xi_4^{(6)} + \frac{3}{16}\sqrt{\frac{35}{2}}(\sin\gamma-\sin 3\gamma)\xi_6^{(6)}$
	4	88/945	$\frac{3}{4}\sqrt{\frac{3}{22}}(5\cos\gamma+7\cos 3\gamma)\xi_0^{(4)} - \frac{9}{2}\sqrt{\frac{5}{22}}\sin\gamma\,\xi_2^{(4)} + \frac{3}{4}\sqrt{\frac{105}{22}}(-\cos\gamma+\cos 3\gamma)\xi_4^{(4)}$
	3	8/63	$\frac{3}{2}\sqrt{\frac{7}{2}}\sin 3\gamma\,\xi_2^{(3)}$
	0	4/9	$\frac{3}{2}\cos 3\gamma\,\xi_0^{(0)}$ $\left[=\frac{3}{\sqrt{2}}\cos 3\gamma\right]$

(1) Order the basis monomials Φ_{NtLL}, for $0 \leqslant N \leqslant v_{\max}$, by increasing N, and then by increasing t when multiple basis monomials of the same L occur for a given N [30]. These functions may then be labeled with a single counting index, as Φ_{Li}, with $i = 1, \ldots, D_{v_{\max}L}$. The dimension $D_{v_{\max}L}$ of the seniority-truncated L-space is given by (A.2).
(2) Calculate the overlaps $\langle\Phi_{Lj}|\Phi_{Li}\rangle$ for $1 \leqslant i, j \leqslant D_{v_{\max}L}$, using (11).
(3) Determine the linear transformation necessary to bring the Φ_{Li} into an orthonormal set by the Gram–Schmidt procedure. The result is a matrix of orthogonalization (and normalization) coefficients T_{Lij} for the L-space, in terms of which the

$$\Psi_{Li} = \sum_{j=1}^{D_{v_{\max}L}} T_{Lij}\Phi_{Lj} \tag{18}$$

are the desired spherical harmonics, in order of increasing seniority.

In step (1), if angular momentum multiplicity occurs at a given N, the ordering of the Φ_{NtL} sharing the *same* N is, in principle, arbitrary. However, choosing a different ordering for the Φ_{NtL} gives rise, after Gram–Schmidt orthogonalization, to a different, equally valid, set of spherical harmonics at the corresponding seniority ($v = N$). That is, the spherical harmonics $\Psi_{v\alpha L}$ ($\alpha = 1, \ldots, d_{vL}$) span a seniority-degenerate subspace, and the ordering of the Φ_{NtL} in the orthonormalization process determines which of the possible unitarily-equivalent bases for the subspace is selected as the "spherical harmonics".

Note that the overlaps of the Φ_{NtLL} obey a parity selection rule. Since Φ_{NtLL} is a product of N factors of $\mathcal{Q}$, it has parity $(-)^N$ under the $\mathbb{R}^5$ parity operation, which takes $\mathcal{Q}_m \to -\mathcal{Q}_m$. The overlap of two functions of opposite $\mathbb{R}^5$-parity [31] vanishes, so $\langle\Phi_{N't'LL}|\Phi_{NtLL}\rangle$ is nonzero only if $N + N'$ is even. The $\Psi_{v\alpha LL}$ resulting from the orthonormalization process therefore retain definite $\mathbb{R}^5$-parity $(-)^v$ and are constructed only from the Φ_{NtLL} of this same parity.

Hence, by the $\mathbb{R}^5$ parity selection rule, all the Φ_{NtLM} with $N \leqslant 3$ are already orthogonal and therefore *are* the spherical harmonics with $v \leqslant 3$, to within normalization. The necessary normalization factors $\mathcal{N}_{v\alpha L}$, such that $\Psi_{v\alpha L} = \mathcal{N}_{v\alpha L}^{-1/2}\Phi_{NtL}$, and resulting spherical harmonics, for $v \leqslant 3$, are summarized in Table 1. The table also provides a glossary relating the $\Psi_{v\alpha L}$ to Hamiltonian ($L = 0$) and electric quadrupole ($L = 2$) operators commonly referenced in physical applications. More generally, even for $v > 3$, the two lowest-seniority $\Psi_{v\alpha L}$

for a given value of L are proportional to the Φ_{NtL} with $N = v$. Other higher-seniority $\Psi_{v\alpha L}$ are nontrivial linear combinations (18) of the Φ_{NtL} with $N \leqslant v$.

2.4. Triple overlap integrals

For the determination of SO(5) Clebsch–Gordan coefficients (Section 2.5), we need to calculate triple overlap integrals

$$\langle \Psi_3 | \hat{\Psi}_2 | \Psi_1 \rangle \equiv \int \Psi_3^*(\gamma, \Omega) \Psi_2(\gamma, \Omega) \Psi_1(\gamma, \Omega) \sin 3\gamma \, d\gamma \, d\Omega. \tag{19}$$

In this expression, $\hat{\Psi}_2$ is interpreted as an operator which acts multiplicatively, *i.e.*, $\hat{\Psi}_2|\Psi_1\rangle$ has as its wave function $\Psi_2(\gamma, \Omega)\Psi_1(\gamma, \Omega)$. For angular momentum coupled functions, we need only the reduced matrix elements $\langle \Psi_3^{(L_3)} \| \hat{\Psi}_2^{(L_2)} \| \Psi_1^{(L_1)} \rangle$ defined by the Wigner–Eckart theorem [26]

$$\langle \Psi_{3M_3}^{(L_3)} | \hat{\Psi}_{2M_2}^{(L_2)} | \Psi_{1M_1}^{(L_1)} \rangle = \frac{1}{(2L_3+1)^{1/2}} \left(\begin{array}{cc|c} L_1 & L_2 & L_3 \\ M_1 & M_2 & M_3 \end{array} \right) \langle \Psi_3^{(L_3)} \| \hat{\Psi}_2^{(L_2)} \| \Psi_1^{(L_1)} \rangle, \tag{20}$$

where the quantity in parentheses is an SO(3) Clebsch–Gordan coefficient.

The Wigner–Eckart theorem is easily inverted (*e.g.*, Ref. [8]) by application of the Clebsch–Gordan unitarity condition, to give the reduced matrix element in a computationally convenient form in terms of the coupled action of $\hat{\Psi}_2^{(L_2)}$ on $|\Psi_1^{(L_1)}\rangle$. Namely,

$$\langle \Psi_3^{(L_3)} \| \hat{\Psi}_2^{(L_2)} \| \Psi_1^{(L_1)} \rangle = (2L_3+1)^{1/2} \langle \Psi_{3M_3}^{(L_3)} | [\hat{\Psi}_2^{(L_2)} \times |\Psi_1^{(L_1)}\rangle]_{M_3}^{(L_3)}, \tag{21}$$

where $[\hat{\Psi}_2^{(L_2)} \times |\Psi_1^{(L_1)}\rangle]_{M_3}^{(L_3)}$ has wave function

$$[\Psi_2^{(L_2)}(\gamma, \Omega) \times \Psi_1^{(L_1)}(\gamma, \Omega)]_{M_3}^{(L_3)} = \sum_{M_1 M_2} \left(\begin{array}{cc|c} L_1 & L_2 & L_3 \\ M_1 & M_2 & M_3 \end{array} \right) \Psi_{2M_2}^{(L_2)}(\gamma, \Omega) \Psi_{1M_1}^{(L_1)}(\gamma, \Omega), \tag{22}$$

following the convention (14) for the coupled product of tensors. The functions $\xi_{KM}^{(L)}$ ($M = 0, \pm 1, \ldots, \pm L$), regarded as components of a spherical tensor $\xi_K^{(L)}$, obey the coupling rule

$$\begin{aligned} [\xi_{K_2}^{(L_2)}(\Omega) \times \xi_{K_1}^{(L_1)}(\Omega)]^{(L)} = {} & \frac{(1+\delta_{K_1+K_2})^{1/2}}{(1+\delta_{K_1})^{1/2}(1+\delta_{K_2})^{1/2}} \left(\begin{array}{cc|c} L_1 & L_2 & L \\ K_1 & K_2 & K_1+K_2 \end{array} \right) \xi_{K_1+K_2}^{(L)}(\Omega) \\ & + \frac{(1+\delta_{K_1-K_2})^{1/2}}{(1+\delta_{K_1})^{1/2}(1+\delta_{K_2})^{1/2}} \left\{ \begin{array}{ll} (-)^{L_2} \left(\begin{array}{cc|c} L_1 & L_2 & L \\ K_1 & -K_2 & K_1-K_2 \end{array} \right) \xi_{K_1-K_2}^{(L)}(\Omega) & K_1 \geqslant K_2 \\ (-)^{L_1} \left(\begin{array}{cc|c} L_1 & L_2 & L \\ -K_1 & K_2 & -K_1+K_2 \end{array} \right) \xi_{-K_1+K_2}^{(L)}(\Omega) & K_1 \leqslant K_2 \end{array} \right\}, \end{aligned} \tag{23}$$

obtained by direct application of (16). It follows that [33]

$$\begin{aligned} \langle \Psi_3^{(L_3)} \| \hat{\Psi}_2^{(L_2)} \| \Psi_1^{(L_1)} \rangle = {} & \frac{16\pi^2}{(2L_3+1)^{1/2}} \int \left[\sum_{\substack{K_1,K_2,K_3 \\ \text{even}}} \frac{(1+\delta_{K_3})^{1/2}}{(1+\delta_{K_1})^{1/2}(1+\delta_{K_2})^{1/2}} \right. \\ & \left. \times \left[\left(\begin{array}{cc|c} L_1 & L_2 & L_3 \\ K_1 & K_2 & K_3 \end{array} \right) + \left\{ \begin{array}{ll} (-)^{L_2} \left(\begin{array}{cc|c} L_1 & L_2 & L_3 \\ K_1 & -K_2 & K_3 \end{array} \right) & K_1 \geqslant K_2 \\ (-)^{L_1} \left(\begin{array}{cc|c} L_1 & L_2 & L_3 \\ -K_1 & K_2 & K_3 \end{array} \right) & K_1 \leqslant K_2 \end{array} \right\} \right] F_{1K_1}(\gamma) F_{2K_2}(\gamma) F_{3K_3}(\gamma) \right] \sin 3\gamma \, d\gamma. \end{aligned} \tag{24}$$

2.5. SO(5) ⊃ SO(3) *Clebsch–Gordan coefficients*

Representations of SO(5) couple to form new representations according to SO(5) Clebsch–Gordan coefficients. If the SO(5) representations are labeled according to the SO(5) ⊃ SO(3) ⊃ SO(2) subalgebra chain (1), each coupling coefficient may be written as the product of an SO(3)-reduced Clebsch–Gordan coefficient and an ordinary SO(3) Clebsch–Gordan coefficient, according to the Racah factorization lemma [34] (see Ref. [35] for a general discussion). We term the SO(3)-reduced factor an SO(5) ⊃ SO(3) Clebsch–Gordan coefficient. Coupling coefficients, such as these, which are reduced with respect to a subalgebra are also known as "isoscalar factors" [36].

In the context of the SO(5) spherical harmonics, only the symmetric representations $(v, 0)$ of SO(5) arise. These are related by the SO(5) ⊃ SO(3) Clebsch–Gordan coefficients $\left(\begin{array}{cc|c} (v_1,0) & (v_2,0) & (v_3,0) \\ \alpha_1 L_1 & \alpha_2 L_2 & \alpha_3 L_3 \end{array} \right)$, where the α_1, α_2, and α_3 are multiplicity indices, corresponding to the multiplicity in the $\Psi_{v\alpha L}$. Let $\{\chi_{\alpha_1 L_1 M_1}^{(v_1,0)}\}$ and $\{\chi_{\alpha_2 L_2 M_2}^{(v_2,0)}\}$ denote orthonormal bases for SO(5) representations of seniority v_1 and v_2, respectively. Then an orthonormal basis for an SO(5) tensor-coupled product irrep of seniority v is defined by

$$[\chi^{(v_2,0)} \otimes \chi^{(v_1,0)}]_{\alpha LM}^{(v,0)} = \sum_{\substack{\alpha_1,L_1,\alpha_2,L_2 \\ M_1,M_2}} \left(\begin{array}{cc|c} (v_1,0) & (v_2,0) & (v,0) \\ \alpha_1 L_1 & \alpha_2 L_2 & \alpha L \end{array} \right) \left(\begin{array}{cc|c} L_1 & L_2 & L \\ M_1 & M_2 & M \end{array} \right) \chi_{\alpha_2 L_2 M_2}^{(v_2,0)} \otimes \chi_{\alpha_1 L_1 M_1}^{(v_1,0)}. \tag{25}$$

The SO(5) ⊃ SO(3) Clebsch–Gordan coefficients enter into the SO(5) Wigner–Eckart theorem, which governs matrix elements of SO(5) ⊃ SO(3) tensor operators. The Racah factorization lemma may be used to write the SO(5) Wigner–Eckart theorem in terms of SO(3)-reduced quantities as

$$\langle \Psi_{v_3 \alpha_3 L_3} \| \hat{\Psi}_{v_2 \alpha_2 L_2} \| \Psi_{v_1 \alpha_1 L_1} \rangle = \sqrt{2L_3+1} \left(\begin{array}{cc|c} (v_1,0) & (v_2,0) & (v_3,0) \\ \alpha_1 L_1 & \alpha_2 L_2 & \alpha_3 L_3 \end{array} \right) \langle \Psi_{v_3} \| \hat{\Psi}_{v_2} \| \Psi_{v_1} \rangle, \tag{26}$$

where $\langle \Psi_{v_3} \| \hat{\Psi}_{v_2} \| \Psi_{v_1} \rangle$ is an SO(5)-reduced (doubly-reduced) matrix element. The factor $\sqrt{2L_3+1}$ compensates for the corresponding factor absorbed into the definition of the SO(3)-reduced matrix element in (20). The SO(5) $\supset$ SO(3) Clebsch–Gordan coefficients satisfy the normalization condition

$$\sum_{\substack{\alpha_1 L_1 \\ \alpha_2 L_2}} \left(\begin{array}{cc|c} (v_1,0) & (v_2,0) & (v_3,0) \\ \alpha_1 L_1 & \alpha_2 L_2 & \alpha_3 L_3 \end{array} \right)^2 = 1 \tag{27}$$

from unitarity, where the phases of the Clebsch–Gordan coefficients are real by convention. The values for L occurring within a given SO(5) representation $(v,0)$, and their multiplicities, are governed by the multiplicity formula (A.1). The Clebsch–Gordan coefficients vanish unless L_1, L_2, and L_3 satisfy the triangle inequality ($|L_1 - L_2| \leqslant L_3 \leqslant L_1 + L_2$). The values of v_1, v_2, and v_3 likewise must satisfy the triangle inequality ($|v_1 - v_2| \leqslant v_3 \leqslant v_1 + v_2$), as well as the parity constraint that $v_1 + v_2 + v_3$ be even.

The SO(5) $\supset$ SO(3) Clebsch–Gordan coefficient $\left(\begin{array}{cc|c} (v_1,0) & (v_2,0) & (v_3,0) \\ \alpha_1 L_1 & \alpha_2 L_2 & \alpha_3 L_3 \end{array} \right)$ follows immediately from the corresponding SO(3)-reduced matrix element $\langle \Psi_{v_3 \alpha_3 L_3} \| \Psi_{v_2 \alpha_2 L_2} \| \Psi_{v_1 \alpha_1 L_1} \rangle$, by (26), once the SO(5)-reduced matrix element $\langle \Psi_{v_3} \| \Psi_{v_2} \| \Psi_{v_1} \rangle$ is known. In fact, from (26) and the normalization condition (27), we obtain

$$\langle \Psi_{v_3} \| \hat{\Psi}_{v_2} \| \Psi_{v_1} \rangle^2 = \sum_{\substack{\alpha_1 L_1 \\ \alpha_2 L_2}} \frac{\langle \Psi_{v_3 \alpha_3 L_3} \| \hat{\Psi}_{v_2 \alpha_2 L_2} \| \Psi_{v_1 \alpha_1 L_1} \rangle^2}{2L_3+1}, \tag{28}$$

for each L_3 and α_3. This yields the SO(5)-reduced matrix element in terms of the summed squares of the computed SO(3)-reduced matrix elements, to within an arbitrary phase, which is chosen to be unity.

Explicit closed-form expressions for the SO(5)-reduced matrix element have been given for the case $\langle \Psi_{v\pm1} \| \Psi_1 \| \Psi_v \rangle$, *i.e.*, for the quadrupole tensor [3]. Moreover, by numerical inspection of the normalization sums for an extensive set of computed SO(3)-reduced matrix elements, we find [37] that the SO(5)-reduced matrix elements are given by

$$\begin{aligned} \langle \Psi_{v_3} \| \Psi_{v_2} \| \Psi_{v_1} \rangle = {} & \frac{1}{4\pi} \sqrt{\frac{(2v_1+3)(2v_2+3)}{(v_3+2)(v_3+1)}} \frac{(\frac{1}{2}\sigma+1)!}{(\frac{1}{2}\sigma - v_1)!(\frac{1}{2}\sigma - v_2)!(\frac{1}{2}\sigma - v_3)!} \\ & \times \sqrt{(\sigma+4) \frac{(\sigma - 2v_1 + 1)!(\sigma - 2v_2 + 1)!(\sigma - 2v_3 + 1)!}{(\sigma+3)!}}, \end{aligned} \tag{29}$$

with $\sigma \equiv (v_1 + v_2 + v_3)$. This conjectured expression has been verified exhaustively for all combinations of values for v_1, v_2, and v_3 likely to be considered in nuclear collective model calculations. However, we stress that is has not been proved in full generality. Use of the expression (29) for $\langle \Psi_{v_3} \| \Psi_{v_2} \| \Psi_{v_1} \rangle$ in the SO(5) Wigner–Eckart theorem (26) allows each SO(5) $\supset$ SO(3) Clebsch–Gordan coefficients to be extracted directly from the corresponding SO(3)-reduced matrix elements (24), without the need to calculate matrix elements for all L_1 and L_2 values involved in the normalization condition (27). [The use of (29) in the code is described in Section 4.2.] The validity of the conjecture, for given v_1, v_2, and v_3, may be established by calculating the normalization sum for the underlying computed SO(3)-reduced matrix elements or, equivalently, by explicitly verifying that the extracted coefficients satisfy (27).

The SO(5) $\supset$ SO(3) Clebsch–Gordan coefficients obey symmetry relations [10]

$$\left(\begin{array}{cc|c} (v_2,0) & (v_1,0) & (v_3,0) \\ \alpha_2 L_2 & \alpha_1 L_1 & \alpha_3 L_3 \end{array} \right) = (-)^{L_1+L_2-L_3} \left(\begin{array}{cc|c} (v_1,0) & (v_2,0) & (v_3,0) \\ \alpha_1 L_1 & \alpha_2 L_2 & \alpha_3 L_3 \end{array} \right) \tag{30}$$

and

$$\left(\begin{array}{cc|c} (v_3,0) & (v_2,0) & (v_1,0) \\ \alpha_3 L_3 & \alpha_2 L_2 & \alpha_1 L_1 \end{array} \right) = (-)^{L_1+L_2-L_3} \sqrt{\frac{d_{v_1}(2L_3+1)}{d_{v_3}(2L_1+1)}} \left(\begin{array}{cc|c} (v_1,0) & (v_2,0) & (v_3,0) \\ \alpha_1 L_1 & \alpha_2 L_2 & \alpha_3 L_3 \end{array} \right), \tag{31}$$

where $d_v = \frac{1}{6}(v+1)(v+2)(2v+3)$ is the dimension of the SO(5) representation $(v,0)$, obtained from the Weyl formula (*e.g.*, Ref. [35]). Hence, it is only necessary to calculate the Clebsch–Gordan coefficient for one permutation of (v_1, v_2, v_3).

3. Implementation

3.1. Overview

The computer code for construction of SO(5) $\supset$ SO(3) spherical harmonics and calculation of SO(5) $\supset$ SO(3) Clebsch–Gordan coefficients is implemented as a set of packages for Mathematica 6 [15]. Mathematica provides native support for symbolic arithmetic. In the present context, this allows all calculations to be carried out exactly, in terms of expressions involving square roots of rational numbers.

The basic algorithm for the calculation of SO(5) $\supset$ SO(3) Clebsch–Gordan coefficients, as described in Section 2, involves three main computational tasks:

(1) construction of the monomials (12) comprising the basis of highest-weight functions,
(2) calculation of the overlaps (11) of these monomials, as needed for the orthonormalization process, and
(3) calculation of triple overlaps (24), as needed for the SO(5) $\supset$ SO(3) Clebsch–Gordan coefficients.

For practical implementation, two algorithmic refinements are made to this scheme. These relate to the internal representation of the functions $F_K(\gamma)$ (Section 3.2) and to the recognition (and full utilization) of extensive redundancies among the calculations involved in

evaluating different triple overlap integrals (Section 3.3). Together, an efficient treatment of these aspects of the implementation extends the range of applicability of the method (for calculation in exact arithmetic) from a maximal seniority of approximately 10 to seniorities of $\gtrsim 100$, thereby easily yielding more than sufficient SO(5) ⊃ SO(3) Clebsch–Gordan coefficients for nuclear structure calculations.

To understand the considerations underlying the efficient implementation of the algorithm, let us more closely consider the structure of the calculation. The computationally most demanding task is evaluation of the overlap or triple overlap integrals in the Φ_{NtL} basis. Recall that this involves first constructing the function of γ appearing in the integrand of (11) or (24) and then evaluating the integral with respect to γ. The integrand is built from the generating functions (15), using (12) and (17). The integrand is thus a polynomial in the trigonometric functions $\cos\gamma$, $\sin\gamma$, $\cos 2\gamma$, $\sin 2\gamma$, $\cos 3\gamma$, and $\sin 3\gamma$ or, therefore, by multiple-angle identities, a polynomial in $\cos\gamma$ and $\sin\gamma$. For the overlap $\langle\Phi_{N_2t_2LM}|\Phi_{N_1t_1LM}\rangle$, the resulting polynomial requires powers of $\cos\gamma$ and $\sin\gamma$ as high as N_1+N_2, or, for the triple overlap $\langle\Phi_{N_3t_3L_3}\|\hat{\Phi}_{N_2t_2L_2}\|\Phi_{N_1t_1L_1}\rangle$, as high as $N_1+N_2+N_3$. The integral may be evaluated exactly, but simplification of the polynomial and integration with standard symbolic algebra software becomes prohibitively inefficient for the construction of spherical harmonics with $\nu \gtrsim 10$. Alternatively, attempts at brute-force numerical integration are hampered by the highly-oscillatory nature of such polynomials in trigonometric functions. Thus, it is seen that evaluation of the overlap integrals is the defining computational challenge.

An effective solution arises from the realization that any polynomial of degree n in $\cos\gamma$ and $\sin\gamma$ can be decomposed as a finite sum of exponentials

$$f(\gamma)=\sum_{k=-n}^{n} a_k e^{ik\gamma}, \tag{32}$$

i.e., as a finite Fourier series, of degree n. Integration of exponentials is trivial. Such a Fourier expansion method was, in fact, used in the final version of the code used to calculate the Clebsch–Gordan coefficients tabulated in Ref. [10]. In the present implementation, from the very beginning of the calculation, we simply represent all $F_K(\gamma)$ coefficients, starting with those of the integrity basis functions (15), as finite Fourier series (32). That is, every function is replaced by a list of Fourier coefficients $\{a_{-n},\ldots,a_0,\ldots,a_n\}$. Then, when the integrand in (11) or (24) is constructed as a function of γ, it is already manifestly Fourier expanded, and the γ integration is straightforward.

3.2. Fourier series representation of functions

When the functions of γ are represented as Fourier sums (32), there are three basic arithmetic operations which must be carried out on the corresponding sets of Fourier coefficients. Addition of two functions $f(\gamma)$ and $g(\gamma)$ is accomplished by addition of their Fourier coefficients. Multiplication of a function by a constant is simply accomplished by multiplication of the coefficients by that constant. Multiplication of two functions $f(\gamma)$ and $g(\gamma)$ by each other gives rise to a convolution of the coefficients. Specifically, let $f(\gamma)$ and $g(\gamma)$ be given by Fourier sums $f(\gamma)=\sum_{r=-m}^{m} a_r(e^{i\gamma})^r$ and $g(\gamma)=\sum_{s=-n}^{n} b_s(e^{i\gamma})^s$. Expanding the product and collecting like powers of $e^{i\gamma}$ yields the product rule

$$f(\gamma)g(\gamma)=\sum_{k=-(m+n)}^{m+n} c_k(e^{i\gamma})^k \tag{33}$$

with the new Fourier coefficients given by

$$c_k=\sum_{t=\max(-2m-k,-2n+k)}^{\min(2m-k,2n+k)} a_{\frac{1}{2}(k+t)}\,b_{\frac{1}{2}(k-t)}. \tag{34}$$

This is essentially the Fourier convolution theorem, in discrete form.

For real-valued functions which are even in γ, the coefficients a_k are pure real and obey the symmetry condition $a_{-k}=a_k$. Similarly, for odd real-valued functions, the coefficients are pure imaginary and obey the symmetry $a_{-k}=-a_k$. For instance, the functions arising in the definition of the generating functions (15) are $\cos m\gamma=[(e^{+i\gamma})^m+(e^{-i\gamma})^m]/2$ and $\sin m\gamma=[(e^{+i\gamma})^m-(e^{-i\gamma})^m]/(2i)$, which are even and odd, respectively. In either case, only coefficients with $k\geqslant 0$ need be stored, and only real-valued coefficients are required, provided a factor of i is absorbed into the definition of the series for odd functions.

Thus, we use the representation

$$f(\gamma)=\left(\frac{1}{i}\right)^g\sum_{k=0}^{n}\frac{a_k}{1+\delta_k}\left[(e^{+i\gamma})^k+(-)^g(e^{-i\gamma})^k\right], \tag{35}$$

with $g=0$ for even functions and $g=1$ for odd functions. This is effectively a Fourier cosine series or a Fourier sine series, for the even and odd cases, respectively.

The definite integrals needed for the calculation are of the form $\int_0^{\pi/3} f(\gamma)\,d\gamma$. Moreover, only odd integrands ($g=1$) arise in the problem. The definite integral of an odd series (35) on the "sector" $0\leqslant\gamma\leqslant\pi/3$ is

$$\int_0^{\pi/3} f(\gamma)\,d\gamma=\sum_{k=1}^{n}\frac{2a_k}{k}\left[1-\cos\frac{(k \bmod 6)\pi}{3}\right]. \tag{36}$$

Evaluation of this sum requires only a limited set of trigonometric values, namely, $\cos k\pi/3$ ($k=0,1,\ldots,5$).

The necessary definitions for working with Fourier representations of functions are contained in the subpackage `FourierSum`. The Fourier sum (35) is represented symbolically by the expression

```
FourierSum[BohrGamma, g, {a0, a1, ..., an}],
```

where g indicates the symmetry ($g = 0$ or 1), and the a_k are the real-valued Fourier coefficients as defined in (35). (The tag `BohrGamma` simply serves to indicate that the argument is γ, since the package allows for more general possibilities.) Thus, for example, $\cos 2\gamma$ is represented as

```
FourierSum[BohrGamma,0,{0,0,1/2}].
```

The coefficients which arise in the present calculations are rational numbers or square roots of rational numbers, and they are maintained as exact symbolic expressions throughout the calculation.

The package defines addition of two `FourierSum` expressions, multiplication by a constant, and multiplication of two `FourierSum` expressions as extensions to the usual Mathematica `+` and `*` operations. The function `IntegrateSector[r,f]` returns the integral given in (36). The function `FourierSumToTrig[f]` is also provided, to convert `FourierSum` expressions back into ordinary symbolic expressions in terms of trigonometric functions.

3.3. Evaluation of matrix elements

The task of computing matrix elements (triple overlap integrals) of the SO(5) ⊃ SO(3) spherical harmonics is most conveniently carried out by first calculating the matrix elements of the original monomial basis functions Φ_{NtL}, that is, the $\langle \Phi_{N_3 t_3 L_3} \| \hat{\Phi}_{N_2 t_2 L_2} \| \Phi_{N_1 t_1 L_1} \rangle$. The desired matrix elements $\langle \Psi_{\nu_3 \alpha_3 L_3} \| \hat{\Psi}_{\nu_2 \alpha_2 L_2} \| \Psi_{\nu_1 \alpha_1 L_1} \rangle$ in the orthonormal spherical harmonic basis then follow immediately from the Gram–Schmidt transformation (18). It is simplest to write this using the counting index labeling within an L-space, as

$$\langle \Psi_{L_3 i_3} \| \hat{\Psi}_{L_2 i_2} \| \Psi_{L_1 i_1} \rangle = \sum_{j_1 j_2 j_3} T_{L_3 i_3 j_3} T_{L_2 i_2 j_2} T_{L_1 i_1 j_1} \langle \Phi_{L_3 j_3} \| \hat{\Phi}_{L_2 j_2} \| \Phi_{L_1 j_1} \rangle. \tag{37}$$

As described in the preceding section, we have transformed the relatively intractable integration problem into the more manageable task of constructing products of $F_K(\gamma)$ functions in Fourier representation. Therefore, the computational burden now lies primarily in evaluating the discrete Fourier convolutions (33)–(34). Although the operations involved are in principle simple arithmetic, the number of iterations required for a single convolution is substantial, growing as the square of the degrees of the Fourier sums involved, and the arithmetic itself involves symbolic simplification of expressions involving square roots of rational numbers.

The challenge, therefore, lies in minimizing the number and complexity of the Fourier convolutions which must be evaluated. The problem is best approached by noting that the matrix elements are not to be calculated singly, but rather in aggregate, that is, as the set of all matrix elements of an operator $\hat{\Phi}_{N_2 t_2 L_2}$ between L-spaces L_1 and L_3. The integrand in the expression (24) for the matrix element is a sum over products of $F_K(\gamma)$ functions, and products of the exact same pairs of $F_K(\gamma)$ functions arise, redundantly, in the evaluation of many different matrix elements.

A few straightforward observations allow us to remove these calculational redundancies. Most obviously, every matrix element $\langle \Phi_{N_3 t_3 L_3} \| \hat{\Phi}_{N_2 t_2 L_2} \| \Phi_{N_1 t_1 L_1} \rangle$ involving the same ket $|\Phi_{N_1 t_1 L_1}\rangle$ and operator $\hat{\Phi}_{N_2 t_2 L_2}$ will also involve the same products between $F_K(\gamma)$ functions from $\Phi_{N_1 t_1 L_1}(\gamma, \Omega)$ and $\Phi_{N_2 t_2 L_2}(\gamma, \Omega)$. In the notation of (21), it is therefore advantageous to calculate the coupled action of $\hat{\Phi}_{N_2 t_2 L_2}$ on any given $|\Phi_{N_1 t_1 L_1}\rangle$, namely, $[\hat{\Phi}_{N_2 t_2 L_2} \times |\Phi_{N_1 t_1 L_1}\rangle]^{(L_3)}$, only once, and to reuse this intermediate result for the matrix element with each bra $\langle \Phi_{N_3 t_3 L_3}|$.

More significant, though, is the observation that all powers of $\Phi_3 \propto \cos 3\gamma$ factor out of the summations in (21). (This will be more clearly apparent below.) Thus, the integrands involved in the calculation of many different $\langle \Phi_{N_3 t_3 L_3} \| \hat{\Phi}_{N_2 t_2 L_2} \| \Phi_{N_1 t_1 L_1} \rangle$, sharing the same total label $t = t_1 + t_2 + t_3$, are actually identical. Even greater reduction in the number of convolutions needed is obtained by first evaluating the integrand only for those monomials involving no powers of Φ_3 ($t_1 = t_2 = t_3 = 0$) and only then multiplying by the relevant power $(\cos 3\gamma)^t$.

In practice, the entire process is based on operations involving the coefficient functions $F_K(\gamma)$ which describe functions on S_4, as in (7). The relevant definitions are provided by the subpackage `WignerDSum`. A function on S_4 is represented as the expression

```
WignerDSum[L,{F0,F2,...,F⌊L⌋2}],
```

where L is the angular momentum and $\lfloor L \rfloor_2$ denotes the greatest *even* integer less than or equal to L. The F_K, in turn, are `FourierSum` expressions (Section 3.2). Thus, for example, the generating function Φ_1 from (15) is represented by

```
WignerDSum[2,{
  FourierSum[BohrGamma,0,{0,1/2}],
  FourierSum[BohrGamma,1,{0,1/2}]
}]
```

Operations of addition of two functions and multiplication by a constant are readily defined, by entry-wise operations on the lists of $F_K(\gamma)$ coefficients. These operations are defined by the package as extensions to the usual Mathematica `+` and `*` operations.

To obtain the coupled action $[\hat{\Phi}_{N_2 t_2 L_2} \times |\Phi_{N_1 t_1 L_1}\rangle]^{(L_3)}$, we evaluate the coupled product $[\Phi_{N_2 t_2 L_2}(\gamma, \Omega) \times \Phi_{N_1 t_1 L_1}(\gamma, \Omega)]^{(L_3)}$. The calculation follows in a straightforward fashion from the coupling rule (23) for the functions $\xi_K^{(L)}$. The coupling operation is provided by the `WignerDSum` package as the function `TensorCouple[Ψ1,Ψ2,L]`.

However, the monomials $\Phi_{N_2 t_2 L_2}(\gamma, \Omega)$ and $\Phi_{N_1 t_1 L_1}(\gamma, \Omega)$ must first themselves be constructed, from the definition (12). As noted in Section 2.3, multiplication of highest-weight functions is identical to stretched ($L = L_1 + L_2$) tensor coupling. The stretched product rule (17) is simply the $L = L_1 + L_2$ special case of the more general coupling rule (23) for the $\xi_K^{(L)}$. Therefore, the Φ_{NtL} are also constructed in the code by use of this same function `TensorCouple`, as

$$\Phi_{NtL} = \left[\left[\Phi_1^{(2)}\right]^{n_1} \times \left[\Phi_2^{(2)}\right]^{n_2} \times \left[\Phi_3^{(0)}\right]^{n_3} \times \left[\Phi_4^{(3)}\right]^{n_4}\right]^{(L)}, \tag{38}$$

where $\Phi_1^{(2)}$ is the tensor with highest-weight component $\Phi_1(\gamma,\Omega)$, *etc.*, and $L = 2n_1 + 2n_2 + 3n_4$ (Section 2.3). To complete the calculation of the matrix element, the overlap with $\langle\Phi_{N_3t_3L_3}|$ must be evaluated. In fact, the function `TensorCouple` also suffices for this purpose. The sum of products of $F_K(\gamma)$ arising in the overlap integral (11) is readily expressed in coupled form. By the coupling rule (23),

$$\left[\Psi_2^{(L)} \times \Psi_1^{(L)}\right]_0^{(0)} = \frac{2}{(2L+1)^{1/2}} \sum_{\substack{K=0 \\ \text{even}}}^{L} F_{1K}(\gamma) F_{2K}(\gamma). \tag{39}$$

This follows from the basic expression for $L = 0$ Clebsch–Gordan coefficients, much like the usual scalar product result $[T_2^{(L)} \times T_1^{(L)}]_0^{(0)} = (-)^L (2L+1)^{-1/2} \sum_M (-)^M T_{1M}^{(L)} T_{2-M}^{(L)}$.

It remains then to carry out the integration over γ, by use of `IntegrateSector` (Section 3.2). If we define $\langle f(\gamma)\rangle \equiv 8\pi^2 \int_0^{\pi/3} f(\gamma) \sin 3\gamma \, d\gamma$, where the factor of $8\pi^2$ results from the integration over Euler angles, then the reduced matrix element deduced from the overlap (21) is simply

$$\langle \Phi_{N_3t_3L_3} \| \Phi_{N_2t_2L_2} \| \Phi_{N_1t_1L_1} \rangle = \left\langle \left[\Phi_{N_3t_3L_3} \times (\Phi_{N_2t_2L_2} \times \Phi_{N_1t_1L_1})^{(L_3)} \right]_0^{(0)} \right\rangle. \tag{40}$$

Expressing the overlap in terms of a coupled product does not change the underlying calculation (and at most affords a convenient economy of coding). However, this formulation does permit the factorization of $(\cos 3\gamma)^t$ from the integrand to be expressed in an especially symmetric (and explicit) form. Observe that $\Phi_3^{(0)} \propto \cos 3\gamma$ is a scalar, and, therefore, unlike the other generating functions, it factors out of the coupled product defining the monomial in (38), and subsequently out of the couplings in the zero-coupled product in (40). Hence, if we label each of the monomials by its exponents with respect to each of the generating functions, the integral factorizes as

$$\left[\Phi^{(L_3)}_{[n_1',n_2',n_3',n_4']} \times \left(\Phi^{(L_2)}_{[\nu_1,\nu_2,\nu_3,\nu_4]} \times \Phi^{(L_1)}_{[n_1,n_2,n_3,n_4]}\right)^{(L_3)}\right]_0^{(0)} = \left[\Phi^{(L_3)}_{[n_1',n_2',0,n_4']} \times \left(\Phi^{(L_2)}_{[\nu_1,\nu_2,0,\nu_4]} \times \Phi^{(L_1)}_{[n_1,n_2,0,n_4]}\right)^{(L_3)}\right]_0^{(0)} \Phi_{[0,0,t,0]}, \tag{41}$$

where $t = n_3' + \nu_3 + n_3$ is the *total* exponent of $\Phi_3^{(0)}$ occurring in the product. Note that only monomials of the form $\Phi_{[n_1,n_2,0,n_4]}$, with $n_3 = 0$, are actually needed in the calculation, along with $\Phi_{[0,0,t,0]} = (\sqrt{2}\cos 3\gamma)^t$.

The mechanics of the optimized calculation of matrix elements therefore proceed as follows. The monomials $\Phi_{[n_1,n_2,0,n_4]}$ are constructed by (38). To eliminate redundancy, this is done recursively, that is, by multiplication of the monomial of one lower degree in n_1, n_2, or n_4 by the appropriate generating function, and all the intermediate results are cached. Then the successive coupled products in (41) are constructed and cached: $(\Phi^{(L_2)}_{[\nu_1,\nu_2,0,\nu_4]} \times \Phi^{(L_1)}_{[n_1,n_2,0,n_4]})^{(L_3)}$ (stage I), $[\Phi^{(L_3)}_{[n_1',n_2',0,n_4']} \times (\Phi^{(L_2)}_{[\nu_1,\nu_2,0,\nu_4]} \times \Phi^{(L_1)}_{[n_1,n_2,0,n_4]})^{(L_3)}]_0^{(0)}$ (stage II), and finally the full integrand with $\Phi_{[0,0,t,0]}$ included (stage III).

For matrix elements within an L-space, Hermiticity reduces the number of independent matrix elements nearly by half. Since, under complex conjugation, Φ_{NtL} satisfies $\Phi^*_{NtLM} = (-)^{L-M}\Phi_{NtL-M}$, it follows [26] that

$$\langle \Phi_{N_3t_3L_3} \| \hat{\Phi}_{N_2t_2L_2} \| \Phi_{N_1t_1L_1} \rangle = (-)^{L_3+L_2-L_1} \langle \Phi_{N_1t_1L_1} \| \hat{\Phi}_{N_2t_2L_2} \| \Phi_{N_3t_3L_3} \rangle^*. \tag{42}$$

As a specific example of the computational savings provided by the caching of intermediate products, consider the calculation of matrix elements of $\Phi_{112} \propto \mathcal{Q}$ within the space $L_1 = L_3 = 40$, for all monomials of degree $\leqslant 50$. [This calculation yields the SO(5) $\supset$ SO(3) Clebsch–Gordan coefficients with $\nu_2 = 1$ and $L_2 = 2$, for all ν_1 and $\nu_3 \leqslant 50$.] There are $D_{50,40} = 154$ basis functions and thus 23 716 matrix elements to be calculated, or 11 935 after the relation (42) is taken into account. Evaluation of the coupled action of Φ_{112} (stage I) involves only 21 couplings, since the coupling is only carried out for basis functions with $n_3 = 0$. Evaluation of the scalar couplings (stage II) constitutes the bulk of the calculation. Whereas each of the couplings evaluated in stage I involves a low-L, low-degree factor (Φ_{112}), in stage II both factors, $\Phi^{(L_3)}_{[n_1',n_2',0,n_4']}$ and $(\Phi^{(L_2)}_{[\nu_1,\nu_2,0,\nu_4]} \times \Phi^{(L_1)}_{[n_1,n_2,0,n_4]})^{(L_3)}$, are typically of high L (hence each contains many F_K terms) and high degree with respect to γ (hence many terms are involved in the Fourier sums). A total of 231 such couplings are necessary. Many more distinct expressions, namely, 3001, must be evaluated at stage III, but each entails only a single multiplication of scalar functions (Fourier convolution) and is therefore not computationally intensive.

Total execution times for evaluation of these matrix elements within each L-space, as well as the dimensions of these spaces, are shown in Fig. 2. It is seen that calculations for higher L are essentially more demanding than those for lower L, even if the bases for the L-spaces are of the same size. For higher L, a larger number of F_K terms are involved in each calculation. Furthermore, the basis monomials tend to involve higher powers of those generating functions which carry angular momentum ($\Phi_1^{(2)}$, $\Phi_2^{(2)}$, and $\Phi_4^{(3)}$), in preference to $\Phi_3^{(0)}$, lessening the extent to which the optimizations discussed above can simplify the calculation.

The full, optimized process of evaluating the matrix elements of a monomial $\Phi_{N_2t_2L_2}$ between two L-spaces L_1 and L_3 is carried out by the function `CalculateMonomialMatrix`. The considerations just described also apply to eliminating redundancies in the evaluation of the overlaps needed for the orthonormalization process.

4. Use of the computer code

4.1. Installation

The Computer Physics Communications Program Library deposit associated with this article contains Mathematica package files `GammaHarmonic.m`, `FourierSum.m`, `WignerDSum.m`, `GramSchmidt.m`, and `Cache.m`, in ASCII text format. Annotated code is included for the packages in both Mathematica notebook format and Portable Document Format. The deposit also includes a Mathematica notebook demonstrating the use of the code (`Example.nb`) and example output files containing tabulations of Clebsch–Gordan coefficients (see Section 4.2).

All package files must be placed in a directory in the Mathematica file search path, as explained in the Mathematica documentation [15], or else in the current working directory for Mathematica. The package `GammaHarmonic` must then be loaded, by evaluating `Get["GammaHarmonic`"]`, as demonstrated in `Example.nb`.

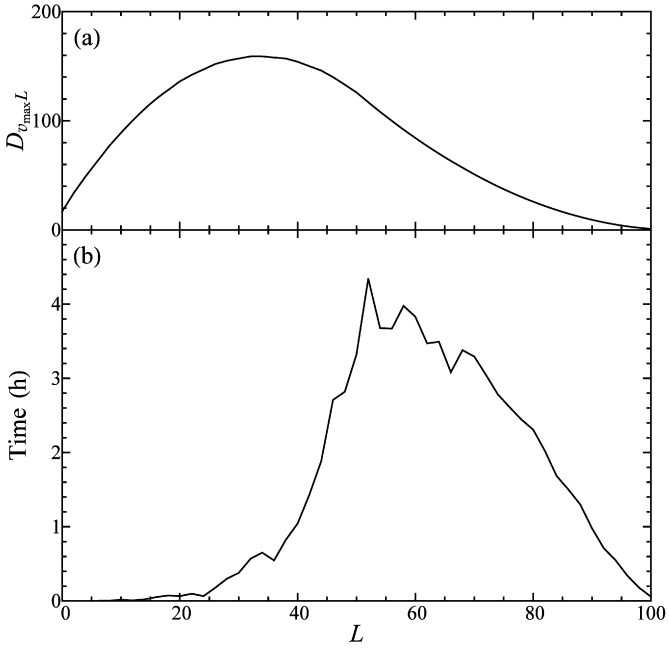

Fig. 2. Basis sizes and corresponding execution times, for calculating the matrix elements of $\Psi_{112} \propto \mathcal{Q}$ between the spherical harmonics with $v \leqslant 50$. (a) The number of basis functions $D_{v_{\max}L}$ ($v_{\max} = 50$), for L even. (b) Time for evaluating the matrix elements within a single L-space ($L_1 = L_3 \equiv L$), again only shown for L even. (The basis dimensions and, consequently, execution times are significantly smaller for L odd.) All times are for calculations carried out under Mathematica 6 for Linux, running on a 2.2 GHz Advanced Micro Devices Opteron processor.

Table 2
Control functions for SO(5) ⊃ SO(3) spherical harmonic and SO(5) ⊃ SO(3) Clebsch–Gordan coefficient generation.

Function	Description
`ConstructQNSet[`$v_{\max}$`,`$L_{\max}$`]`	Constructs a list of monomial (N, L, t, K) labels for each L-space.
`ConstructMonomials[`$v_{\max}$`,`$L_{\max}$`]`	Precaches the Φ_{NtL} constituting the monomial basis.
`ConstructMonomialMatrices[`$v_{\max}$`,`$L_{\max}$`,{`L_2`,`i_2`}]`	Calculates the matrix elements $\langle \Phi_{L_3 i_3} \| \hat{\Phi}_{L_2 i_2} \| \Phi_{L_1 i_1} \rangle$ in the monomial basis, by evaluation of the triple overlap integrals.
`ConstructBasisGST[`$v_{\max}$`,`$L_{\max}$`]`	Constructs the Gram–Schmidt transformation coefficients.
`ConstructBasisMatrices[`$v_{\max}$`,`$L_{\max}$`,{`L_2`,`i_2`}]`	Calculates the matrix elements $\langle \Psi_{L_3 i_3} \| \Psi_{L_2 i_2} \| \Psi_{L_1 i_1} \rangle$ in the spherical harmonic basis, by Gram–Schmidt transformation of the monomial matrix elements.
`WriteSO5CGTable[`$v_{\max}$`,`$L_{\max}$`,{`L_2`,`i_2`},`*`filename`*`]`	Writes a tabulation of SO(5) ⊃ SO(3) Clebsch–Gordan coefficients, as defined in the text, including both the exact rational and floating-point values.
`ReadSO5CGTable[`$v_{\max}$`,`$L_{\max}$`,{`L_2`,`i_2`},`*`filename`*`]`	Reads back a tabulation of SO(5) ⊃ SO(3) Clebsch–Gordan coefficients, as defined in the text.

4.2. Instructions

The `GammaHarmonic` package provides calculation control functions to carry out the several steps involved in constructing and tabulating a set of SO(5) ⊃ SO(3) Clebsch–Gordan coefficients. The syntax for each of the control functions is given in Table 2. Here, we provide basic instructions for carrying out these calculational tasks. A worked example, with sample input and output, is given in the Mathematica notebook `Example.nb`.

(1) The labeling scheme for the basis monomials must first be set up, using `ConstructQNSet` (see Table 2 for the appropriate syntax). This function assembles and stores a list of (N, L, t, K) labels for the monomials ($N \leqslant v_{\max}$) spanning each L-space ($L \leqslant L_{\max}$) [38].
(2) The necessary monomials Φ_{NtL} for the calculation must be constructed, with `ConstructMonomials`. Only monomials with $n_3 = 0$ are evaluated, for the reasons discussed in Section 3.3.
(3) The function `ConstructMonomialMatrices` is then used to construct matrix elements $\langle \Phi_{L_3 i_3} \| \hat{\Phi}_{L_2 i_2} \| \Phi_{L_1 i_1} \rangle$ in the monomial basis, by the process discussed in Section 3.3. The function calculates all matrix elements for a given L_2 and i_2, between all L-spaces L_1 and L_3, up to $L_{\max}$, subject to the triangle inequality. This calculation should be carried out for any (L_2, i_2) which contribute, in (37), to the final spherical harmonic matrix elements of interest. For nuclear structure applications, these would typically include $(L_2, i_2) = (2, 1)$, for the electric quadrupole operator, and $(L_2, i_2) = (0, 2)$, needed for $\cos^n 3\gamma$ contributions to the potential in the Hamiltonian. The calculation must also be carried out for $(L_2, i_2) = (0, 1)$, *i.e.*, for the identity operator Φ_{010}, since this provides the overlaps needed for the Gram–Schmidt orthonormalization.
(4) The function `ConstructBasisGST` must be used to generate the Gram–Schmidt transformation coefficients T_{Lij}.
(5) Finally, the function `ConstructBasisMatrices` is used to calculate the reduced matrix elements $\langle \Psi_{L_3 i_3} \| \hat{\Psi}_{L_2 i_2} \| \Psi_{L_1 i_1} \rangle$ of the spherical harmonics, by Gram–Schmidt transformation (37) of the previously-calculated monomial matrix elements.

The SO(5) ⊃ SO(3) Clebsch–Gordan coefficients follow from these computed SO(3)-reduced matrix elements, by the SO(5) Wigner–Eckart theorem (26) and the normalization condition (27), as described in Section 2.5. Individual Clebsch–Gordan coefficients may be

accessed with the function `SO5ClebschGordan[`$\nu_{\max}$`,{`ν_1,L_1,α_1`},{`ν_2,L_2,α_2`},{`ν_3,L_3,α_3`}]`. So that the coefficients can be extracted independently, without requiring computation of matrix elements for all L_1 and L_2 values encountered in the normalization sum (27), the function `SO5ClebschGordan` directly applies the expression (29) for the SO(5)-reduced matrix element in the SO(5) Wigner–Eckart theorem.

The function `WriteSO5CGTable` outputs a tabulation of SO(5) ⊃ SO(3) Clebsch–Gordan coefficients sharing the same ν_2, α_2, and L_2. These correspond to spherical harmonic matrix elements sharing the same $\hat{\Psi}_{\nu_2\alpha_2 L_2}$. Coefficients are listed in order of increasing L_3, L_1, ν_3, α_3, ν_1, and α_1 (that is, with the last of these indices varying most rapidly). Only coefficients with $L_1 \leqslant L_3$ are tabulated, in recognition of the symmetry relation (31), and only those coefficients for which nonzero values are allowed under the SO(3) triangle inequality and SO(5) selection rules (Section 2.5) are included.

The Clebsch–Gordan coefficients are written both exactly and as floating point numbers. The exact value of a Clebsch–Gordan coefficient can be expressed as the signed square root of a rational number, $\pm\sqrt{a/b}$. The magnitude of each value is squared in the output, to eliminate the need for radicals, so the value written is $\pm a/b$. Because the numerators and denominators appearing in these rational numbers can be large (exceeding 400 decimal digits, for instance, for $\nu_{\max} = 50$), the floating point value is also given. This is meant to facilitate input by external programs written in languages which do not provide native support for arbitrary-length integers. Each row of the tabulation has the form

$$\nu_1\ L_1\ \alpha_1\ \nu_2\ L_2\ \alpha_2\ \nu_3\ L_3\ \alpha_3\ x \quad \pm a/b,$$

where x is the floating point representation of $\pm a/b$.

Tabulated coefficients may be read back with `ReadSO5CGTable`. The corresponding SO(3)-reduced matrix elements are recovered and stored as matrices `BasisOperatorMatrix[`$\nu_{\max}$`,{`L_2,i_2`},{`L_3,L_1`}]`, which may then be used, for instance, for ACM calculations in Mathematica. When using the matrix elements calculated by the code, it should be noted that the factor of $8\pi^2$ which arises from the integration over Euler angles has been suppressed in the actual calculations. (This choice is made in order to eliminate the symbol π from input and output.) If the true normalization is desired, all computed matrix elements must be multiplied by $(8\pi^2)^{-1/2}$.

Two example tabulations of SO(5) ⊃ SO(3) Clebsch–Gordan coefficients are included with the Computer Physics Communications Program Library deposit. These contain coefficients with $(\nu_2, L_2) = (1, 2)$ and $(3, 0)$ [that is, $(L_2, i_2) = (2, 1)$ and $(0, 2)$], for all seniorities ν_1 and ν_3 up to $\nu_{\max} = 50$ and for all allowed values of L_1 and L_3 at these seniorities ($L_{\max} = 100$). The tabulations are given in the files `basis-50-100-cg-2-1.dat` and `basis-50-100-cg-0-2.dat`. (The numerical labels indicate $\nu_{\max}$, $L_{\max}$, L_2, and i_2, respectively.) The tabulated coefficients are of sufficient extent to support basic nuclear structure calculations with the ACM.

Intermediate results may be saved to files at various stages of the calculation, and later retrieved, allowing computations to be resumed or extended [39] at a later time. In particular, monomial matrix elements may be saved with `WriteMonomialMatrices` and subsequently read back with `ReadMonomialMatrices` (see `Example.nb` and the internal program documentation). Similar functions are defined to write and read back the Gram–Schmidt transformation coefficients and to write out the SO(3)-reduced matrix elements of the spherical harmonics in matrix format.

4.3. Explicit expressions for the SO(5) ⊃ SO(3) spherical harmonics

Explicit expressions for the SO(5) ⊃ SO(3) spherical harmonics, as functions of γ and the Euler angles (Table 1), are not needed for diagonalization of the collective model Hamiltonian or calculation of transition matrix elements in the ACM framework. The SO(5) ⊃ SO(3) Clebsch–Gordan coefficients suffice. However, if ACM calculations are carried out in an SU(1, 1) × SO(5) basis, probability distributions $P(\beta, \gamma)$ for the wave functions in coordinate space can then be obtained by combining the known radial wave functions $R_n^{\lambda}(\beta)$ [3] and the expressions for the $\Psi_{\nu\alpha L}(\gamma, \Omega)$. The general procedure is given in the appendix of Ref. [9], and example probability distributions may be found in Figs. 3 and 4 of that reference.

The function `ConstructBasisWaveFunctions[`$\nu_{\max}$`,`$L_{\max}$`]` explicitly constructs the spherical harmonics $\Psi_{\nu\alpha L}(\gamma, \Omega)$, by taking linear combinations of the monomials Φ_{NtL}, according to the Gram–Schmidt transformation (18). The spherical harmonics may be converted from Fourier representation to symbolic expressions involving trigonometric functions by use of `FourierSumToTrig` (Section 3.2), as demonstrated in `Example.nb`. A normalization factor of $(8\pi^2)^{-1/2}$ must be restored in these results, as indicated in Table 1, if the true normalization is desired.

4.4. Algebraic collective model infrastructure

If ACM calculations are to be carried out within Mathematica, the `GammaHarmonic` package provides several additional functions which can facilitate this process. As already noted (Section 4.2), the package provides the necessary function (`ReadSO5CGTable`) for input of previously-calculated SO(5) ⊃ SO(3) Clebsch–Gordan coefficients. The function `TruncateBasisMatrices` may then be used to truncate the stored matrices of SO(3)-reduced matrix elements to lower $\nu_{\max}$, in order to reduce the product space dimensions for ACM calculations. The `GammaHarmonic` package also defines several functions (`SO5LSpaceSize`, `SO5Branching`, `SO5LSpaceSeniorities`, *etc.*) based on the SO(5) ⊃ SO(3) dimension and branching formulas of Appendix A (see the internal program documentation). These functions are of use in indexing the SU(1, 1) × SO(5) basis functions and constructing the seniority contribution to the kinetic energy operator.

5. Conclusion

The computational methods described in this article, as implemented in the accompanying computer code, make possible the calculation of a sufficient set of SO(5) ⊃ SO(3) Clebsch–Gordan coefficients to support fully converged nuclear structure calculations with the algebraic collective model (ACM). The SU(1, 1) × SO(5) algebraic structure of the ACM basis permits matrix elements of an essentially unlimited set of potential and kinetic energy operators to easily be constructed. The Bohr collective model in the resulting calculational scheme is thus genuinely an *algebraic* collective model. The availability of SO(5) ⊃ SO(3) Clebsch–Gordan coefficients, in conjunction with

a large body of analytic expressions for β matrix elements [3,4], makes it possible to algebraically construct the matrix elements for any collective model Hamiltonian expressible as a polynomial in the collective quadrupole moments and canonical momenta. Algebraic expressions for matrix elements of a variety of other operators, including the term β^{-2} occurring in the Davidson potential [40,41], have also been derived [3,4].

The calculated SO(5) ⊃ SO(3) Clebsch–Gordan coefficients now permit the diagonalization of the Bohr Hamiltonian for potentials of essentially arbitrary γ stiffness. This allows application of the ACM to the full range of nuclear quadrupole rotational–vibrational structure, from spherical oscillator to axial rotor to triaxial rotor. With an appropriate optimized choice of β basis functions [3], fully converged calculations can be carried out very efficiently, providing a valuable tool for studying collective motion in nuclei.

The SU(1, 1) × SO(5) framework also opens the door for more detailed exploration of the formal relationship between the Bohr collective model and the interacting boson model (IBM) [11], through the U(6) ⊃ U(5) ⊃ SO(5) and U(6) ⊃ SO(6) ⊃ SO(5) bases. Algebraic collective model methods have already been applied [13] to calculation of collective states within the SO(6) limit of the IBM. The availability SO(5) ⊃ SO(3) Clebsch–Gordan coefficients enables such studies to be enhanced and extended.

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Appendix A. Branching and multiplicity for the reduction SO(5) ⊃ SO(3)

The multiplicity of each SO(3) irrep (L) within the SO(5) irrep $(v, 0)$ is needed in the code, both to determine the SO(5) ⊃ SO(3) branching for the basis and to convert between the $(v\alpha L)$ and (Li) labeling schemes. The result of Refs. [7,42] can be expressed more compactly as

$$d_{vL} = \left(\left\lfloor \frac{1}{3}(v-b)\right\rfloor + 1\right)\theta_{v-b} - \left\lfloor \frac{1}{3}(v-L+2)\right\rfloor\theta_{v-L+2}, \tag{A.1}$$

where $b \equiv L/2$ for L even or $(L+3)/2$ for L odd. The step function θ_k is unity for $k \geqslant 0$ and zero otherwise. The dimension $D_{v_{\max}L} \equiv \sum_{v=0}^{v_{\max}} d_{vL}$ of the basis for a given L-space, truncated at seniority $v \leqslant v_{\max}$, is consequently

$$D_{v_{\max}L} = \left[f(v_{\max}-b, 3) + (v_{\max}-b+1)\right]\theta_{v_{\max}-b} - f(v_{\max}-L+2, 3)\theta_{v_{\max}-L+2}, \tag{A.2}$$

where $f(n, m) \equiv \sum_{k=0}^{n} \lfloor k/m \rfloor$ is given by

$$f(n, m) = \lfloor n/m \rfloor \left[n + 1 - \frac{1}{2}m\left(\lfloor n/m \rfloor + 1\right)\right]. \tag{A.3}$$

References

[1] A. Bohr, B.R. Mottelson, Nuclear Deformations, Nuclear Structure, vol. 2, World Scientific, Singapore, 1998.
[2] D.J. Rowe, Nucl. Phys. A 735 (2004) 372.
[3] D.J. Rowe, P.S. Turner, Nucl. Phys. A 753 (2005) 94.
[4] D.J. Rowe, J. Phys. A 38 (2005) 10181.
[5] G. Gneuss, U. Mosel, W. Greiner, Phys. Lett. B 30 (1969) 397.
[6] G. Gneuss, U. Mosel, W. Greiner, Phys. Lett. B 31 (1970) 269.
[7] J.M. Eisenberg, W. Greiner, Nuclear Models: Collective and Single-Particle Phenomena, 3rd ed., Nuclear Theory, vol. 1, North-Holland, Amsterdam, 1987.
[8] D.J. Rowe, J.L. Wood, Fundamentals of Nuclear Models: Foundational Models, World Scientific Singapore, in press.
[9] M.A. Caprio, Phys. Rev. C 72 (2005) 054323.
[10] D.J. Rowe, P.S. Turner, J. Repka, J. Math. Phys. 45 (2004) 2761.
[11] F. Iachello, A. Arima, The Interacting Boson Model, Cambridge University Press, Cambridge, 1987.
[12] F. Iachello, P. Van Isacker, The Interacting Boson-Fermion Model, Cambridge University Press, Cambridge, 1991.
[13] D.J. Rowe, G. Thiamova, Nucl. Phys. A 760 (2005) 59.
[14] M.A. Caprio, F. Iachello, Nucl. Phys. A 781 (2007) 26.
[15] Mathematica 6, Wolfram Research, Inc., Champaign, Illinois, 2007.
[16] N. Kemmer, D.L. Pursey, S.A. Williams, J. Math. Phys. 9 (1968) 1224.
[17] S.A. Williams, D.L. Pursey, J. Math. Phys. 9 (1968) 1230.
[18] L. Wilets, M. Jean, Phys. Rev. 102 (1956) 788.
[19] D.R. Bès, Nucl. Phys. 10 (1959) 373.
[20] E. Chacón, M. Moshinsky, R.T. Sharp, J. Math. Phys. 17 (1976) 668.
[21] E. Chacón, M. Moshinsky, J. Math. Phys. 18 (1977) 870.
[22] S. De Baerdemacker, K. Heyde, V. Hellemans, J. Phys. A 40 (2007) 2733.
[23] The generating functions that we use can also be derived by methods similar to those used in deriving an "integrity basis" [43] for the SO(3) invariants in the universal enveloping algebra of SU(3) and by construction of a generating function for the character of the reducible SO(3) representation on $L^2(S_4)$ [44].
[24] P.O. Hess, M. Seiwert, J. Maruhn, W. Greiner, Z. Phys. A 296 (1980) 147.
[25] D. Troltenier, P.O. Hess, J.A. Maruhn, in: K. Langanke, J.A. Maruhn, S.E. Koonin (Eds.), Computational Nuclear Physics 1: Nuclear Structure, Springer-Verlag, Berlin, 1991, p. 105.
[26] A.R. Edmonds, Angular Momentum in Quantum Mechanics, 2nd ed., Investigations in Physics, vol. 4, Princeton University Press, Princeton, New Jersey, 1960.
[27] A. Bohr, Mat. Fys. Medd. Dan. Vid. Selsk. 26 (14) (1952).
[28] Use of left-to-right coupling (*e.g.* Ref. [26]) for the SO(3) tensor product would introduce phase factors of the form $(-)^{L_1+L_2-L_3}$ in some of the *intermediate* results (namely, those which explicitly involve the tensor coupling operation) of the following sections. However, the choice of convention has no effect on the final computed matrix elements or SO(5) ⊃ SO(3) Clebsch–Gordan coefficients.
[29] Strictly speaking, the degree of an arbitrary polynomial in the components $\mathcal{Q}_m$ of the quadrupole tensor is not well defined. Since $\mathcal{Q}\cdot\mathcal{Q} \equiv \sum_m |\mathcal{Q}_m|^2 = 1$, a polynomial may be multiplied by arbitrary factors of $\mathcal{Q}\cdot\mathcal{Q}$ with no effect. The definition of degree must therefore be restricted to polynomials that cannot be reduced to polynomials of lower degree by means of the identity $\mathcal{Q}\cdot\mathcal{Q} = 1$. This condition is automatically satisfied by the highest-weight functions obtained as products (12) of generating functions.

[30] See, however, endnote [38] regarding the ordering of monomials of the same L and N.
[31] The $\mathbb{R}^5$-parity quantum number has variously been termed γ-parity [19], d-parity [32], and q-parity [10] in different nuclear collective model contexts.
[32] N. Pietralla, P. von Brentano, A. Gelberg, T. Otsuka, A. Richter, N. Smirnova, I. Wiedenhöver, Phys. Rev. C 58 (1998) 191.
[33] The expression (24) is equivalent to equation (A.4) of Ref. [9]. However, in comparing the expressions, note that Ref. [9] follows a different normalization convention for the reduced matrix element in the Wigner–Eckart theorem and for the coefficients $F_K(\gamma)$.
[34] G. Racah, Phys. Rev. 76 (1949) 1352.
[35] B.G. Wybourne, Classical Groups for Physicists, Wiley, New York, 1974.
[36] A.R. Edmonds, Proc. R. Soc. London A 268 (1962) 567.
[37] D.J. Rowe, T.A. Welsh, M.A. Caprio, in preparation.
[38] The order in which the labels are stored determines the order of orthogonalization in the Gram–Schmidt procedure. By default, the convention of Section 2.3 is followed in the case of multiplicities, namely, monomials are orthonormalized in order of *increasing* t. However, the opposite ordering (*decreasing* t) was used for the tabulation in Ref. [10] which yields a unitarily equivalent but distinct set of values. The code will employ the latter convention if the option `Order->-1` is given to `ConstructQNSet`.
[39] If calculations have already been completed through $L_{\max} = L_{\max,0}$, they may be continued from this point onward (to higher $L_{\max}$) by specifying the option `Last->`$L_{\max,0}$ to any of the calculation control functions (Table 2) or input/output functions. Alternatively, by this mechanism, calculations for different sets of L-spaces may be carried out concurrently on multiple processors or systems.
[40] J.P. Elliott, J.A. Evans, P. Park, Phys. Lett. B 169 (1986) 309.
[41] D.J. Rowe, C. Bahri, J. Phys. A 31 (1998) 4947.
[42] T. Kishimoto, T. Tamura, Nucl. Phys. A 163 (1971) 100.
[43] B.R. Judd, W. Miller Jr., J. Patera, P. Winternitz, J. Math. Phys. 15 (1974) 1787.
[44] T.A. Welsh, D.J. Rowe, in preparation.