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ALGEBRAIC MANIPULATION OF THE STATES ASSOCIATED WITH THE U(5) ⊃ O(5) ⊃ O(3) CHAIN OF GROUPS: ORTHONORMALIZATION AND MATRIX ELEMENTS

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A collection of procedures able to perform algebraic manipulations for the orthonormalization and for the calculation of matrix elements between the states associated with the U(5) ⊃ O(5) ⊃ O(3) chain of groups is presented. These procedures combine both the exact- and the bigfloat-arithmetic modes and thus return arbitrarily accurate results; this is particularly relevant to the Gram–Schmidt orthonormalization, where strong cancellations usually pose serious problems in all floating-point implementations.

PROGRAM SUMMARY

Title of program: PHIMANIP

Catalogue number: ABJA

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

Computer: VAX 8650

Operating System: VMS Version 4.7

Programming languages used: REDUCE

High speed storage required: depends on the problem, minimum 0.5 Mbytes

No. of bits in a word: 32

No. of lines in combined program and test deck: 665

Keywords: U(5) ⊃ O(5) ⊃ O(3) chain of groups, interacting boson approximation, geometrical collective model, five-dimensional harmonic oscillator, quadrupole vibrations of the nucleus, wave functions for γ-degree of freedom, Gram–Schmidt orthonormalization, matrix elements in the β, γ plane, exact arithmetic, bigfloat arithmetic, computer-assisted algebra, REDUCE

Nature of physical problem
Group theoretical ideas and, in particular, states associated with the U(5) ⊃ O(5) ⊃ O(3) chain of groups are widely used to describe properties of nuclei, both within the framework of the interacting boson approximation and of the geometric collective models of the Frankfurt group. Among the many processes and properties this chain has been applied to, prominent are the low-energy nuclear spectra, Coulomb excitation and medium-energy proton scattering, and the photoabsorption of the giant dipole resonance in deformed nuclei.

Method of solution
Implementation of Gram–Schmidt orthonormalization in exact arithmetic upon the wave functions generated by the program PHISYM [1]. Direct calculation of matrix elements [2,3] by implementation of relevant integrations over the β- and γ-degrees of freedom through the use of algebraic recurrence relations and with the help of LET rules.

Restrictions on the complexity of the problem
The available computer memory in combination with the automatic space allocations of REDUCE is the most severe restriction. This situation may be alleviated by splitting the calculation into several smaller steps.

Typical running time
This depends strongly on the complexity of the problem and cannot be estimated in advance.

References
[1] C. Yannouleas and J.M. Pacheco, Comput. Phys. Commun. 52 (1988) 85.
[2] E. Chacón and M. Moshinsky, J. Math. Phys. 18 (1977) 870.
[3] P.O. Hess, M. Seiwert, J. Maruhn and W. Greiner, Z. Phys. A296 (1980) 147.

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LONG WRITE-UP

1. Introduction

In a previous paper [1] (hereafter referred to as paper I), we presented a REDUCE program that calculates algebraically the γ-dependent part of the states associated with the $U(5) \supset O(5) \supset O(3)$ chain of groups. These states form a complete basis that spans [2] the five-dimensional space for quadrupole deformations of a nucleus or the space for a nuclear Hamiltonian in the IBA model [3] built out of d bosons.

Given the usefulness of this chain*, considerable effort within the framework of group theory has been invested in providing analytic specifications of the states associated with it. In fact, four rather lengthy papers [4–7] that offer closed analytic results are now available. Yet, these states, as presented in refs. [4–7], are not normalized and not orthogonal in some quantum numbers. More important, in spite of their analytic form, the γ-dependent part of these states involves a prohibitive degree of algebraic manipulations which cannot be carried out by hand.

Until now, numerical computation has been used [3,8] in the handling of these states, but such an approach neutralizes many of the advantages of the algebraic group theoretical method. Fortunately, the recently introduced symbolic and algebraic codes like REDUCE [9] and MACSYMA [10] offer a powerful tool for the algebraic handling of such situations.

Paper I presented the first step in a research program aiming at using computer-assisted algebra for handling the γ-dependent part - denoted by $\phi_K^{\lambda\mu L}(\gamma)$ - of the states associated with the $U(5) \supset O(5) \supset O(3)$ chain of groups. Specifically, paper I presented a REDUCE program - called PHISYM - that calculates this part by a direct implementation of the analytic expressions derived by Chacón and Moshinsky ** [6]. The purpose of the present paper is to complete this effort by offering REDUCE procedures that orthonormalize these states with respect to all indices and, subsequently, calculate matrix elements between them. This orthonormalization of the basis states is a prerequisite for the evaluation of the matrix elements that appear in the many physical applications [2,3,8,11–13]. As will be elaborated later, these matrix elements are expressed as a product of two integrals, one over the radial variable β and the second over the angular variable γ. We will present REDUCE procedures for the calculation of both integrals.

These procedures are grouped in one program under the name PHIMANIP. The program PHIMANIP, in conjunction with the program PHISYM, forms a powerful tool offering an easy access to many complicated aspects of nuclear structure and of the physics of rotating nuclei. Special care has been taken that the program PHIMANIP is user-friendly, namely, the user does not need to have extensive knowledge of REDUCE in order to use it; most of the necessary additional REDUCE statements are built in with special auxiliary procedures.

Apart from the easy accessibility to the subject of the $U(5) \supset O(5) \supset O(3)$ chain of groups, a central advantage of the present algebraic programs is the possibility of choosing between exact and arbitrary floating-point-precision arithmetic provided by the REDUCE system, a fact that drastically enhances the accuracy of the calculations. This exact arithmetic is particularly crucial [14] for the Gram–Schmidt orthonormalization method that appears as a necessary step in the handling [11,12] of the $\phi_K^{\lambda\mu L}(\gamma)$'s.

The plan of the present paper is as follows:

1. Section 2 summarizes the Gram–Schmidt orthonormalization method as adopted to the present case; it also describes the relevant matrix elements that appear in physical applications, as well as some auxiliary mathematical steps;
2. Section 3 describes the different procedures necessary for an integral algebraic manipulation of the states of the $U(5) \supset O(5) \supset O(3)$ chain of groups;

* For a complete description of its physical significance, see the introduction in paper I.

** For a concise description of these expressions, see paper I.

3. Section 4 describes how to use these procedures and offers typical examples;
4. Finally, Section 5 provides a discussion on future perspectives.

2. Mathematical background

The states associated with the chain U(5) ⊃ O(5) ⊃ O(3) are the eigenstates of the five-dimensional harmonic oscillator. The labeling of these states is done through five quantum numbers $\{N, \lambda, \mu, L, M\}$. Specifically, N gives the number of phonons present in the corresponding state; λ is referred to as the seniority and reflects the number of phonons which do not contribute to pairs coupled to angular momentum zero. L and M are the quantum numbers for the total angular momentum and its projection in the laboratory frame, respectively. The fifth quantum number, denoted here by μ, is related to the number of phonon triplets coupled to momentum zero.

2.1. Orthonormalization

It turns out that a convenient way of spanning the coordinate space for the five-dimensional harmonic oscillator is to consider the three Euler angles θ_i, $i = 1, 2, 3$ and the two intrinsic β and γ shape variables [15,6]. The corresponding eigenstates are written as

$$|N\lambda\mu LM\rangle = F_{n_\beta}^{\lambda}(\beta)\sqrt{\frac{2L+1}{8\pi^2}}\,C_L^{\lambda\mu}\sum_{K\geq 0}\phi_K^{\lambda\mu L}(\gamma) \times\frac{\left[D_{M,K}^{L*}(\theta_i)+(-)^L D_{M,-K}^{L*}(\theta_i)\right]}{(1+\delta_{K0})}, \qquad (1)$$

where $D_{M,K}^{L*}$ are the usual rotation matrices [16] and the β-dependent part, $F_{n_\beta}^{\lambda}(\beta)$, is expressed through associated Laguerre polynomials [6] as follows:

$$F_{n_\beta}^{\lambda}(\beta) = \left[\frac{2n_\beta!\kappa^{\lambda+5/2}}{(n_\beta+\lambda+3/2)!}\right]^{1/2} \times\beta^{\lambda}L_{n_\beta}^{\lambda+3/2}(\kappa\beta^2)\,e^{-\kappa\beta^2/2}. \qquad (2)$$

In eq. (1), the indices N and n_β are connected through the relation $N = 2n_\beta + \lambda$, while in eq. (2) $\kappa = M\omega/\hbar$, where ω is the frequency of the oscillator and M an appropriate inertial parameter.

Unlike paper I, explicit care has been taken here to display the normalization constants. The overlap of two kets like eq. (1) involves a five-dimensional integration over the two intrinsic degrees of freedom, β and γ, and the three Euler angles. The contribution of β to the normalization constant is the square root in eq. (2); the corresponding contribution of the integration over the Euler angles, which involves the integral of two rotation matrices [16], is given by $\{(2L+1)/(8\pi^2)\}^{1/2}$. The part that corresponds to the gamma integration is denoted by $C_L^{\lambda\mu}$ and is given by

$$\left[C_L^{\lambda\mu}\right]^{-2} = \int_0^{\pi}\sum_{K\geq 0}\frac{2\left[\phi_K^{\lambda\mu L}(\gamma)\right]^2}{(1+\delta_{K0})}\sin(3\gamma)\,d\gamma = \mathcal{N}_L^{\lambda\mu}. \qquad (3)$$

It should be noticed that the normalization constant in eq. (3) involves the trace over the intrinsic angular-momentum projections K.

The kets in eq. (1) are orthogonal in the four indices $\{N, \lambda, L, M\}$. However, they are not necessarily orthogonal in the index μ; this, as will be later elaborated, can be easily checked with the present code. Specifically, the nonorthogonality occurs when different values of μ correspond to the same value of λ, namely, when degeneracies in energy with respect to μ appear, since $N = 2n_\beta + \lambda$. The relation of λ to μ is given by

$$\tfrac{1}{2}L \leq \lambda - 3\mu \leq L, \quad \text{when } L \text{ is even}, \qquad (4)$$

and by

$$\tfrac{1}{2}(L+3) \leq \lambda - 3\mu \leq L, \quad \text{when } L \text{ is odd}. \qquad (5)$$

There are no μ-degeneracies for the first few angular momenta $L = 0, 2, 3, 4, 5$ and $L = 7$ (but not for L = 6). The range of angular momenta that corresponds to a given *maximum* μ-degeneracy can be determined by the relation [11]

$$6(n\mu d_{\max} - 1) \leq L \leq (6(n\mu d_{\max} - 1) + 5). \qquad (6)$$

where $n\mu d_{\max}$ denotes the maximum μ-degeneracy. For example, for momenta $12 \leq L \leq 17$ a

maximum of three basis states have to be orthogonalized.

We adopt the Gram–Schmidt method to the problem of orthonormalizing the kets $|N\lambda\mu LM\rangle$ of eq. (1). In the present case, this method amounts to the following: Assume that the first 1, 2,..., i kets are already *orthogonalized* and denoted by a tilde over them, while the rest of the kets, $i+1,\ldots,$ are not. Also assume that their norms, $\mathcal{N}_L^{\lambda\mu}$, are available. Then the $\tilde{\phi}_K^{\lambda\mu(i+1)L}(\gamma)$'s that correspond to the *orthogonal*, but as yet *unnormalized*, $(i+1)$-ket are given by the expression

$$\tilde{\phi}_K^{\lambda\mu(i+1)L}(\gamma) = \phi_K^{\lambda\mu(i+1)L}(\gamma) - \sum_{j=1}^{i} \tilde{\phi}_K^{\lambda\mu(j)L}(\gamma) \times(\lambda,\ \mu(j),\ L\,|\,\lambda,\ \mu(i+1),\ L)/\mathcal{N}_L^{\lambda\mu(j)}. \tag{7}$$

In eq. (7), $(\ldots\,|\,\ldots)$ denotes the γ-overlap of two kets, $|N'\lambda'\mu'LM\rangle$ and $|N''\lambda''\mu''LM\rangle$, and is given by

$$(\lambda',\ \mu',\ L\,|\,\lambda'',\ \mu'',\ L) = \int_0^{\pi} \sum_{K\geq 0} \frac{2\phi_K^{\lambda'\mu'L}(\gamma)\phi_K^{\lambda''\mu''L}(\gamma)}{(1+\delta_{K0})} \sin(3\gamma)\,d\gamma. \tag{8}$$

Of course, before applying eq. (7) to the next step $(i+2)$, the norm of the function $\tilde{\phi}^{\lambda\mu(i+1)L}(\gamma)$ must be evaluated according to eq. (3).

2.2. Matrix elements

The implementation of the Gram–Schmidt method described in the previous subsection yields a complete and *orthonormal* basis of states having the form of eq. (1), but with the untilded $\phi_K^{\lambda\mu L}(\gamma)$'s replaced by the tilded $\tilde{\phi}_K^{\lambda\mu L}(\gamma)$'s. The next natural step is the calculation of matrix elements between these states. In the different physical applications, the most general matrix element [6] that can appear has the form

$$\left\langle N''\lambda''\mu''L''M''\left|\beta^{2\rho+\lambda}T_M^{\lambda\mu L}(\beta,\gamma,\theta_i)\right|N'\lambda'\mu'L'M'\right\rangle, \tag{9}$$

where the operator $T_M^{\lambda\mu L}(\beta,\gamma,\theta_i)$ is given by

$$T_M^{\lambda\mu L}(\beta,\gamma,\theta_i) = \sum_K \tilde{\phi}_K^{\lambda\mu L}(\gamma) D_{M,K}^{L*}(\theta_i). \tag{10}$$

Notice that, in this subsection, the indices K will be free to run over both positive and negative values. This is equivalent to restricting them to nonnegative values, because of the symmetry properties of the $\tilde{\phi}_K^{\lambda\mu L}(\gamma)$'s, namely

$$\tilde{\phi}_{-K}^{\lambda,\mu,L}(\gamma) = (-)^L \tilde{\phi}_K^{\lambda\mu L}(\gamma). \tag{11}$$

This symmetry property is automatically taken into account by the program PHISYM.

After the integration over the Euler angles has been carried out, the matrix element of eq. (9) is expressed as the product of two integrals, one over β and the other over γ, namely

$$\left\langle N''\lambda''\mu''L''M''\left|\beta^{2\rho+\lambda}T_M^{\lambda\mu L}(\beta,\gamma,\theta_i)\right|N'\lambda'\mu'L'M'\right\rangle = (\lambda',\ n'_\beta;\ \lambda'',\ n''_\beta;\ 2\rho+\lambda)_{\text{beta}} \times(-)^{L'+L''+M'+M''} \times\langle L,\ L'',\ M,\ -M''\,|\,L',\ -M'\rangle \times(\lambda\mu L;\ \lambda'\mu'L';\ \lambda''\mu''L''), \tag{12}$$

where the integral over β is given by

$$(\lambda',\ n'_\beta;\ \lambda'',\ n''_\beta;\ 2\rho+\lambda)_{\text{beta}} = \int_0^{\infty} F_{n''_\beta}^{\lambda''}(\beta)\beta^{2\rho+\lambda}F_{n'_\beta}^{\lambda'}(\beta)\beta^4\,d\beta, \tag{13}$$

while the integral over γ is given by

$$(\lambda\mu L;\ \lambda'\mu'L';\ \lambda''\mu''L'') = \sum_{K,K',K''} (-)^{L-L'}\langle L,\ L',\ K,\ K'\,|\,L'',\ -K''\rangle \times\int_0^{\pi} \tilde{\phi}_K^{\lambda\mu L}(\gamma)\tilde{\phi}_{K'}^{\lambda'\mu'L'}(\gamma)\tilde{\phi}_{K''}^{\lambda''\mu''L''}(\gamma)\sin(3\gamma)\,d\gamma. \tag{14}$$

In eqs. (12) and (14), the symbol $\langle\ldots\,|\,\ldots\rangle$ stands for the usual Clebsch–Gordan coefficients [16]. The quantity defined by eq. (14) plays the role of the reduced Wigner coefficient (RWC) (3j symbol) for the O(5) ⊃ O(3) chain of groups, as discussed in ref. [6].

It should be noticed that for $\lambda = 0$, $\mu = 0$, $L = 0$ and $L' = L''$ the RWC of eq. (14) reduces precisely to the γ-overlap of two functions as given by eq. (8). This is the reason why we use for its definition the usual Clebsch–Gordan coefficients $\langle \dots | \dots \rangle$, instead of the usual 3j symbol as in ref. [6]. In this last case, an extra factor of $1/\sqrt{2L'+1}$ would have appeared.

It should also be noticed that the integral over beta (eq. (13)) scales with the harmonic oscillator constant κ as $\kappa^{-(2\rho+\lambda)/2}$.

There are selection rules for the integral (13) and the RWC (14). In particular, the selection rules for the reduced Wigner coefficient (14) are

$$|L - L''| \le L' \le L + L'' \tag{15}$$

for the angular momenta (resulting from the Clebsch–Gordan coefficients), and

$$\lambda + \lambda' + \lambda'' = \text{even}, \quad |\lambda - \lambda''| \le \lambda' \le \lambda + \lambda'' \tag{16}$$

for the seniorities [11].

For the matrix element over beta (eq. (13)) we consider the standard case of a power being an integer of the form $2\rho + \lambda$ with $\rho \ge 0$. Then, in the case with $\lambda + \lambda' + \lambda'' = \text{even}$, namely when the corresponding integral over gamma may be non-vanishing, the following selection rule applies [11]:

$$\left|2(n'_\beta - n''_\beta) + (\lambda' - \lambda'')\right| \le 2\rho + \lambda. \tag{17}$$

In many frequent physical applications [2,8,13], one expands the potential energy surface of a deformed nucleus or some IBA-type hamiltonian as a polynomial in powers of $\cos(3\gamma)$, instead of using the general operators $T^{\lambda\mu L}_M(\beta, \gamma, \theta_i)$. Although the powers of $\cos(3\gamma)$ can be expressed as a linear combination of $\tilde{\phi}_0^{3\mu,\mu,0}(\gamma)$'s - since in this case the ϕ's are proportional to the Legendre polynomials of degree μ, namely $P_\mu(\cos(3\gamma)) \sim \tilde{\phi}_0^{3\mu,\mu,0}(\gamma)$ - we prefer to present a separate procedure that directly evaluates the matrix elements of $\cos^m(3\gamma)$, namely

$$(\lambda', \mu', L|\cos^m(3\gamma)|\lambda'', \mu'', L) = \int_0^\pi \sum_{K\ge 0} \frac{2\phi_K^{\lambda'\mu'L}(\gamma)\phi_K^{\lambda''\mu''L}(\gamma)}{(1+\delta_{K0})} \times \cos^m(3\gamma)\sin(3\gamma)\,d\gamma, \tag{18}$$

as well as another procedure that evaluates directly the matrix elements of $\beta^{2\rho+3m}\cos^m(3\gamma)$.

2.3. Auxiliary steps

As produced by the program PHISYM, the wave functions $\phi_K^{\lambda\mu L}(\gamma)$ are trigonometric polynomials of $\sin(\gamma)$ and $\cos(\gamma)$, where the powers of $\cos(\gamma)$ are limited to one and zero. For the algebraic integration over the variable γ, it is then sufficient to expand the $\sin(3\gamma)$ and the additional $\cos(3\gamma)$'s and to implement the following three definite integrals [17]:

$$\int_0^\pi \sin^{2m}(\gamma)\,d\gamma = \frac{(2m-1)!!}{2^m m!}\pi, \tag{19}$$

$$\int_0^\pi \sin^{2m+1}(\gamma)\,d\gamma = \frac{2^{m+1}m!}{(2m+1)!!} \tag{20}$$

and

$$\int_0^\pi \sin^m(\gamma)\cos(\gamma)\,d\gamma = 0, \quad \text{for any integer } m. \tag{21}$$

With respect to the integral over β (eq. (13)), a fast and elegant algebraic technique can be used for the standard case when $\rho \ge 0$. In this case, with $x = \kappa\beta^2$, the following two recurrence relations [18,19] for the associated Laguerre polynomials can be utilized to equalize the left $\{n'_\beta, \lambda'\}$ and right $\{n''_\beta, \lambda''\}$ indices, namely

$$L_m^\alpha(x) = L_m^{\alpha+1}(x) - L_{m-1}^{\alpha+1}(x) \tag{22}$$

and

$$xL_m^\alpha(x) = (2m+\alpha+1)L_m^\alpha(x) - (m+\alpha)L_{m-1}^\alpha(x) - (m+1)L_{m+1}^\alpha(x). \tag{23}$$

Then, one implements the orthonormalization relation [19] for the associated Laguerre polynomials, namely

$$\int_0^\infty e^{-x}x^\alpha L_m^\alpha(x)L_n^\alpha(x) = \frac{(m+\alpha)!}{m!}\delta_{mn}. \tag{24}$$

3. Description of symbolic program

The procedures and operators included in the program PHIMANIP are summarized in table 1 and table 2, their names being listed in column 1. These procedures are divided into two categories, namely auxiliary (table 1) and main-purpose (table 2) procedures. Table 1 also lists three procedures already available in the program PHISYM, but which are indispensable for the running of the program PHIMANIP. These three procedures provide the initial wave functions $\phi_K^{\lambda\mu L}(\gamma)$ (PHI's), the conversion of trigonometric expressions of $\sin(3\gamma)$ and $\cos(3\gamma)$ into powers of $\sin(\gamma)$ and $\cos(\gamma)$ and the usual Clebsch–Gordan coefficients. Column 2 lists the arguments of each procedure, whereas column 3 offers a brief description of the corresponding function.

Notice that the functions $\phi_K^{\lambda\mu L}(\gamma)$ must be calculated initially with the procedure PHI (LAMBDA, MU, L, K), but subsequently they must be stored as a special subscribed operator APHI(LAMBDA, MU, L, K).

All procedures that are designed to evaluate matrix elements always return a value corresponding to properly normalized wave functions $\phi_K^{\lambda\mu L}(\gamma)$. These procedures are easily distinguishable since they have FLAG as a first argument. This argument can take two values, namely EXACT or BFLOAT. This allows the user to decide, at any stage, whether the procedure should perform the calculation in exact or in bigfloat arithmetic. The bigfloat option is advantageous in the common situation where the norms are very large numbers, since the REDUCE simplification of the corresponding square roots is very tedious in exact arithmetic. Special care has been taken so that the bigfloat option is activated only immediately before the calculation of these large square roots. In this way, the tracing over the intrinsic projections K is always done in exact arithmetic, a fact that guarantees high accuracy (see section 3.6).

The precision with which bigfloat calculations are performed can be entered or changed at any stage simply by typing "PRECISION v" after the prompt; the default value is 16, corresponding to REAL*8 in Fortran. When exiting, all procedures in the program PHIMANIP leave the REDUCE environment switched on in exact arithmetic.

The procedures that have FLAG as an argument are the following five: ME, MEG, MEB, MECOS, and MEGCOS.

From the point of view of their function, all the procedures and operators are grouped into three different trees (cf. fig. 1). However, each procedure and each operator can be called independently according to the user's needs.

On top of the usual REDUCE messages [9], a

Table 1
Auxiliary procedures and operators and previous procedures

	Arguments	Brief description
Auxiliary procedures:		
CHECKAPHI	(LAMBDA,MU,L)	Checks availability of APHI's
MKAPHI	(LAMBDA,MU,L)	Constructs wave functions APHI's for all permitted values of K
CLEARAPHI	(LAMBDA,MU,L)	Deletes wave functions APHI's
Previous procedures:		
PHI	(LAMBDA,MU,L,K)	Calculates wave functions PHI's
CONV	(exp)	Expands $\sin(3\gamma)$ and $\cos(3\gamma)$ in powers of $\cos(\gamma)$ and $\sin(\gamma)$
CG	(L1,L2,L3,M1,M2,M3)	Returns usual Clebsch–Gordan coefficients
Auxiliary operators:		
DEFINT	(exp)	Performs the definite integration of $\sin^m(\gamma)\cos^n(\gamma)$, $n = 0$ or 1, eqs. (19–21)
HU	(lagp(m, α))	Implements recurrence relation (22) for associated Laguerre polynomial, L_m^α
FX	(lagp(m, α))	Implements recurrence relation (23) for associated Laguerre polynomial, L_m^α

Table 2a
Main-purpose procedures

Main-purpose procedures	Arguments	Brief description
GS	(LAMBDA,L)	Performs the Gram-Schmidt orthonormalization of APHI's for given LAMBDA and L
NORMAPHI	(LAMBDA,MU,L)	Calculates the norm of APHI's
GAMMAOVERLAP	(LAMBDA1,MU1 LAMBDA2,MU2,L)	Returns the gamma overlap for two APHI's with the same L, eq. (8)
ME	(FLAG, N1,LAMBDA1,MU1,L1,M1, N2,LAMBDA2,MU2,L2,M2 N3,LAMBDA3,MU3,L3,M3)	Returns the complete matrix element of $\beta^{2\rho+\lambda}T_M^{\lambda\mu L}(\beta, \gamma, \theta_i)$ in eq. (12), N2 = ρ, ρ ≥ 0 $T_M^{\mu L} \Rightarrow 2$
MEG	(FLAG, LAMBDA1,MU1,L1,M1, LAMBDA2,MU2,L2,M2, LAMBDA3,MU3,L3,M3)	Returns the Euler-angles plus the gamma contribution to the matrix element of eq. (12) (RWC × Clebsch–Gordan × phase), $T_M^{\mu L} \Rightarrow 2$
RWC	(LAMBDA1,MU1,L1, LAMBDA2,MU2,L2, LAMBDA3,MU3,L3)	Returns the reduced Wigner coefficient for the chain O(5) ⊃ O(3), eq. (14), λ, μ, $L \Rightarrow 1$
TRIPLINT	(LAMBDA1,MU1,L1,K1, LAMBDA2,MU2,L2,K2, LAMBDA3,MU3,L3,K3)	Returns the integral of three given $\phi_K^{\lambda\mu L}(\gamma)$'s appearing in RWC
MEB	(FLAG, LAMBDA1,NBETA1, LAMBDA2,NBETA2,POWER)	Returns the integral over beta, eq. (13), κ = 1, POWER = 2ρ + λ, ρ ≥ 0
MECOS	(FLAG, N1,LAMBDA1,MU1,L1,M1, N2,LAMBDA2,MU2,L2,M2, RHO,POWERG)	Returns the matrix element of $\beta^{\text{POWERB}}[\cos(3\gamma)]^{\text{POWERG}}$ between two kets (cf. eq. (1)), POWERB = 2 × RHO + 3 × POWERG
MEGCOS	(FLAG, LAMBDA1,MU1,LAMBDA2, MU2,L,POWER)	Returns the matrix element of $[\cos(3\gamma)]^{\text{POWER}}$, eq. (18), POWER ≥ 0

number of informational and warning messages, as well as error messages, are built-in in the program PHIMANIP. To suppress the former messages, the user needs only to type "FLAGMSG: = MSGOFF" after the prompt. To reactivate them, it is enough to type "FLAGMSG: = MSGON". The error messages, however, are built with the REDUCE statement "REDERR" and cannot be suppressed.

Table 2b
Note:

FLAG ⇒	EXACT or BFLOAT
1 ⇒	left indices
2 ⇒	indices in the middle or right indices
3 ⇒	right indices

In the following, we will describe in detail the particulars for each procedure. In addition, although the extra messages in the present program are self-explanatory when appearing during the execution of a specific procedure, we present a full listing of them so that the user can easily distinguish between them and the usual REDUCE messages.

3.1. Auxiliary procedures

CHECKAPHI – This procedure, built-in in almost all the main procedures, returns an error message in the case when the required wave functions APHI are not available yet. If the APHI's have been calculated previously, it returns a warning message to that effect.

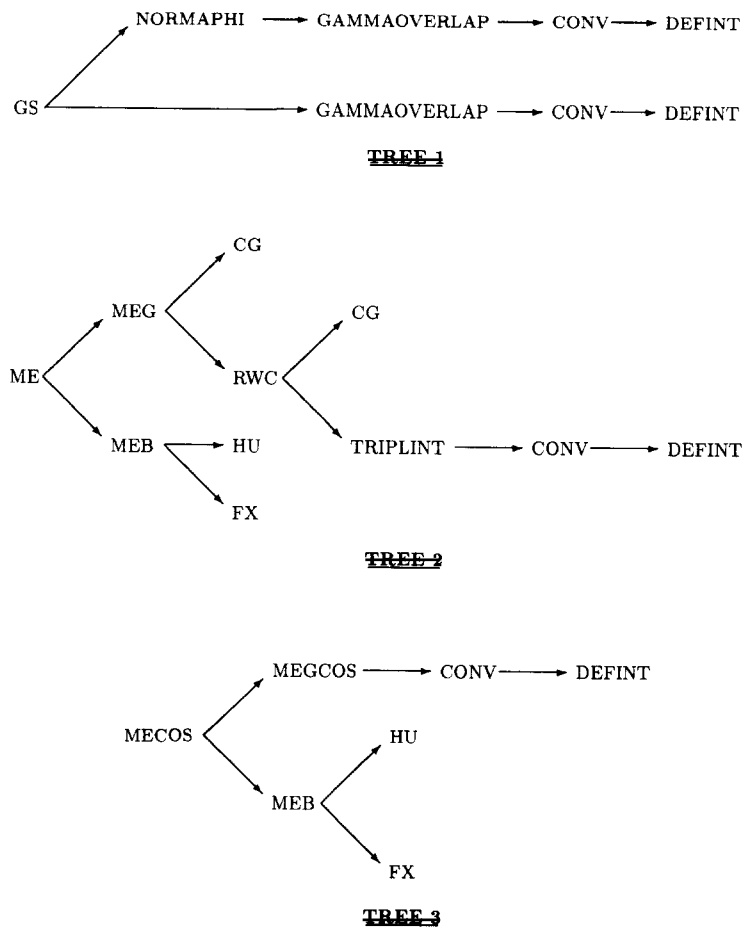

Fig. 1.

MKAPHI – By calling the procedure PHI of the program PHISYM, it creates the wave functions APHI for all permitted intrinsic projections K that correspond to given values of (LAMBDA, MU, L). If the APHI's are already available, MKAPHI does not call the procedure PHI again; instead, it simply displays the APHI's.

CLEARAPHI – It is used to delete existing APHI's, if the user so wishes.

3.2. Previous procedures

PHI – This is the top-level procedure from the program PHISYM. This procedure returns the initial wave functions $\phi_K^{\lambda\mu L}(\gamma)$ that are unnormalized and nonorthogonal in some indices μ. It is called by the procedure MKAPHI.

CONV – This procedure converts the trigonometric functions obtainable through this program (as well as through the program PHISYM) into a polynomial in powers of $\sin(\gamma)$ multiplied at most by a first power of $\cos(\gamma)$. This procedure is instrumental in the sense that it enables one to restrict the range of integration formulas in the operator DEFINT to the three cases given by eqs. (19)–(21).

CG – It calculates the standard Clebsch–Gordan coefficients of O(3).

3.3. Auxiliary operators

DEFINT – This operator performs definite integration of expressions which are linear combinations of integrals of trigonometric functions of

the form exhibited in eqs. (19)–(21). It is constructed as a linear operator. DEFINT is always applied to an integrand which has been converted previously through the application of the procedure CONV. A group of LET rules allows the mere substitution of the integrands in the l.h.s. of eqs. (19)–(21) by the integration result in the r.h.s.

HU – It implements recurrence relation (22) for the associated Laguerre polynomials. It is constructed as a linear operator which can be applied recursively. The substitutions involved are implemented by a LET rule. The associated Laguerre polynomial in its argument must be denoted as "lagp(m, α)".

FX – It implements recurrence relation (23) for the associated Laguerre polynomials. Like HU, it is constructed as a linear operator which can be applied recursively. The associated Laguerre polynomial in its argument must also be denoted as "lagp(m, α)".

3.4. Main procedures

GS – It performs the Gram–Schmidt orthonormalization according to subsection 2.1, eqs. (7), (8) and (3). If there are no μ-degeneracies, this procedure simply calls NORMAPHI, whereas in the opposite case eq. (7) is implemented using the procedures displayed in the Tree 1 of fig. 1. Prior to calling any other procedure, GS determines how many (if any) μ-degeneracies exist for the required values of the pair (LAMBDA, L), and informs the user about that effect. Upon exit, the contents of the operator APHI have been overwritten with the *orthogonalized* expressions while the corresponding norms have been stored in the operator NORM(LAMBDA, MU, L).

NORMAPHI – It calculates, with respect to the γ-variable, the norm of APHI's, eq. (3). This is achieved (see Tree 1) by calling GAMMAOVERLAP, which evaluates eq. (8) for $\lambda' = \lambda'' = \lambda$ and $\mu' = \mu'' = \mu$. Upon exit, the norm has been stored in the operator NORM(LAMBDA, MU, L).

GAMMAOVERLAP – It evaluates eq. (8). It calls CONV before applying operator DEFINT which performs the final definite integrations. It should be noted that there is only one value L for the angular momenta as an argument to this procedure. This is due to the fact that the γ-overlap of two ket states with different values of L is always zero (cf. the Glebsch-Gordan coefficient in eq. (12)). However, the selection rules for the seniorities (eq. (16)) are not built in this procedure. This allows for an additional check concerning the orthogonality with respect to different seniorities (cf. section 2.1).

ME – This procedure evaluates the complete matrix element between two kets in eq. (12). It is the top level procedure of the Tree 2 in fig. 1. It checks first the selection rules for gamma (cf. eqs. (15)–(16)). If successful, it proceeds to evaluate the β-part by calling MEB. If the β-result is nonzero, it calls CHECKAPHI to determine whether the necessary wave functions APHI are available and proceeds to evaluate the γ-part of the matrix element by calling MEG. As displayed in Tree 2, this procedure consists basically of the selection rules and the subsequent decisions on whether to call MEG and MEB.

MEG – Calculates the Euler-angles part plus γ-part in ME. It consists essentially of the reduced Wigner coefficient (RWC) of O(5) ⊃ O(3) multiplied by a usual Clebsch–Gordan coefficient and a phase (see eq. (12)). Here the intermediate result is divided by the square root of the product of the norms for APHI1 and APHI3, so that the matrix elements ME and MEG correspond to properly normalized states.

RWC – Evaluates the reduced Wigner coefficient of O(5) ⊃ O(3) given in eq. (14). Since this equation involves a linear combination of products of three wave functions APHI, only the different coefficients are determined in the present procedure, leaving the γ-integration of the three APHI's for the procedure TRIPLINT (see Tree 2). Unlike MEG, the division with the corresponding norms is not enforced here. If the user wishes to calculate the RWC for normalized APHI's, he must implement this division through an additional, but simple REDUCE statement.

TRIPLINT – For each term in the triple summation over the intrinsic projections K, K', K'' in eq. (14) for which the corresponding Clebsch–Gordan coefficient is nonzero, TRIPLINT performs the γ-integration of the product of three *unnormalized* wave functions APHI. This

step is done in a way quite analogous to GAMMAOVERLAP, namely procedure CONV is first used and then the operator DEFINT is called.

MEB – This procedure calculates the β-integral corresponding to eq. (13) for $\kappa = 1$ (see eq. (2)). The selection rule (17) is first verified. As pointed out in subsection 2.3, the integration over beta is accomplished by utilizing the recurrence relations (22) and (23) in order to transform the initial β-matrix element into a linear combination of orthonormalization integrals for the associated Laguerre polynomials (cf. eq. (24)). For most physical purposes, it is sufficient to restrict the power ρ in eq. (9) to be a non-negative integer. This is assumed throughout this paper. The method adopted for the integration over the β-variable fails when ρ is a negative integer. In this particular case, an error message will be displayed, stating that the present algebraic technique is unable to deal with such integrals.

MECOS – This procedure is the top level procedure in the Tree 3 of fig. 1. It returns the matrix element of $\beta^{\mathrm{POWERB}}\cos(3\gamma)^{\mathrm{POWERG}}$ between two kets specified by eq. (1), where POWERB = 2 × RHO + 3 × POWERG. It first checks the selection rules for gamma (see next procedure). If successful, it calls MEB in order to evaluate the β-part (see Tree 3); if the β-part is nonzero, it proceeds to call MEGCOS in order to evaluate the γ-part.

MEGCOS – This procedure has structure analogous to GAMMAOVERLAP, but with the additional feature of a $\cos(3\gamma)$ raised to a natural power "sandwiched" between the two wave functions APHI (cf. eq. (18)). The selection rules for these matrix elements are taken into account by considering all the possible degrees of the Legendre polynomials, appearing in the expansion of a given $\cos^m(3\gamma)$ (cf. Table 12.1 in ref. [19]). Since the Legendre polynomials correspond to wave functions PHI for momentum zero, only states with the same value of L will be coupled by $\cos^m(3\gamma)$; therefore, we keep with the practice of GAMMAOVERLAP and use only one value of L as an argument for this procedure. As with MEG the final result corresponds to properly normalized $\phi_K^{\lambda\mu L}(\gamma)$'s, since the division with the square root of the norms of APHI's is performed here.

3.5. Messages

3.5.1. Error messages

(***** aphi's(, , ,) not available
***** the other K's are probably missing);
***** the first argument must be BFLOAT or EXACT;
(***** the combination L = , , lambda = , ,
***** is not possible);
***** N is different from 2 * NBETA + LAMBDA or NBETA < 0;
***** present algebraic method is unapplicable;
***** (lambda1 + lambda2 + power) is an odd integer.

In addition to the above error messages that correspond to the program PHIMANIP, the following four error messages are built-in in the program PHISYM:

***** Case for L = 1 does no exist;
***** required projection K does not exist;
***** (lambda − 3 * mu) < L/2 .or. (lambda − 3 * mu) > L;
***** (lambda − 3 * mu) < (L + 3)/2 .or. (lambda − 3 * mu) > L.

3.5.2. Informational and warning messages

*** done;
*** aphi's (, ,) are available;
*** number of degenerate states:;
*** values of different possible mu's:;
*** no mu-degeneracy;
*** WARNING: aphi's should have been GS' ed;
*** WARNING: aphi1 and aphi3 should have been GS' ed.

The last two warnings indicate that procedure GS should have been called before calling the present procedure.

In addition to these messages, the results of ME and MECOS are displayed in a table form. Apart from the complete final result that is saved in the corresponding REDUCE workspace, this table displays the intermediate results of MEB (beta result) and MEG (gamma result). The suppression and reactivation of this table display depends on the value of FLAGMSG described earlier.

3.6. Accuracy of calculations

In floating-point arithmetic, a straightforward implementation of the Gram–Schmidt process is not advisable [14]. Indeed, extensive cancellations in the summation over positive and negative contributions appear as a rule in this case. The same problem, in floating-point arithmetic, also appears in the calculation of the gamma overlap of eq. (8) for two different set of indices λ and μ, since the trace over K is involved.

This, however, does not constitute a problem for the algebraic codes, since they use exact arithmetic. Indeed, as mentioned earlier, particular care has been taken in the writing of the program so that the implementation of the Gram–Schmidt method is always carried efficiently in exact arithmetic.

4. How to use the program: Examples

After calling the system REDUCE, one needs to input both the program PHISYM and the program PHIMANIP from previously prepared files. In the test run output, we will assume that these two files are named "phisym.red" and "phimanip.red", respectively.

The first three examples illustrate the use of the program in interactive mode, while the fourth example illustrates the use of the program in batch mode.

4.1. Example 1

This example shows the implementation of the Gram–Schmidt orthonormalization method (section 2.1). For angular momentum $L = 6$, there are two degenerate states when $\lambda = 9$ with $\mu = 1$ and $\mu = 2$. Indeed, before the orthonormalization, the gammaoverlap of these two states is different from zero. After the calling of procedure GS, the gammaoverlap is precisely zero. The full sequence of the corresponding input commands is given in the test run output.

4.2. Example 2

In this example, we present the evaluation of a particular case for the general matrix element of eq. (12). The T operator has been chosen to agree with $(-\cos(3\gamma))$. This corresponds to the potential-energy-surface term which generates the prolate-oblate asymmetry [8,13] in the geometrical model. The corresponding procedure is ME.

Since the operator T was restricted to agree with $(-\cos(3\gamma))$, the result of ME can also be reached through the procedure MECOS.

A complete description of the different steps and indices involved in this example is given in the test run output.

4.3. Example 3

The purpose of this example is to illustrate the autonomous functioning of each procedure in one of the trees of fig. 1. The partial beta and gamma results displayed in the tables of the previous example are reproduced by calling the procedures MEB, MEG, and MEGCOS.

The result of RWC agrees with that of MEG and MEGCOS when the division with the square roots of the corresponding norms is taken into account.

An examination of the test run output allows for a direct comparison between the indices in these procedures and in the procedures of the previous examples.

4.4. Example 4

This example shows how to use the programs PHISYM and PHIMANIP in batch mode. The warning messages have been suppressed and precision 16 has been chosen to calculate two different cases by calling procedure MEGCOS. The APHI's used have been orthonormalized first by calling procedure GS.

Notice that RES1 is accurate to 16 significant digits. RES2 is exact, however, in spite of the bigfloat option, since its vanishing is produced through the tracing over the index K before the bigfloat mode is activated when dividing with the square root of the norms.

5. Discussion and future perspectives

The exact arithmetic provided by REDUCE constitutes a powerful advantage in the manipulation of the states associated with the U(5) ⊃ O(5) ⊃ O(3) chain of groups. This is particularly relevant in the case of the Gram–Schmidt orthonormalization.

The related facility of using arbitrary floating-point arithmetic offers additional flexibility in handling the square roots, and thus speeding up the calculation, while preserving the desired relative accuracy.

To take full advantage of the possibilities inherent in the present programs, an elaborate scheme of input-output for intermediate results is advisable in order to bypass the internal-space limitations imposed by REDUCE. This scheme is currently under development. It is designed to enable the input of bigfloated intermediate results without loss of precision by using extensive text manipulation.

References

[1] C. Yannouleas and J.M. Pacheco, Comput. Phys. Commun. 52 (1988) 85.
[2] M. Moshinsky, Nucl. Phys. A338 (1980) 156.
[3] R.F. Casten and D.D. Warner, Rev. Mod. Phys. 60 (1988) 389.
[4] T.M. Corrigan, F.J. Margetan and S.A. Williams, Phys. Rev. C14 (1976) 2279.
[5] E. Chacón, M. Moshinsky and R.T. Sharp, J. Math. Phys. 17 (1976) 668.
[6] E. Chacón and M. Moshinsky, J. Math. Phys. 18 (1977) 870.
[7] A. Gheorghe, A.A. Raduta and V. Ceausescu, Nucl. Phys. A296 (1978) 228.
[8] M. Seiwert, J.A. Maruhn and P.O. Hess, Phys. Rev. C30 (1984) 1779.
[9] A.C. Hearn, REDUCE User's Manual, Version 3.3, (The Rand Corporation, Santa Monica, 1987).
[10] MACSYMA User's Guide (Symbolics, USA, 1988).
[11] P.O. Hess, M. Seiwert, J. Maruhn and W. Greiner, Z. Phys. A296 (1980) 147.
[12] G. Wenes, N. Yoshinaga and A.E.L. Dieperink, Nucl. Phys. A443 (1985) 472.
[13] J.M. Pacheco, C. Yannouleas and R.A. Broglia, Phys. Rev. Lett. 61 (1988) 294.
[14] J.H. Wilkinson, The Algebraic Eigenvalue Problem (Oxford Univ. Press, New York, 1965).
[15] A. Bohr, Kgl. Dan. Vid. Selk, Mat. Fys. Medd. 26 (1952) 14.
[16] A.R. Edmonds, Angular Momentum in Quantum Mechanics (Princeton Univ. Press, NJ, 1957).
[17] W. Gröbner and N. Hofreiter, Integraltafel II (Springer, Wien, 1975) nos. 331.23a, 331.27, 331.28.
[18] M. Abramowitz and I.A. Segun, Handbook of Mathematical Functions (Dover, New York, 1968) no. 22.7.30.
[19] G. Arfken, Mathematical Methods for Physicists (Academic Press, New York, 1970) exercise 13.2.7, eq. 13.48.

TEST RUN OUTPUT

```
REDUCE 3.3, 15-Jan-88 ...

1: in "phisym.red"$

2: in "phimanip.red"$

%  ****************  E x a m p l e  1  *************

3: mkaphi(9,1,6);

*** done

4: mkaphi(9,2,6);

*** done

5: gammaoverlap(9,1,9,2,6);

*** aphi's(9,1,6) are available

*** aphi's(9,2,6) are available

    4416
 - ------
    539

6: gs(9,6);

*** number of degenerate states: 2

*** values of different possible mu's:

1

2

*** aphi's(9,1,6) are available

*** aphi's(9,2,6) are available

*** done

7: gammaoverlap(9,1,9,2,6);

*** aphi's(9,1,6) are available

*** aphi's(9,2,6) are available

0

% ***************** End of example 1 *****************

%  ****************  E x a m p l e  2  *************

8: mkaphi(8,1,6);

*** done

9: mkaphi(3,1,0);

*** done

10: gs(8,6);

*** no mu-degeneracies

*** value of mu: 1

*** aphi's(8,1,6) are available

*** done

11: me(   exact, 13,9,1,6,6, 2,3,1,0,0, 10,8,1,6,6);

*** aphi's(9,1,6) are available

*** aphi's(3,1,0) are available

*** aphi's(8,1,6) are available

*** WARNING: aphi1 and aphi3 should have been GS' ed

-----------------------------------------------------

*** RESULTS FOR ME( 13,9,1,6,6,

                   2,3,1,0,0,

                   10,8,1,6,6)

diff. phi components for T(3,1,0,0):

                  2
COS(G)*(4*SIN(G)  - 1)

power  of  beta : 7

                        14985*SQRT(23)
beta     result :  - ----------------
                          4*SQRT(2)

                      63*SQRT(2057)
gamma    result : -----------------
                     187*SQRT(16399)

complete result :

    944055*SQRT(2057)
 - -------------------
     748*SQRT(1426)

-----------------------------------------------------

12: mecos(exact, 13,9,1,6,6,  10,8,1,6,6,  2,1);

*** aphi's(9,1,6) are available

*** aphi's(8,1,6) are available

*** WARNING: aphi's should have been GS' ed
```

```
*** RESULTS FOR MECOS( 13,9,1,6,6,

                      10,8,1,6,6,

                      2,1)

power  of  beta : 7

                     14985*SQRT(23)
beta     result :  - ---------------
                       4*SQRT(2)

                      63*SQRT(2057)
gamma    result :  - -----------------
                     187*SQRT(16399)

complete result :

 944055*SQRT(2057)
-------------------
  748*SQRT(1426)

% ********** End of example 2 **********

%  **********   E x a m p l e  3  **********

13: meb(exact, 9,2, 8,1, 7);

    14985*SQRT(23)
 - ---------------
      4*SQRT(2)

14: meg(exact, 9,1,6,6, 3,1,0,0, 8,1,6,6);

*** aphi's(9,1,6) are available

*** aphi's(3,1,0) are available

*** aphi's(8,1,6) are available

*** WARNING: aphi1 and aphi3 should have been GS' ed

  63*SQRT(2057)
-----------------
 187*SQRT(16399)

15: rwc(9,1,6,   3,1,0,   8,1,6  );

*** aphi's(9,1,6) are available

*** aphi's(3,1,0) are available

*** aphi's(8,1,6) are available

 97200
-------
  187

16: megcos(exact, 9,1,  8,1,   6,1);

*** aphi's(9,1,6) are available

*** aphi's(8,1,6) are available

*** WARNING: aphi's should have been GS' ed

     63*SQRT(2057)
 - -----------------
    187*SQRT(16399)

% ********** End of example 3 **********
```

```
% **********  E x a m p l e  4  *******

$r rsys:reduce
off int;
off echo;

flagmsg:=msgoff;

FLAGMSG := MSGOFF

in "phisym.red"$

in "phimanip.red"$

mkaphi(31,7,10)$
mkaphi(31,8,10)$
mkaphi(32,8,10)$
mkaphi(32,9,10)$

gs(31,10)$
gs(32,10)$

precision 16;

16

write res1:=megcos(bfloat,31,7,32,8,10,1)$

RES1 := 0.015 72734 97917 0488

write res2:=megcos(bfloat,31,7,32,9,10,1)$

RES2 := 0

% ********** End of e x a m p l e 4 ****
```