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AN ALGEBRAIC PROGRAM FOR THE STATES ASSOCIATED WITH THE U(5) ⊃ O(5) ⊃ O(3) CHAIN OF GROUPS

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A REDUCE program is presented that calculates algebraically the γ-dependent part of the states associated with the U(5) ⊃ O(5) ⊃ O(3) chain of groups, familiar from nuclear-structure problems. The method of solution is a direct implementation of the analytic expressions given by Chacón and Moshinsky.

PROGRAM SUMMARY

Title of program: PHISYM

Catalogue number: ABFN

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 language 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: 261

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, 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
Direct implementation of algebraic expressions in ref. [1].

Restrictions on the complexity of the problem
The available computer memory in combination with the automatic space allocations of REDUCE is the severest restriction in the present full arithmetic version. 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. (See the test run output for specific examples.)

Reference
[1] E. Chacón and M. Moshinsky, J. Math. Phys. 18 (1977) 870.

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* A more effective approach is the preparation of "bigfloat" versions. Work in this respect is in progress.

LONG WRITE-UP

1. Introduction

The concept of symmetries has found applications in various branches of physics. In particular, one of the recent important developments in nuclear physics has been the application of symmetry ideas and algebraic techniques to nuclear structure [1,2]. In this approach the Hamiltonian of the system is invariant under a certain class of transformations which form a group. Assuming such a Hamiltonian and such a group, the powerful and elegant techniques of group theory can be applied. These techniques, however, involve complicated algebraic manipulations. The degree of complication is such that in several physically important cases – like the case of the recently discovered octupole-deformed nuclei (see, part 1 in ref. [2]) – closed analytic results are still far from being produced in spite of the power of the group theoretical analysis. Invariably, one had to use numerical analysis to go beyond the limitations of human capability for algebraic manipulation.

Recently, however, a new advanced technique in computational physics was made available with the introduction of symbolic and algebraic computer codes like REDUCE [3] and MACSYMA [4]. Computer-assisted algebra is useful to fields where the scientist is confronted with a prohibitive degree of algebraic manipulations [5–7]. It can naturally be of great assistance to the field of the applications of group theory to nuclear physics.

The aim of the present paper is to motivate such a development by presenting a specific first example. In particular, we present a REDUCE program which calculates the states characterized by irreducible representations of the U(5) ⊃ O(5) ⊃ O(3) chain of groups. The particular physical significance of this chain and its applications will be discussed briefly in the rest of the introduction.

Much of the group theoretical work in nuclear physics has centered around the Interacting Boson Approximation (IBA) model [1] and its extensions [8]. In IBA, one assumes that the low-lying excitations can be described by a Hamiltonian built out of bosons with angular momentum 0 (s bosons) or 2 (d bosons). The usefulness of such a Hamiltonian is manifested when the corresponding group structure is invoked. A group decomposition shows that there are three distinct chains, namely U(5) ⊃ O(5) ⊃ O(3), a five-dimensional harmonic oscillator, SU(3) ⊃ O(3), an axial rotor, and O(6) ⊃ O(5) ⊃ O(3), a γ-unstable rotor. For each of these three limits, the characteristic wave functions are eigenstates of specific terms of the IBA Hamiltonian. While many examples of nuclei exist that correspond, at least partially, to the above three limits, most often this is not the case. In this case, one has to diagonalize the IBA Hamiltonian in a truncated space spanned by the states characterized by irreducible representations of one of the above chains, preferably the U(5) ⊃ O(5) ⊃ O(3), which corresponds to quadrupole vibrations. As an example of such a calculation we mention ref. [9] for the low-lying spectrum of ^{168}Er.

Group theoretical ideas are not restricted to the IBA model. Indeed, in practice many phenomenological calculations of nuclear spectroscopy have been carried out by the Frankfurt group, and it was soon realized [10,11] that the chain U(5) ⊃ O(5) ⊃ O(3) provided the link towards connecting the IBA with the geometrical collective model of the Frankfurt group. The geometric Hamiltonian of the Frankfurt group extends the Bohr vibrational Hamiltonian [12] to potential energy surfaces nonlinear in the quadrupole coordinates, thus being able to describe rotational and transitional nuclei as well. As with the case of the IBA, it was realized that the states associated with the chain U(5) ⊃ O(5) ⊃ O(3) form also the physically meaningful basis for the diagonalization [10,13] of the geometric Hamiltonian (for specific applications of this method to ^{238}U and ^{168}Er, see refs. [14,15]).

The usefulness of this chain is not restricted to low-energy static nuclear properties. Indeed, multi-step processes such as those encountered in Coulomb excitation and in medium-energy proton scattering and described with the IBA [16–18], or the photon absorption of the giant dipole resonance in deformed nuclei – described either in a geometric model [19,20] or in the IBA [20] –

require the use of the states associated with the U(5) ⊃ O(5) ⊃ O(3) chain as an ingredient in all calculations.

Given the importance of this chain, substantial effort within the framework of group theory has been devoted in providing an exact and algebraic determination of the states characterized by its irreducible representations. In fact, four rather lengthy papers [21,22,13,23] addressing this problem were published almost simultaneously and closed analytic results were presented. In spite of their closed analytic form, the γ-dependent part of these wave functions is very tedious to be algebraically manipulated by hand. Moreover, these states were not normalized and not orthogonal in some quantum numbers. The algebraic solution of the orthonormalization problem was addressed in several subsequent publications [24–26], but the results were mixed from the point of view of enhancing the efficiency of computational needs.

The present status is that, in spite of the algebraic nature and of the extent of a successful implementation of group theoretical methods to the problem, numerical computation [15,9,26] is utilized to construct in practice the states of the U(5) ⊃ O(5) ⊃ O(3) chain, a procedure that negates many of the advantages of the algebraic method. In particular, in the case of IBA, the standard computer code is PHINT [27] which is a FORTRAN program. In contrast to the numerical computation, our approach is to develop algebraic computer programs for the manipulation of the states of the U(5) ⊃ O(5) ⊃ O(3) chain. Among the many advantages, we mention the full-precision arithmetic particularly suitable for high-power trigonometric polynomials with alternating coefficients as in the present case, the efficient algebraic integration over the γ coordinate during the implementation of the Gram–Schmidt orthonormalization procedure and the easy tabulation of intermediate results for immediate use in subsequent steps.

Therefore, in a first step, we present here a REDUCE program which calculates the γ-dependent part of the states characterized by irreducible representations of the U(5) ⊃ O(5) ⊃ O(3) chain of groups. In a subsequent publication, we intend to present the algebraic codes for their orthonormalization. For the analytical expressions, we follow the work of Chacón and Moshinsky [13].

2. States associated with the U(5) ⊃ O(5) ⊃ O(3) chain of groups

As mentioned in the introduction, 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 by considering the full chain reduction displayed in table 1, leading to the four quantum numbers $\{N, \lambda, L, M\}$.

Specifically, N gives the number of phonons present in the corresponding state; λ is the seniority, and L and M are the quantum numbers for the total angular momentum and its projection in the laboratory frame, respectively. On top of these four quantum numbers, a fifth one, related to the number of phonon triplets coupled to momentum zero and denoted here by μ, is needed to yield a fully defined and complete set of states.

It turns out that a convenient way of spanning the five-dimensional coordinate space for the harmonic oscillator is to consider the three Euler angles θ_i, $i = 1, 2, 3$ and the two intrinsic β and γ shape variables [12,13]. The corresponding eigenstates are written as

$$|N\lambda\mu LM\rangle = F_N^{\lambda}(\beta) \sum_{K\geq 0} \phi_K^{\lambda\mu L}(\gamma)\left[D^{L*}_{M,K} + (-)^L D^{L*}_{M,-K}\right] /(1+\delta_{K0}), \quad (1)$$

where $F_N^{\lambda}(\beta)$ is expressed through appropriate Laguerre polynomials [13] and $D^{L*}_{M,K}$ are the usual rotation matrices [28]. Notice that $N = 2n + \lambda$, where n is an integer.

In the present work, we are interested in the γ-dependent part of eq. (1). This part is denoted by $\phi_K^{\lambda\mu L}(\gamma)$. Due to symmetry considerations,

Table 1

Group	U(5) ⊃ O(5) ⊃ O(3) ⊃ O(2)			
Quantum number	N	λ	L	M

$\phi_K^{\lambda\mu L}(\gamma)$ is nonzero for even values of the projection K as follows:

$$\begin{aligned} &K = 0, 2, \ldots, L \quad \text{for } L = \text{even}, \\ &K = 2, \ldots, L-1 \quad \text{for } L = \text{odd}. \end{aligned} \tag{2}$$

The analytic expressions for the $\phi_K^{\lambda\mu L}(\gamma)$ are summarized in tables 2 and 3. Two cases, one for even angular momentum and another for odd angular momentum are distinguished. In the odd case, one introduces an auxiliary even momentum and utilizes corresponding expressions from table 2. In table 2, notice that the lower index in $S_K^{2r}(\gamma)$ is restricted to even values, and that $\langle \cdots | \cdots \rangle$ is the usual Clebsch–Gordan coefficient. With respect to ref. [13], the redundant factor $\pi^{-5/4}2^{(\lambda+\mu+\tau)/2}$ in $F_n^{\sigma\tau\mu}(\cos 3\gamma)$ and the $(1/\sqrt{3})$ in $g_k^{(3)}(\gamma)$ have been omitted here.

The wave functions $\phi_K^{\lambda\mu L}(\gamma)$ form a complete but nonorthonormal set. Symbolic programs for their orthonormalization, as well as for evaluating the matrix elements of potential terms of the form $\cos^m(3\gamma)$ will be presented in a future publication.

3. Description of symbolic program

At the top level, the calculation of the wave functions $\phi_K^{\lambda\mu L}(\gamma)$ follows the flow chart in fig. 1,

Table 2
Angular momentum L = even

$$\phi_K^{\lambda\mu L}(\gamma) = \sum_n G_K^{nL}(\gamma) F_n^{\sigma\tau\mu}(\cos 3\gamma); \quad \sigma + \tau = L/2,\ \sigma + 2\tau + 3\mu = \lambda,\ \sigma, \tau, \mu \geq 0,$$

$$G_K^{nL}(\gamma) = (-\sqrt{2})^n \sum_{K'K''} \langle L-2n, 2n, K', K'' \mid LK \rangle S_{K'}^{L-2n}(\gamma) S_{K''}^{2n}(-2\gamma);$$

$$S_K^{2r}(\gamma) = \left[\frac{(2r+K)!(2r-K)!}{(4r)!}\right]^{1/2} \sum_{q=K/2}^{[r/2+K/4]} \binom{r}{2q-K/2} \binom{2q-K/2}{q} (\sqrt{6})^r \left(\frac{1}{2\sqrt{3}}\right)^{2q-K/2} (\cos\gamma)^{r+K/2-2q} (\sin\gamma)^{2q-K/2};$$

$$F_n^{\sigma\tau\mu}(\cos 3\gamma) = (-1)^{\mu+\tau-n} 2^{-n/2} \sum_{r=0}^{[(\mu+\tau-n)/2]} C_{rn}^{\sigma\tau\mu} 2^{-r} (\cos 3\gamma)^{\mu+\tau-n-2r};$$

$$C_{rn}^{\sigma\tau\mu} = \frac{3^n \sigma!\lambda!(-)^r 2^r (2\mu+2\tau-2r)!(3r)!}{2^{\mu+n} n!(2\lambda+1)!r!(\mu+\tau-r)!(\mu+\tau-n-2r)!} \sum_{s=\max(n-\tau,0)}^{\min(\sigma,\lambda,3r-\tau+n)} \frac{(-)^s 4^s (\tau+s)!(2\lambda+1-2s)!}{s!(\sigma-s)!(\tau-n+s)!(3r-\tau+n-s)!(\lambda-s)!};$$

$$0 \leq n \leq \frac{L}{2}; \quad \frac{L}{2} \leq \lambda - 3\mu \leq L$$

Table 3
Angular momentum $\bar{L}$ = odd

$$\phi_K^{\lambda\mu\bar{L}}(\gamma) = \sum_n G_K^{n\bar{L}}(\gamma) \bar{F}_n^{\sigma\tau\mu}(\cos 3\gamma); \quad L = \bar{L} - 3,\ \lambda = \bar{\lambda} - 3,\ (L = \text{even});$$

$$G_K^{n\bar{L}}(\gamma) = \sum_{Kk} \langle L3Kk \mid \bar{L}\bar{K} \rangle G_K^{nL}(\gamma) g_k^{(3)}(\gamma); \quad g_k^{(3)}(\gamma) = \sin 3\gamma(\delta_{k2} - \delta_{k,-2});$$

$$\bar{F}_n^{\sigma\tau\mu}(\cos 3\gamma) = (-1)^{\mu+\tau-n} 2^{-n/2} \sum_{r=0}^{[(\mu+\tau-n)/2]} \bar{C}_{rn}^{\sigma\tau\mu} 2^{-r} (\cos 3\gamma)^{\mu+\tau-n-2r};$$

$$\bar{C}_{rn}^{\sigma\tau\mu} = \frac{3^n \sigma!(\lambda+3)!(-)^r 2^r (2\mu+2\tau+1-2r)!(3r)!}{2^{\mu+n} n!(2\lambda+7)!r!(\mu+\tau-r)!(\mu+\tau-n-2r)!} \sum_{s=\max(n-\tau,0)}^{\min(\sigma,\lambda+3,3r-\tau+n)} \frac{(-)^s 4^s (\tau+s)!(2\lambda+7-2s)!}{s!(\sigma-s)!(\tau-n+s)!(3r-\tau+n-s)!(\lambda+3-s)!};$$

$$0 \leq n \leq \frac{L}{2}; \quad \frac{\bar{L}+3}{2} \leq \bar{\lambda} - 3\mu \leq \bar{L}$$

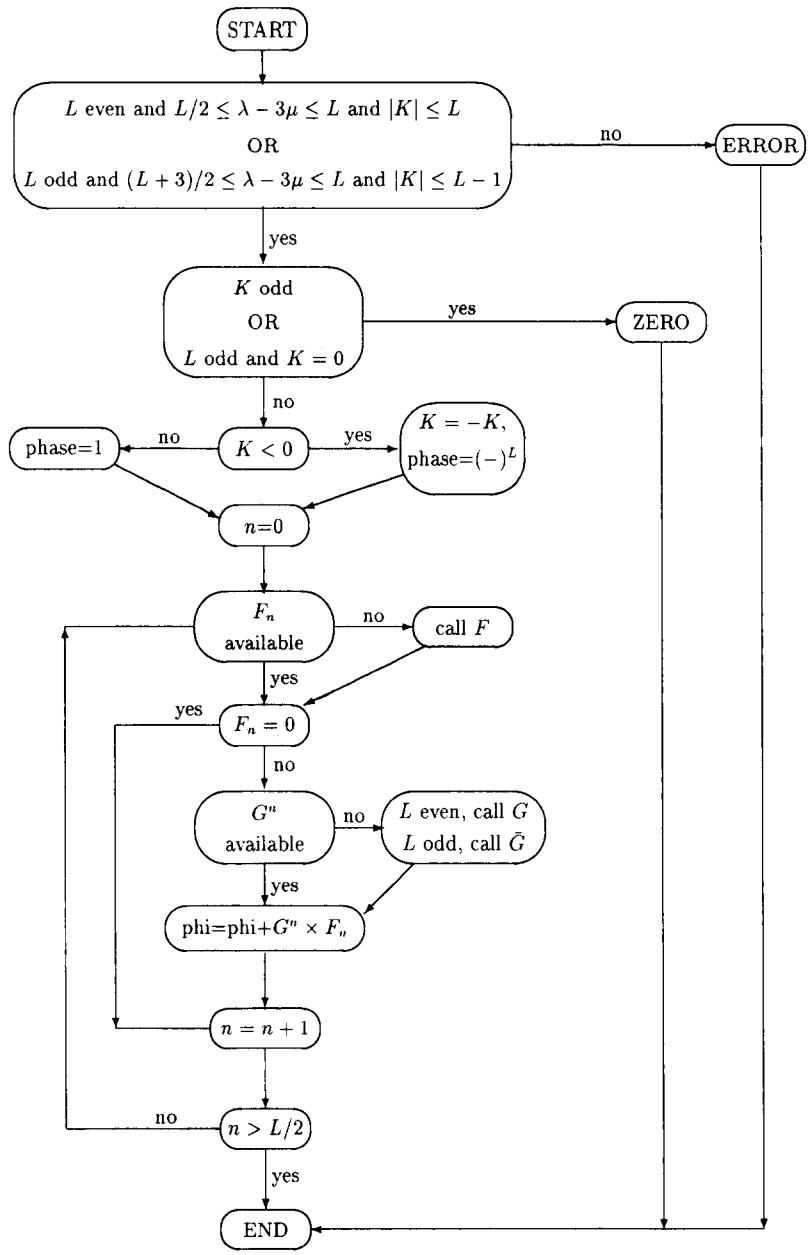

Fig. 1.

where $G(\bar{G})$ and $F(\bar{F})$ are the functions tabulated in tables 2 and 3. At a second level, the functions $G(\bar{G})$, $F(\bar{F})$ are calculated with the help of S, $C(\bar{C})$ and DLT (delta function). The wave function $\phi_K^{\lambda\mu L}(\gamma)$ is represented by PHI(lam, mu, L, K). The expressions for F and $\bar{F}$ were modified in such a way that they can be calculated with the same procedure (named F). The same is true for the coefficients C and $\bar{C}$.

Because of the structure of these functions, it is likely that they will be required more than once during the same REDUCE session. Therefore, their

repeated evaluation can be avoided by storing them in the operators AS, AG and AF, respectively; this results in an additional saving of time while computing different functions $\phi_K^{\lambda\mu L}(\gamma)$.

The evaluation of the different functions requires two auxiliary quantities: a table of factorials, which is stored in array FAC and Clebsch–Gordan coefficients which are computed using procedure CG. Finally, the functional dependence of the functions $\phi_K^{\lambda\mu L}(\gamma)$ in terms of γ is controlled using the auxiliary procedure CONV. In the present case, CONV sets the dependence of $\phi_K^{\lambda\mu L}(\gamma)$ exclusively in terms of powers of $\sin(\gamma)$ and $\cos(\gamma)$. This form will be particularly useful for symbolic integrations involving these functions. Since in this REDUCE program full precision is kept throughout the calculation, the value returned for a given $\phi_K^{\lambda\mu L}(\gamma)$ corresponds to its actual analytic form. Moreover, the powerfulness of the symbolic manipulation can be verified, e.g., in the case of the calculation of the functions G; indeed, once the analytical expressions for S are known, the SUBSTITUTION command makes it trivial to compute the functions G. Notice that the G's are expressed as linear combinations of products of the form $S(\gamma)S(-2\gamma)$ (cf. table 2).

4. How to run the program, examples

After calling REDUCE, the program PHISYM must be input from a previously prepared file using the command IN. Afterwards, all that is necessary to do is to type,

```
phi(lambda, mu, L, K);
```

substituting lambda, mu, L and K by the desired integer values.

Example 1. Producing all nonzero projections K for a given L

We give all the intrinsic projections K for momentum $L=4$ with $\lambda=10$ and $\mu=2$. The corresponding REDUCE statement is:

```
for i := 0 step 2 until 4
  do write a(i) := phi(10, 2, 4, i);
```

The results are exhibited in the test run output.

Example 2. Case of even angular momentum L

In ref. [9] the IBA was used to calculate the low-lying spectrum of ^{168}Er. This case corresponds to a space of 16 bosons. The calculation was extended up to angular momentum eight. We produce here the three $\phi_0^{\lambda\mu 8}(\gamma)$ with highest seniorities that contribute to the basis of ref. [9]. The REDUCE statements are given in the test run output, together with the corresponding analytic results. The chosen values for λ and μ correspond to the most complicated cases. The rest of the contributions to the basis can be easily computed by using analogous statements.

Example 3. Case of odd angular momentum L

Ref. [15] calculated the low-lying spectrum of ^{168}Er using the geometrical collective model. Up to thirty phonons were used to construct the truncated basis. Among the $\phi_4^{\lambda\mu 5}(\gamma)$ in this basis, we produce here the two contributions with highest seniorities. The REDUCE statements are given in the test run output.

Acknowledgement

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TEST RUN OUTPUT

```
2: on time;

%                          *** EXAMPLE 1 ***


5: operator a;

6: for i:=0 step 2 until 4 do write a(i):=phi(10,2,4,i);

                                  10              8             6
A(0) :=  - (90*(1680*SIN(G)   - 4120*SIN(G)  + 3585*SIN(G)  - 1320*

                        4            2
     SIN(G)  + 185*SIN(G)  - 6))/SQRT(70)

                                                 8             6
A(2) :=  - (45*SQRT(105)*SIN(G)*COS(G)*(672*SIN(G)  - 1376*SIN(G)  +

                        4            2
     930*SIN(G)  - 231*SIN(G)  + 16))/(7*SQRT(5))

                    2            8             6             4
A(4) := (45*SIN(G) *(672*SIN(G)  - 1648*SIN(G)  + 1386*SIN(G)  - 456*

                2
     SIN(G)  + 47))/2

Time: 14230 ms


%                       *** EXAMPLE 2 ***

7:phi(15,3,8,0);

                                       14              12
(31185*SQRT(78)*COS(G)*(345216*SIN(G)   - 1172064*SIN(G)   + 1571544*

          10             8             6             4
    SIN(G)   - 1054010*SIN(G)  + 368450*SIN(G)  - 63183*SIN(G)  +

               2
    4392*SIN(G)  - 72))/(46748*SQRT(165))

Time: 17670 ms

8:phi(16,3,8,0);

                                    16              14
(315*SQRT(78)*(19227648*SIN(G)   - 75203904*SIN(G)   + 120208560*

                12              10             8
     SIN(G)   - 101142828*SIN(G)   + 48027305*SIN(G)  -

                6             4             2
     12771994*SIN(G)  + 1757407*SIN(G)  - 102480*SIN(G)  +

     1464))/(572*SQRT(165))

Time: 8410 ms

9:phi(16,4,8,0);

                                    16              14
(35*SQRT(78)*(7594752*SIN(G)   - 78018816*SIN(G)   + 213073440*

                12              10             8
     SIN(G)   - 260926992*SIN(G)   + 163475795*SIN(G)  -

                6             4             2
     52956256*SIN(G)  + 8256928*SIN(G)  - 510720*SIN(G)  +

     7296))/(12341472*SQRT(165))

Time: 9270 ms

%                          *** EXAMPLE 3 ***

10:phi(28,8,5,4);

                          2                26                24
 - (495*SQRT(42)*SIN(G) *(1100742656*SIN(G)   - 7661748224*SIN(G)   +

                              22              20
       23796318208*SIN(G)   - 43497439232*SIN(G)   + 51969116160*

             18              16              14
       SIN(G)   - 42621236736*SIN(G)   + 24520274688*SIN(G)   -

                          12              10              8
       9936357184*SIN(G)   + 2806490492*SIN(G)   - 538283525*SIN(G)

                          6             4             2
       + 66909728*SIN(G)  - 4975312*SIN(G)  + 190976*SIN(G)  - 2688))

/(4864*SQRT(35))

Time: 12560 ms

11:phi(29,8,5,4);

                          2                26
 - (1485*SQRT(42)*SIN(G) *COS(G)*(1100742656*SIN(G)   - 7430012928*

             24              22              20
       SIN(G)   + 22347972608*SIN(G)   - 39500005376*SIN(G)   +

                          18              16
       45556353024*SIN(G)   - 35998569984*SIN(G)   + 19913177856*

             14              12              10
       SIN(G)   - 7741221696*SIN(G)   + 2092331644*SIN(G)   -

                          8             6             4
       382985525*SIN(G)  + 45298188*SIN(G)  - 3194744*SIN(G)  +

                       2
       115904*SIN(G)  - 1536))/(128*SQRT(35))

Time: 8010 ms
```