Symbolic-Numeric Algorithm for Calculations in Geometric Collective Model of Atomic Nuclei

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Abstract. We developed a symbolic–numeric algorithm involving a set of effective symbolic and numerical procedures for calculations of low lying energy spectra and eigenfunctions of atomic nuclei. The eigenfunctions are expanded over the orthonormal noncanonical $U(5)\supset O(5)\supset O(3)$ basis in Geometric Collective Model. We give implementation of the algorithm and procedures in Wolfram Mathematica. We present benchmark calculations of energy spectrum, quadrupole moment and the reduced upwards transition probability $B(E2)$ for the nucleus ^{186}Os.

Keywords: Orthonormal non-canonical basis · Groups $U(5)\supset SO(5)\supset SO(3)$ · Irreducible representations · Gram-Schmidt orthonormalization · Geometric Collective Model · Spectral characteristic · Atomic nuclei

1 Introduction

The Bohr–Mottelson (B-M) collective model [2,3] has gained widespread acceptance in calculations of vibrational-rotational quadrupole spectra and electromagnetic transitions in atomic nuclei [4,8,17]. Among others it was applied for such nuclei as: uranium [14], Pt, Os and W isotopes [15]. Some results were also obtained for the super-heavy deformed nuclei [12] where a fit of microscopically derived potential energy surfaces proposed in [9,21–23] has been performed with the help of numerical (FORTRAN) application of the geometric collective model (GCM) [13,20].

Key problems in such numerical large-scale calculations of spectral characteristics of the GCM with the octahedral O_h point symmetry as well as the

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general Bohr Hamiltonian [18,19] are round-off errors appearing in calculation of high-power polynomials. These polynomials with alternating coefficients and strong numerical cancellations are observed in the Gram–Schmidt orthonormalization of the nonorthogonal set of basis eigenfunctions that we investigated in [7] using both integer and floating point arithmetics implemented in Wolfram Mathematica [25].

In the present paper, we propose some development of effective symbolic procedures for calculations of the spectral characteristic of atomic nuclei in GCM. We give the implementation of the developed procedures in Wolfram Mathematica and performance of benchmark calculations. We analyze round-off errors in calculation of high-power polynomials with alternating coefficients. We show that strong cancellation in Gram–Schmidt orthonormalization usually pose serious problems in numerical calculations [7,14,15,20,26,27].

The structure of the paper is following. In Sect. 2, we describe the statement of the problem separated into subsections corresponding to procedures (subroutines) involving the GCM code. We give the benchmark examples of their execution summing up them in the Tables that show computer memory and execution time with respect to ranges of the quantum numbers involved in the runs: construction of GCM Hamiltonian, construction of orthonormal $U(5)\supset O(5)\supset O(3)$ basis, calculation of β- and γ-dependent matrix elements, and composition of Hamiltonian matrices of algebraic eigenvalue problem. In Sect. 3, benchmark calculations of energy spectrum, quadrupole moment and the reduced upwards transition probability $B(E2)$ for ^{186}Os are presented. Finally, in Sect. 4, the summary of main results and conclusions are given. In Appendices A and B, the sets of input parameters for atomic nuclei and boundary value problem for GCM model are presented.

The CPU times of the benchmark calculations give required estimates for choosing appropriate versions of the presented symbolic-numeric algorithms and programs. The computations were performed with Wolfram Mathematica 10.1 on PC Intel i7-36030QM, CPU 2.40 GHz, RAM 8 GB, 64-bit Windows 8.

2 The Statement of the Problem and Subroutines

Hamiltonian. The classical nuclear collective Hamiltonian constructed in the so called laboratory frame has the general form [20]

$$\hat{H} = \hat{T}(\pi, \alpha) + \hat{V}(\alpha). \tag{1}$$

Quantum description of the collective motions in GCM is performed by using the quadrupole deformation coordinates, $\hat{\alpha}^{[2]} = \alpha_{2m}, m = -2, -1, 0, 1, 2$, and the corresponding conjugate momenta, $\hat{\pi}^{[2]} = \pi_{2m}, m = -2, -1, 0, 1, 2$, subjected to commutation relations $[\hat{\pi}^{[2]}_m, \hat{\alpha}^{[2]}_{m'}] = -\imath\hbar\delta_{mm'}$. The kinetic energy is constructed to contain the two lowest-order terms proportional to the square of the momenta determined in a nonstandard form accepted in [20]:

$$\hat{T} = \frac{1}{B_2}[\hat{\pi} \times \hat{\pi}]^{[0]} + \frac{P_3}{3}\left\{\left[[\hat{\pi} \times \hat{\alpha}]^{[2]} \times \hat{\pi}\right]^{[0]}\right\}, \tag{2}$$

where $\{\ldots\}$ means the sum over all permutations, and B_2 and P_3 are kinetic-energy parameters. For such nonstandard definition of the parameter B_2 with respect to standard one (see Eq. (2)), it will be multiplied by factor $2/\sqrt{5}$. So, in the practice of GCM calculations, the rescaled parameter $\bar{B}_2 = 2B_2/\sqrt{5}$ is really used. The tensor product of spherical tensors $A^{[l_1]}$ and $B^{[l_2]}$ is defined as

$$[A^{[l_1]} \otimes B^{[l_2]}]^{[l]} = \sum_{m_1,m_2} (l_1 m_1 l_2 m_2 | lm) A^{[l_1]}_{m_1} B^{[l_2]}_{m_2},$$

where $(l_1 m_1 l_2 m_2 | lm)$ are SO(3) Clebsch–Gordan coefficients [24]. All terms in the Hamiltonian are coupled to angular momentum 0, i.e., to rotational scalars.

Potential Energy. For the potential energy we use a polynomial expansion up to the sixth order in the deformation variables β and γ specified by the intrinsic deformation coordinates $\hat{a}^{[2]} = a_{2m'}$. The intrinsic frame is defined as coinciding to principal axes of the nucleus. It is determined by a set of three Euler angles $\Omega \in S^3(\Omega)$ and new deformation variable $\alpha_{2m} = \sum_{m'} D^{2*}_{mm'}(\Omega) a_{2m'}$, where $D^{2*}_{mm'}(\Omega)$ denotes the Wigner functions of irreducible representations of SO(3) group [24] (marker * denotes the complex conjugate operation). The choice of principal axes requires the following constraints: $a_{2-2} = a_{22}$, $a_{2-1} = a_{21} = 0$. The β and γ variables are defined as: $a_{20} = \beta\cos\gamma$, $a_{22} = (1/\sqrt{2})\beta\sin\gamma$. The potential energy is assumed in the following form:

$$\hat{V}(\beta,\gamma) = \sum_{\rho=2}^{6} \sum_{m=0}^{2} \beta^\rho \cos^m(3\gamma) \hat{V}_{\rho,m}, \tag{3}$$

where potential parameters $\hat{V}_{\rho,m}$ read as:

$$\begin{aligned} &\hat{V}_{2,0} = C_2 \tfrac{1}{\sqrt{5}};\ \ \hat{V}_{3,1} = -C_3\sqrt{\tfrac{2}{35}};\ \ \hat{V}_{4,0} = C_4 \tfrac{1}{5};\\ &\hat{V}_{5,1} = -C_5\sqrt{\tfrac{2}{175}};\ \ \hat{V}_{6,2} = C_6 \tfrac{2}{35};\ \ \hat{V}_{6,0} = D_6 \tfrac{1}{5\sqrt{5}}. \end{aligned} \tag{4}$$

Introducing these parameters the potential $\hat{V}(\beta,\gamma)$ takes the form

$$\begin{aligned} &\hat{V}(\beta,\gamma) = C_2 \tfrac{1}{\sqrt{5}}\beta^2 - C_3\sqrt{\tfrac{2}{35}}\beta^3\cos(3\gamma) + C_4\tfrac{1}{5}\beta^4\\ &-C_5\sqrt{\tfrac{2}{175}}\beta^5\cos(3\gamma) + C_6\tfrac{2}{35}\beta^6\cos^2(3\gamma) + D_6\tfrac{1}{5\sqrt{5}}\beta^6. \end{aligned} \tag{5}$$

For practical reason, we rescale $\hat{V}_{\rho,m}$ to $V_{\rho,m}$ in oscillator units of length with respect to the β variable using basis parameters of mass B'_2 and stiffness C'_2:

$$V(\beta,\gamma) = \sum_{\rho=2}^{6} \sum_{m=0}^{2} \beta^\rho \cos^m(3\gamma) V_{\rho,m},\ \ V_{\rho,m} = \hat{V}_{\rho,m} \times \left(\frac{\hbar}{\sqrt{B'_2 C'_2}}\right)^{\rho/2}. \tag{6}$$

Basis States and a Range of the Set of Quantum Numbers. We choose as basic functions the eigenfunctions of the five-dimensional harmonic oscillator

$$\hat{H}_5 = \frac{\sqrt{5}}{2B'_2}[\hat{\pi}\times\hat{\pi}]^{[0]} + \frac{\sqrt{5}C'_2}{2}[\hat{\alpha}\times\hat{\alpha}]^{[0]}. \tag{7}$$

Table 1. The degeneracy $d_{\lambda L} = \mu_{\max} - \mu_{\min} + 1$ for a number of L and λ. The first row of the table is formed by the values of λ and the first column of the table is formed by the values of the angular momentum L. The next columns in non empty square contains the degeneracy $d_{\lambda L}$ depending on accessible values of momentum L and seniority λ.

L, λ	5	10	15	20	25	30	35	40	45	50
0			1			1			1	
2	1	1		1	1		1	1		1
5	1	1		1	1		1	1		1
10	1	2	2	2	2	2	2	2	2	2
15		1	3	2	2	3	2	2	3	2
20		1	2	4	4	3	4	4	3	4
25			1	3	4	4	4	4	4	4
30			1	2	4	6	5	5	6	5
35				1	3	4	6	6	5	6

Table 2. The example of calculations of the total number of states defined by quantum numbers $\nu\lambda$ for a number of L up to the specified value of the $\nu_{\max}$. The first row of the table is formed by the values of $\nu_{\max}$ and the first column of the table is formed by the value of the angular momentum L. The next columns contains the total number of states for corresponding values of L and $\nu_{\max}$.

$L, \nu_{\max}$	5	10	15	20	25	30	35	40	45	50
0	5	14	27	44	65	91	120	154	192	234
2	7	22	45	77	117	165	222	287	360	442
5	2	12	30	57	92	135	187	247	315	392
10	1	12	36	72	121	182	256	342	441	552
15	0	2	16	42	81	132	196	272	361	462
20	0	1	12	36	72	121	182	256	342	441
25	0	0	2	16	42	81	132	196	272	361
30	0	0	1	12	36	72	121	182	256	342
35	0	0	0	2	16	42	81	132	196	272

The basis states can be characterized by irreducible representations of the $U(5) \supset O(5) \supset O(3) \supset O(2)$ chain of groups [7]:

- ν is the number of phonons,
- λ is the number of phonons that are not coupled pairwise to zero (seniority),
- L and M are the numbers of the angular momentum and its projection,
- μ is the additional quantum number, denoting the maximal number of phonon triplets coupled to the angular momentum $L = 0$ and counting degenerated states for $L \geq 6$:

$$\nu = 0, 1, 2, \ldots, \nu_{\max},\ \lambda = \nu, \nu{-}2, \ldots, 1 \text{ or } 0,\ \mu = \mu_{\min}, \mu_{\min}{+}1, \ldots, \mu_{\max}. \tag{8}$$

Here $\nu_{\max}$ is some chosen as the maximum number of phonons. The range of μ (i.e., $\mu_{\min}$ and $\mu_{\max}$) for given λ and L is determined by inequalities:

$$L/2 \le \lambda - 3\mu \le L,\ L = \text{even},\quad (L+3)/2 \le \lambda - 3\mu \le L,\ L = \text{odd}. \tag{9}$$

The solution of inequalities Eqs. (9) gives a range of accessible values of μ at given accessible λ and L:

$$\mu_{\min} = \max\left(0, \texttt{Ceiling}\left(\tfrac{\lambda-L}{3}\right)\right),\ \mu_{\max} = \texttt{Floor}\left(\frac{\lambda-(L+3(L \bmod 2))/2}{3}\right), \tag{10}$$

where $\texttt{Ceiling}(\mu)$ is the lowest integer but not lower than μ and $\texttt{Floor}(\mu)$ is the largest integer not greater than μ.

2.1 The Representation of the Wave Functions in Coordinate Space

The five-dimensional equation of the B-M collective model (7) in the intrinsic frame $\beta \in R^1_+$ and $\gamma, \Omega \in S^4$ with respect to $\Psi^{int}_{\nu\lambda\mu LM} \in L_2(R^1_+ \bigotimes S^4)$ with the measure $d\tau = \beta^4 \sin(3\gamma) d\beta d\gamma d\Omega$ reads as

$$\{H^{(BM)} - E^{BM}_\nu\}\Psi^{int}_{\nu\lambda\mu LM} = 0,\ H^{(BM)} = \frac{\hbar^2}{2B'_2}\left(-\frac{1}{\beta^4}\frac{\partial}{\partial\beta}\beta^4\frac{\partial}{\partial\beta} + \frac{\hat{\Lambda}^2}{\beta^2}\right) + \frac{C'_2}{2}\beta^2. \tag{11}$$

Here $E^{BM}_\nu \equiv E^L_\nu = \hbar\omega'_2(\nu + \frac{5}{2})$ are the eigenvalues of the five-dimensional harmonic oscillator, $\omega'_2 = \sqrt{C'_2/B'_2}$ is the oscillation frequency, $\hbar$ is Planck constant, $\hat{\Lambda}^2$ is the quadratic Casimir operator of O(5) in $L_2(S^4(\gamma, \Omega))$ at nonnegative integers $\nu = 2n_\beta + \lambda$, i.e., at even and nonnegative integers $\nu - \lambda$ determined as

$$(\hat{\Lambda}^2 - \lambda(\lambda+3))\Psi^{int}_{\nu\lambda\mu LM} = 0,\ \hat{\Lambda}^2 = -\frac{1}{\sin(3\gamma)}\frac{\partial}{\partial\gamma}\sin(3\gamma)\frac{\partial}{\partial\gamma} + \sum_{k=1}^{3}\frac{(\hat{\bar{L}}_k)^2}{4\sin^2(\gamma - \frac{2}{3}k\pi)}, \tag{12}$$

where the nonnegative integer λ is the seniority (8) and $(\hat{\bar{L}}_k)^2$ are the angular momentum operators of $\overline{\mathrm{O}(3)}$ along the principal axes in intrinsic frame, i.e., with commutator $[\hat{\bar{L}}_i, \hat{\bar{L}}_j] = -\imath\varepsilon_{ijk}\hat{\bar{L}}_k$ [7].

Eigenfunctions $|\nu\lambda\mu LM\rangle$ of the five-dimensional oscillator (7) in the intrinsic frame (11) have the form

$$\Psi^{int}_{\nu\lambda\mu LM}(\beta, \gamma, \Omega) = \langle\beta\gamma\Omega|\nu\lambda\mu LM\rangle = \sum_{K(even)} \Phi^{int}_{\nu\lambda\mu LK}(\beta, \gamma)\mathcal{D}^{(L)*}_{MK}(\Omega), \tag{13}$$

where $\mathcal{D}^{(L)*}_{MK}(\Omega)$ are the orthonormal Wigner functions with measure $d\Omega$,

$$\mathcal{D}^{(L)*}_{MK}(\Omega) = \sqrt{\frac{2L+1}{8\pi^2}}\frac{D^{(L)*}_{MK}(\Omega) + (-1)^L D^{(L)*}_{M,-K}(\Omega)}{1+\delta_{K0}}; \tag{14}$$

summation over K runs even values K in range:

$$\begin{aligned} K &= 0, 2, \ldots, L \qquad \text{for even integer } L : 0 \le L \le L_{\max}, \\ K &= 2, \ldots, L-1 \qquad \text{for odd integer } L : 3 \le L \le L_{\max}. \end{aligned} \tag{15}$$

$\Phi^{int}_{\nu\lambda\mu LK}(\beta,\gamma)$ are the nonorthogonal components with overlap $\langle\hat{\phi}^{\lambda\mu' L}(\gamma)|\hat{\phi}^{\lambda\mu L}(\gamma)\rangle$

$$\Phi^{int}_{\nu\lambda\mu LK}(\beta,\gamma) = C^{\lambda\mu}_{L} F_{\nu\lambda}(\beta)\hat{\phi}^{\lambda\mu L}_{K}(\gamma), \tag{16}$$

determined by (17), (18) and normalization factor $C^{\lambda\mu}_{L} = (\langle\hat{\phi}^{\lambda\mu L}(\gamma)|\hat{\phi}^{\lambda\mu L}(\gamma)\rangle)^{-1/2}$.

2.2 γ-Dependent Part of the Basis States

The components $\hat{\phi}^{\lambda\mu L}_{K}(\gamma) = (-1)^{L}\hat{\phi}^{\lambda\mu L}_{-K}(\gamma)$ for even K and $\hat{\phi}^{\lambda\mu L}_{K}(\gamma) = 0$ for odd L and $K = 0$ as well as for odd K are determined below according to papers [5,6,17,26]. It should be noted that for these components, $L \neq 1$, $|K| \le L$ for $L =$ even and $|K| \le L-1$ for $L =$ odd:

$$\hat{\phi}^{\lambda\mu L}_{K}(\gamma) = \sum_{n=0}^{n_{\max}} F^{\sigma\tau\mu}_{n\lambda L}(\gamma)\left[G^{nL}_{|K|}(\gamma)\delta_{L,\text{even}} + \bar{G}^{nL}_{|K|}(\gamma)\delta_{L,\text{odd}}\right]; \tag{17}$$

$$K = K_{\min}, K_{\min}+2, \ldots, K_{\max}; \qquad K_{\min} = \begin{cases} 0, & L = \text{even}, \\ 2, & L = \text{odd}; \end{cases} \qquad K_{\max} = \begin{cases} L, & L = \text{even}, \\ L-1, & L = \text{odd}; \end{cases}$$

$$n_{\max} = \begin{cases} L/2, & L = \text{even}, \\ (L-3)/2, & L = \text{odd}; \end{cases} \qquad \delta_{L,\text{even}} = \begin{cases} 1, & L = \text{even}, \\ 0, & L = \text{odd}; \end{cases} \qquad \delta_{L,\text{odd}} = \begin{cases} 0, & L = \text{even}, \\ 1, & L = \text{odd}; \end{cases}$$

where $L/2 \le \lambda - 3\mu \le L$ for $L =$ even, and $(L+3)/2 \le \lambda - 3\mu \le L$ for $L =$ odd;

2.3 Wave Function for γ Degree of Freedom $\hat{\phi}^{\lambda\mu L}_{K}(\gamma)$

Components $\bar{G}^{nL}_{K}(\gamma)$, $G^{nL}_{K}(\gamma)$ and $F^{\sigma\tau\mu}_{n\lambda L}(\gamma)$ in Eq. (17) are calculated by

$$\bar{G}^{nL}_{K}(\gamma) = \sum_{k=3-L,2}^{L-3} \langle L-3, 3, k, K-k|LK\rangle G^{nL-3}_{|k|}(\gamma)\sin 3\gamma(\delta_{K-k,2} - \delta_{K-k,-2});$$

$$G^{nL}_{K}(\gamma) = (-\sqrt{2})^{n} \sum_{k=2n-L,2}^{L-2n} \langle L-2n, 2n, k, K-k|LK\rangle S^{(L-2n)/2}_{|k|}(\gamma) S^{n}_{|K-k|}(-2\gamma);$$

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

$$\times \frac{1}{(r-2q+K/2)!(q-K/2)!q!} (\cos\gamma)^{r+K/2-2q} (\sin\gamma)^{2q-K/2};$$

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

$$C^{\sigma\tau\mu}_{rn\lambda L} = \frac{3^{n}\sigma!\lambda!(-1)^{r}2^{r}(2\mu+2\tau-2r+\delta_{L,\text{odd}})!(3r)!}{2^{\mu+n}n!(2\lambda+1)!r!(\mu+\tau-r)!(\mu+\tau-n-2r)!}$$

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

where $S^{r}_{K}(\gamma)$ is taken to be equal 0, if $\sin\gamma = 0$ or $\cos\gamma = 0$, $F^{\sigma\tau\mu}_{n\lambda L}(\gamma)$ is taken to be equal 0, if $\cos 3\gamma = 0$, $C^{\sigma\tau\mu}_{rn\lambda L}$ is taken to be equal 0, if $\mu+\tau-n-2r < 0$. It has been implemented in Ref. [7].

2.4 Gram–Schmidt Orthogonalization of the Functions $\hat{\phi}_K^{\lambda\mu L}(\gamma)$

Using implementation [7] of orthogonalization of the functions $\hat{\phi}_K^{\lambda\mu L}(\gamma)$ with the Gram–Schmidt method the reduced overlap (a scalar product with integration over γ) is required

$$\langle\hat{\phi}^{\lambda\mu' L}(\gamma)|\hat{\phi}^{\lambda\mu L}(\gamma)\rangle = \int_0^\pi d\gamma \sin(3\gamma) \sum_{K=K_{\min},2}^{K_{\max}} \frac{2\hat{\phi}_K^{\lambda\mu' L}(\gamma)\hat{\phi}_K^{\lambda\mu L}(\gamma)}{1+\delta_{K,0}}. \tag{18}$$

It should be noted that the definition of the reduced overlap integral (18) will be the same for original $\hat{\phi}^{\lambda\mu L}(\gamma)$ as well as for orthogonalized functions $\phi_K^{\lambda\mu L}(\gamma)$.

The degeneracy labelled by μ for the nuclear calculations is small in relevant cases as presented in Table 1, therefore, the original Gram–Schmidt method may be adopted to orthogonalize the functions $\hat{\phi}_K^{\lambda\mu L}(\gamma)$. For large μ, the modified Gram–Schmidt methods will be applied [7].

Application of the Gram–Schmidt method gives the orthogonalized functions

$$\phi_K^{\lambda\mu L}(\gamma) = \hat{\phi}_K^{\lambda\mu L}(\gamma) - \sum_{\mu'=\mu_{\min}}^{\mu-1} \phi_K^{\lambda\mu' L}(\gamma) \frac{\langle\phi^{\lambda\mu' L}(\gamma)|\hat{\phi}^{\lambda\mu L}(\gamma)\rangle}{\langle\phi^{\lambda\mu' L}(\gamma)|\phi^{\lambda\mu' L}(\gamma)\rangle}. \tag{19}$$

This procedure should be applied for all available indexes μ in boundaries given in Eq. (10) and indexes K in boundaries given in Eq. (17).

As produced by the procedure outlined in Eq. (19), the wave functions $\phi_K^{\lambda\mu L}(\gamma)$ are trigonometric polynomials of $\sin(\gamma)$ and $\cos(\gamma)$. For the algebraic integration over the variable γ, it is then sufficient to expand the $\sin(3\gamma)$ and the additional $\cos(3\gamma)$ and to implement the following three definite integrals:

$$\int_0^\pi \sin^{2m}(\gamma)d\gamma = \frac{(2m-1)!!}{2^m m!}\pi, \quad \int_0^\pi \sin^{2m+1}(\gamma)d\gamma = \frac{2^{m+1}m!}{(2m+1)!!}, \quad \int_0^\pi \sin^m(\gamma)\cos(\gamma)d\gamma = 0,$$

for any integer m. For example, the normalization integral for $L = 0$, $\lambda = 27$ and $\mu = 9$ is equal to $\frac{2}{57}$ and shows less than 0.001 sec. computation time on Mathematica. At the same time, direct symbolic integration of this normalization integral takes 436.781 s.

2.5 The Normalized Components $F_{n_\beta}^{\lambda}(\beta)$

The normalized components $F_{n_\beta}^{\lambda}(\beta)$ with the number of nodes $n_\beta = (\nu - \lambda)/2$, adapted for calculations of rescaled matrix elements $V(\beta, \gamma)$ from (6), read as

$$F_{n_\beta}^{\lambda}(\beta) = \sqrt{\frac{2n_\beta!}{\Gamma\left(n_\beta + \lambda + \frac{5}{2}\right)}}\beta^\lambda \exp\left(-\frac{1}{2}\beta^2\right) L_{n_\beta}^{\lambda+\frac{3}{2}}(\beta^2), \tag{20}$$

where $L_{n_\beta}^{\lambda+\frac{3}{2}}(\beta^2)$ is the associated Laguerre polynomial [1].

Table 3. The example of calculations of the matrix elements (27) for a number of L and fixed $\nu_{\max} = 30$. The columns of the table are formed by the value of the angular momentum L, the total number of states $\{\nu\lambda\mu\}$ defined by quantum numbers $\nu\lambda\mu$, the total number of states $\{\lambda\mu\}$ defined by quantum numbers $\lambda\mu$, the total number #MeT of matrix elements (27) in upper triangles of their matrices with $m = 1, 2$, the number #MeN of nonzero matrix elements among #MeT that are given by Eq. (28), the cumulative number #MeZ of angular matrix elements that are calculated equal to 0 among #MeN matrix elements, the maximum memory in MB used to store intermediate data for the current Mathematica session in computation of the overlap integrals, and the CPU time.

L	$\{\nu\lambda\mu\}$	$\{\lambda\mu\}$	#MeT	#MeN	#MeZ	memory	CPU time
0	91	11	132	30	0	0 MB	0.17 s
6	271	37	1406	266	15	3.48 MB	4.09 s
10	326	49	2450	495	80	4.18 MB	28.33 s
15	259	47	2256	534	109	4.45 MB	45.47 s
20	305	62	3906	1010	322	6.26 MB	2.60 min
25	193	50	2550	788	227	6.06 MB	3.08 min
30	174	51	2652	853	138	7.75 MB	5.07 min

In Table 2, we present an example of calculations of the number of functions (20) for a number of L up to the specified value of the $\nu_{\max}$ under condition (9). The presented results show the general tendency: with larger ν, the number of states increases and the calculations involve larger L. If we require larger L the number ν has to be sufficiently large.

2.6 Hamiltonian Matrix Elements and Algebraic Eigenvalue Problem

For the calculation of the matrix elements of the kinetic energy T the gradient formula [11] is applied taking into account the rescaled parameter $\bar{B}_2 = 2B_2/\sqrt{5}$:

$$T^{L}{}_{\nu'\lambda'\mu',\nu\lambda\mu} = (-1)^{\frac{|\nu'-\nu|}{2}} \frac{1}{2}\hbar\sqrt{B_2' C_2'}\,\frac{1}{\bar{B}_2}\langle\nu'\lambda'|\beta^2|\nu\lambda\rangle\delta_{\lambda',\lambda}\delta_{\mu',\mu} \tag{21}$$

$$-\sqrt{\frac{2}{35}}\hbar^{\frac{3}{2}}(B_2' C_2')^{\frac{1}{4}}\frac{P_3}{3}\langle\nu'\lambda'|\beta^3|\nu\lambda\rangle\langle\lambda'\mu' L|\cos(3\gamma)|\lambda\mu L\rangle\left(\delta_{|\nu'-\nu|,1} - 3\delta_{|\nu'-\nu|,3}\right).$$

The potential energy matrix elements V read as

$$V^{L}{}_{\nu'\lambda'\mu',\nu\lambda\mu} = \sum_{\rho=2}^{6}\sum_{m=0}^{2} V_{\rho,m}\langle\nu'\lambda'|\beta^{\rho}|\nu\lambda\rangle\langle\lambda'\mu' L|\cos^{m}(3\gamma)|\lambda\mu L\rangle. \tag{22}$$

Matrix elements of the quantum Hamiltonian (1) read as

$$H^{L}{}_{\nu'\lambda'\mu',\nu\lambda\mu} = T^{L}{}_{\nu'\lambda'\mu',\nu\lambda\mu} + V^{L}{}_{\nu'\lambda'\mu',\nu\lambda\mu}. \tag{23}$$

The eigenvalues E_n^L and the eigenfunctions Ψ_n^L of the quantum Hamiltonian $H = T + V$ (1) are calculated by solving the Schrödinger equation

$$(H - E_n^L)\Psi_n^L = 0. \tag{24}$$

We seek eigenfunctions Ψ_n^L of Hamiltonian (1) in the form of expansion over the basis functions $\Psi_{\nu\lambda\mu}^{int}(\beta, \gamma, \Omega)$ (13)

$$\Psi_n^L(\beta, \gamma, \Omega) = \sum_{\nu\lambda\mu} \Psi_{\nu\lambda\mu}^{int}(\beta, \gamma, \Omega) D_{\nu\lambda\mu,n}(L). \tag{25}$$

Eigenenergies E_n^L are calculated as an algebraic eigenvalue problem

$$\sum_{\nu\lambda\mu} ({H^L}_{\nu'\lambda'\mu',\nu\lambda\mu} - \delta_{\nu'\nu}\delta_{\lambda'\lambda}\delta_{\mu'\mu}E_n^L) D_{\nu\lambda\mu,n}(L) = 0. \tag{26}$$

Here $D_{\nu\lambda\mu,n}(L)$ is the eigenvector of Hamiltonian (23) for the n'th state with the angular momentum L. In Eq. (26), indices ν, λ and μ enumerate the total basis. The total number of different collections of (ν, λ and μ) for given L, and up to given $\nu_{\max}$ is the total dimension of the basis. These values are presented in Tables 3, 4, and 7. In Table 7, Dim is this total number of different (ν, λ and μ) for listed L and up to given $\nu_{\max} = 30$, i.e., the dimension of the Hamiltonian matrix.

2.7 Matrix Elements $\langle \lambda'\mu'L| \cos^m(3\gamma) |\lambda\mu L\rangle$

For computation of potential energy matrix elements the matrix elements of powers $m = 0, 1, 2$ of $\cos(3\gamma)$ should be evaluated, that are defined as

$$\langle \lambda'\mu'L| \cos^m(3\gamma) |\lambda\mu L\rangle = \frac{1}{\sqrt{\langle \phi^{\lambda'\mu'L}(\gamma)|\phi^{\lambda'\mu'L}(\gamma)\rangle \langle \phi^{\lambda\mu L}(\gamma)|\phi^{\lambda\mu L}(\gamma)\rangle}}$$
$$\times \int_0^\pi d\gamma \sin(3\gamma) \cos^m(3\gamma) \sum_{K=K_{\min},2}^{K_{\max}} \frac{2\phi_K^{\lambda'\mu'L}(\gamma)\phi_K^{\lambda\mu L}(\gamma)}{1 + \delta_{K,0}}. \tag{27}$$

Here summation boundaries are the same as in Eq. (18). Obviously this integral is equal to $\delta_{\lambda\mu,\lambda'\mu'}$ when $m = 0$. It should be pointed out that only small part of these integrals are not equal to 0. There are useful simple conditions that allow identify the large part of these integrals that are equal to zero. The appropriate selection rules are

$$\begin{aligned} &\lambda + \lambda' + (m \bmod 2) = \text{ odd}, \\ &|\lambda - \lambda'| \le 3n \text{ and } 3n \le \lambda + \lambda', \text{ where } n = m, m-2, \ldots, 1 \text{ or } 0. \end{aligned} \tag{28}$$

Using conditions (28) saves a lot of computation resources and makes it possible to avoid calculation of most of integrals (27) that actually are equal to 0. Nevertheless, these conditions are not precise and some of matrix elements that pass their test may appear to be equal to 0 after their computation. An example

Table 4. The example of calculations of the matrix elements (27) for a number of $\nu_{\max}$ and fixed $L = 18$. The first column of the table is formed by value of the $\nu_{\max}$, other columns are denoted as in Table 3.

$\nu_{\max}$	$\{\nu\lambda\mu\}$	$\{\lambda\mu\}$	#MeT	#MeN	#MeZ	memory	CPU time
10	2	2	6	3	0	0 MB	0.17 s
15	23	12	156	73	2	3.51 MB	5.80 s
20	81	28	812	312	52	3.93 MB	29.14 s
25	181	45	2070	632	170	4.92 MB	1.12 min
30	323	62	3906	953	294	5.97 MB	1.94 min
35	506	78	6162	1253	405	7.08 MB	2.86 min
40	731	95	9120	1577	530	8.50 MB	4.08 min
45	998	112	12656	1898	654	10.02 MB	5.68 min
50	1306	128	16512	2198	765	11.62 MB	7.65 min

of calculations of the matrix elements (27) is presented in Tables 3 and 4. Each evaluation is performed after quitting the Mathematica kernel. $\{\nu\lambda\mu\}$ is the total number of states defined for given $\nu_{\max}$ by quantum numbers in Eq. (8) under conditions in Eqs. (9) and (10); $\{\lambda\mu\}$ is the total number of states defined only by indices λ and μ, and this number is equal to the total number of different pairs of λ and μ among the states $\{\nu\lambda\mu\}$; #MeT – the cumulative number of angular matrix elements in the upper triangles of matrices for $\cos^m(3\gamma)$ with $m = 1, 2$ on states $\{\lambda\mu\}$, here the number of matrix elements with $m = 0$ are not included, since they all are equal to 1 by definition; #MeN is the number of nonzero matrix elements among #MeT that are given by Eq. (28); #MeZ is the cumulative number of angular matrix elements that are evaluated by equal to 0 by direct computation.

2.8 Matrix Elements $\langle \nu'\lambda'|\beta^\rho|\nu\lambda\rangle$

For the first case $|\lambda - \lambda'| \le \rho$, matrix elements $\langle \nu'\lambda'|\beta^\rho|\nu\lambda\rangle$ read as:

$$\int_0^\infty F^{\lambda'}_{n'_\beta}(\beta)\beta^\rho F^{\lambda}_{n_\beta}(\beta)\beta^4 d\beta = \left[\frac{n'_\beta! n_\beta!}{\Gamma(n'_\beta + \lambda' + \frac{5}{2})\Gamma(n_\beta + \lambda + \frac{5}{2})}\right]^{\frac{1}{2}} \tag{29}$$
$$\times(-1)^{n'_\beta + n_\beta}\Gamma\Big(\frac{1}{2}(\rho + \lambda' - \lambda + 2)\Big)\Gamma\Big(\frac{1}{2}(\rho + \lambda - \lambda' + 2)\Big)$$
$$\times\sum_\sigma \frac{\Gamma\left(\frac{1}{2}(\rho + \lambda' + \lambda + 5) + \sigma\right)}{\sigma!(n'_\beta - \sigma)!(n_\beta - \sigma)!\Gamma\left(\sigma + \frac{1}{2}(\rho + \lambda' - \lambda) - n_\beta + 1\right)} \frac{1}{\Gamma\left(\sigma + \frac{1}{2}(\rho + \lambda - \lambda') - n'_\beta + 1\right)}$$

the summation bounds for $\rho + \lambda' - \lambda$ even are:

$$\max\left(n'_\beta - (\rho + \lambda - \lambda')/2, n_\beta - (\rho + \lambda' - \lambda)/2, 0\right) \le \sigma \le \min(n'_\beta, n_\beta),$$

the summation bounds for $\rho + \lambda' - \lambda$ odd are:

$$0 \le \sigma \le \min(n'_\beta, n_\beta).$$

Table 5. An example of calculations of the matrix elements over β given by Eqs. (29) and (30) for a number of $\nu_{\max}$ when $\rho = 1, \ldots, 6$. The columns of the table are formed by the value of $\nu_{\max}$, the total number of states $\{\nu\lambda\}$ is defined by the quantum numbers $\nu\lambda$ up to the specified value of $\nu_{\max}$, the total number $\#\mathrm{Me}(\beta)$ of different matrix elements over β, the maximum memory in MB used to store intermediate data for the current Mathematica session in computation of the matrix elements, and the CPU time.

$\nu_{\max}$	$\{\nu\lambda\}$	$\#\mathrm{Me}(\beta)$	memory	CPU time
10	36	495	0 MB	0.30 s
20	121	2690	3.27 MB	1.78 s
40	441	12630	5.70 MB	9.06 s
60	961	29970	5.54 MB	24.26 s
80	1681	54710	5.69 MB	49.47 s
100	2601	86850	5.74 MB	1.44 min

For the second case $|\lambda - \lambda'| > \rho$ and the pair of quantities n'_β, λ' and n_β, λ are interchanged when $\lambda > \lambda'$:

$$\int_0^\infty F^{\lambda'}_{n'_\beta}(\beta)\beta^\rho F^{\lambda}_{n_\beta}(\beta)\beta^4 d\beta = \left[\frac{n'_\beta! n_\beta!}{\Gamma(n'_\beta + \lambda' + \frac{5}{2})\Gamma(n_\beta + \lambda + \frac{5}{2})}\right]^{\frac{1}{2}} \tag{30}$$
$$\times(-1)^{n_\beta}\frac{\Gamma\left(\frac{1}{2}(\rho+\lambda'-\lambda+2)\right)}{\Gamma\left(\frac{1}{2}(-\rho+\lambda'-\lambda)\right)}\sum_\sigma(-1)^\sigma\frac{\Gamma\left(\frac{1}{2}(\rho+\lambda'+\lambda+5)+\sigma\right)\Gamma\left(\frac{1}{2}(\lambda'-\lambda-\rho)+n'_\beta-\sigma\right)}{\sigma!(n'_\beta-\sigma)!(n_\beta-\sigma)!\Gamma\left(\sigma+\frac{1}{2}(\rho+\lambda'-\lambda)-n_\beta+1\right)}$$

the summation bounds for $\rho+\lambda'-\lambda$ even are: $\max\left(n_\beta-(\rho+\lambda'-\lambda)/2, 0\right) \le \sigma \le \min(n'_\beta, n_\beta)$, the summation bounds for $\rho+\lambda'-\lambda$ odd are: $0 \le \sigma \le \min(n'_\beta, n_\beta)$.

There are selection rules for the matrix elements over the variable β. The matrix elements are equal to zero when

$$\begin{aligned} &|\nu' - \nu| > \rho, \quad \rho \text{ and } |\nu' - \nu| \text{ have unequal parities,} \\ &|\lambda' - \lambda| > \rho, \quad |\nu' - \nu| \text{ and } |\lambda' - \lambda| \text{ have unequal parities,} \\ &\rho = 4 \text{ and } |\lambda' - \lambda| \neq 0, \quad \rho = 5 \text{ and } |\lambda' - \lambda| = 5. \end{aligned} \tag{31}$$

The formulas of the matrix elements over β Eqs. (29) and (30) are very effective comparing with direct symbolic integration approach. For example, symbolic integration of the matrix element with $n'_\beta = 126, \lambda' = 121, n_\beta = 125, \lambda = 120$, and $\rho = 120$ takes 23.80 s, when Mathematica timing for a computation with Eqs. (29) and (30) returns zero.

In Table 5, we present an example of memory consumption and CPU time of calculations of the matrix elements over β for a number of ν and fixed range of ρ. This interval $\rho = 1, \ldots, 6$ represents all powers of ρ in the expression of the potential energy for the approach adopted in this paper. It should be stressed that the presented procedure is very effective and could be applied for large scale calculations since the quantum numbers managed significantly outperform the ones considered for very large values, e.g., $\lambda \sim 100$ and $\mu \sim 10$.

In Table 6, we present the illustration how the accuracy of calculations depends on the number of significant digits used in computations. The presented results

Table 6. An example of calculations of relative accuracy of the matrix elements over β given by Eq. (30) for a number of ρ when $\nu = 100, \lambda = 70, \nu' = 60, \lambda' = 5$. The first row specifies the number of significant digits used in the corresponding computation. The n.a. indicates that the calculations could not be performed with specified number of significant digits.

ρ, precision	25	26	27	28	32	36	40
1	$2.4 \cdot 10^{-1}$	$1.8 \cdot 10^{-2}$	$3.0 \cdot 10^{-3}$	$3.4 \cdot 10^{-5}$	$3.7 \cdot 10^{-8}$	$1.5 \cdot 10^{-12}$	$2.1 \cdot 10^{-16}$
3	n.a.	$4.8 \cdot 10^{-2}$	$2.4 \cdot 10^{-5}$	$2.4 \cdot 10^{-5}$	$1.3 \cdot 10^{-7}$	$1.9 \cdot 10^{-11}$	$1.7 \cdot 10^{-15}$
5	n.a.	$2.1 \cdot 10^{-3}$	$2.1 \cdot 10^{-3}$	$1.2 \cdot 10^{-3}$	$1.1 \cdot 10^{-7}$	$1.3 \cdot 11^{-10}$	$1.2 \cdot 10^{-16}$
7	n.a.	n.a.	$1.3 \cdot 10^{-1}$	$1.2 \cdot 10^{-3}$	$1.9 \cdot 10^{-7}$	$1.4 \cdot 10^{-10}$	$4.8 \cdot 10^{-15}$
8	n.a.	n.a.	n.a.	$4.5 \cdot 10^{-2}$	$2.4 \cdot 10^{-6}$	$1.4 \cdot 10^{-10}$	$2.2 \cdot 10^{-14}$

gives the background for assertion that large scale calculations of this kind may be performed only symbolically.

3 Benchmark Calculations of GCM for ^{186}Os Nucleus

3.1 The Example of Calculations of Eigenenergies $E_n^{L^\pi}$ (in MeV)

The eigenstates L_n^π are characterized by the angular momentum L, parity $\pi = \pm = (\pm 1)$ [4] and sequence number n for fixed angular momentum starting at the lowest state. The calculated eigenvalues $E_n^{L^\pi}$ of rotational bands of ^{186}Os nucleus are the same as may be produced by the FORTRAN program [20]. In these calculations, the following values of parameters were used: $C_2 = -564.76, C_3 = 733.01, C_4 = 13546., C_5 = -8535.1, C_6 = -41635., D_6 = 0.$, and $C_2' = C2S = 100.$ (in MeV), $B_2 = 112.48$ and $B_2' = B2S = 90.$ (in 10^{-42}MeV s^2), $P_3 = -0.0531$ (in 10^{+42}MeV/s^2), $\hbar = 6.58211828$ (in 10^{-22}MeV s), $\nu_{\max} = NPH = 30$ in expansion of (25). In Table 7, we show a comparison of calculated eigenenergies from algebraic eigenvalue problem (26) and experimental eigenenergies from [15,20]. They are in a good agreement that confirm consistent choice of the parameters of GCM model and our version of the GCM code.

3.2 The Quadrupole Moment Q and Transitions $B(E2)$

The quadrupole operator $Q_m^{(2)}$ is defined as

$$Q_m^{(2)} = \rho_0 R_0^5 \left(\alpha_m^{[2]} - \frac{10}{\sqrt{70\pi}} [\alpha^{[2]} \times \alpha^{[2]}]_m^{[2]} \right), \tag{32}$$

where $\rho_0 = 3Ze/(4\pi R_0^3)$, $R_0 = r_0 A^{1/3}$, $r_0 = 1.1$fm.

The quadrupole moment of nth level with specified L reads as

$$\begin{aligned} Q_n(L) &= \rho_0 R_0^5 \sqrt{\frac{16\pi}{5}} \begin{pmatrix} L & 2 & L \\ -L & 0 & L \end{pmatrix} 10^{-2} \\ &\times \left(\alpha_{n,n}^{[2]}(L,L) - \frac{10}{\sqrt{70\pi}} [\alpha^{[2]} \times \alpha^{[2]}]_{n,n}^{[2]}(L,L) \right), \end{aligned} \tag{33}$$

Table 7. First column shows the labels L_n^π of eigenstates of a given rotational band, where L is the angular momentum, and $\pi = \pm$ is the parity. Dim is a number of components of the eigenvector $D_{\nu\lambda\mu,n}$ in Eq. (26), i.e., Dim is the total number of different (ν, λ and μ) for listed L and up to given $\nu_{\max}$, as well as the dimension of Hamiltonian matrix. Energy calc. are the eigenenergies of algebraic eigenvalue problem, Δ Energy calc.=Energy calc.(L_n^π) - Energy calc.(0_1^+) are the eigenenergies counted of eigenenergy of ground state 0_1^+, Δ Energy exp. are the experimental eigenenergies of rotational bands of ^{186}Os nucleus, all eigenenergies are in MeV.

Level	Code	Dim	Energy calc.	CPU time	Δ Energy calc.	Δ Energy exp.
0_{gs}^+	0_1^+	91	−5.683	5.33 s	0.000	0.000
2_{gs}^+	2_1^+	165	−5.546	23.78 s	0.138	0.137
4_{gs}^+	4_1^+	225	−5.260	58.70 s	0.424	0.433
6_{gs}^+	6_1^+	271	−4.854	1.58 min	0.829	0.867
2_γ^+	2_2^+		−4.937		0.746	0.767
3_γ^+	3_1^+	75	−4.750	4.19 s	0.934	0.910
4_γ^+	4_2^+		−4.596		1.087	1.070
5_γ^+	5_1^+	135	−4.343	17.22 s	1.340	1.275
4_γ^+	4_3^+		−4.174		1.509	1.352
6_γ^+	6_2^+		−4.164		1.520	1.492

where $\begin{pmatrix} L & 2 & L \\ -L & 0 & L \end{pmatrix}$ is 3-j symbol [24]. The reduced upwards transition probability $B(E2)$ is calculated by the expression

$$B_{n_2,n_1}(E2, L_2 \to L_1) = \frac{10^{-4}}{2L_2+1} \times \left[\rho_0 R_0^5 \left(\alpha^{[2]}_{n_2,n_1}(L_2,L_1) - \frac{10}{\sqrt{70\pi}}[\alpha^{[2]} \times \alpha^{[2]}]^{[2]}_{n_2,n_1}(L_2,L_1)\right)\right]^2. \tag{34}$$

3.3 Matrix Elements $\alpha^{[2]}_{n_2,n_1}(L_2,L_1)$ and $[\alpha^{[2]} \times \alpha^{[2]}]^{[2]}_{n_2,n_1}(L_2,L_1)$

Matrix elements $\alpha^{[2]}_{n_2,n_1}(L_2,L_1)$ and $[\alpha^{[2]} \times \alpha^{[2]}]^{[2]}_{n_2,n_1}(L_2,L_1)$ are given by the following expressions

$$\alpha^{[2]}_{n_2,n_1}(L_2,L_1) = \sqrt{(2L_1+1)(2L_2+1)}\sqrt{\frac{\hbar}{\sqrt{B_2'C_2'}}} \times \sum_{\nu_1\lambda_1\mu_1}\sum_{\nu_2\lambda_2\mu_2} \langle \nu_2\lambda_2 L_2|\beta|\nu_1\lambda_1 L_1\rangle\langle\lambda_2\mu_2 L_2|\alpha^{[2]}|\lambda_1\mu_1 L_1\rangle \times D_{\nu_1\lambda_1\mu_1,n_1}(L_1)D_{\nu_2\lambda_2\mu_2,n_2}(L_2), \tag{35}$$

$$[\alpha^{[2]} \times \alpha^{[2]}]^{[2]}_{n_2,n_1}(L_2,L_1) = \sqrt{\frac{1}{7}}\sqrt{(2L_1+1)(2L_2+1)}\frac{\hbar}{\sqrt{B_2'C_2'}} \times \sum_{\nu_1\lambda_1\mu_1}\sum_{\nu_2\lambda_2\mu_2} \langle \nu_2\lambda_2 L_2|\beta^2|\nu_1\lambda_1 L_1\rangle D_{\nu_1\lambda_1\mu_1,n_1}(L_1) \times \langle\lambda_2\mu_2 L_2|[\alpha^{[2]} \times \alpha^{[2]}]^{[2]}|\lambda_1\mu_1 L_1\rangle D_{\nu_2\lambda_2\mu_2,n_2}(L_2). \tag{36}$$

Here $D_{\nu_i\lambda_i\mu_i,n_i}(L_i)$ is the eigenvector of the Hamiltonian (23) for the n_ith state with angular momentum L_i from the algebraic eigenvalue problem (26).

3.4 Matrix Elements $\langle \lambda_1\mu_1 L_1|\alpha^{[2]}|\lambda_2\mu_2 L_2\rangle$

Matrix elements of $\alpha^{[2]}$ are calculated by means of the reduced Wigner coefficients in the chain O(5)⊃O(3) [7]

$$\langle \lambda_1\mu_1 L_1|\alpha^{[2]}|\lambda_2\mu_2 L_2\rangle = (-1)^{L_2-L_1}\frac{1}{\sqrt{2L_1+1}}\frac{1}{N} \times \sum_{K=-K_s(2)}^{K_s}\sum_{K_1=-K_{1s}(2)}^{K_{1s}}\sum_{K_2=-K_{2s}(2)}^{K_{2s}}\langle 2,K,L_2,K_2|L_1,-K_1\rangle \times \int_0^\pi \phi_{K_1}^{\lambda_1\mu_1 L_1}(\gamma)\phi_K^{\lambda=1\mu=0\,L=2}(\gamma)\phi_{K_2}^{\lambda_2\mu_2 L_2}(\gamma)\sin(3\gamma)d\gamma, \tag{37}$$

where $\langle 2,K,L_2,K_2|L_1,-K_1\rangle$ is Clebsch–Gordan coefficient [24], $\phi_K^{\lambda=1\mu=0L=2}(\gamma)$ are the orthogonalized functions calculated from Eq. (19) at $\lambda=1,\mu=0,L=2$. For all K, the summation bounds and normalization factors N are defined as follows:

$$K_s=\begin{cases} L, & L=\text{even},\\ L-1, & L=\text{odd};\end{cases} \qquad N=\begin{cases}\langle\lambda_1\mu_1 L_1|\lambda_1\mu_1 L_1\rangle, & (\lambda_1\mu_1 L_1)=(\lambda_2\mu_2 L_2),\\ \sqrt{\langle\lambda_1\mu_1 L_1|\lambda_1\mu_1 L_1\rangle\langle\lambda_2\mu_2 L_2|\lambda_2\mu_2 L_2\rangle}, & \text{otherwise.}\end{cases}$$

The angular brackets $\langle\lambda\mu L|\lambda\mu L\rangle$ here represent the overlap integrals Eq. (18) $\langle\phi^{\lambda\mu L}(\gamma)|\phi^{\lambda\mu L}(\gamma)\rangle$ of the corresponding functions $\phi^{\lambda\mu L}(\gamma)$.

3.5 Matrix Elements $\langle \lambda_1\mu_1 L_1|[\alpha^{[2]}\times\alpha^{[2]}]^{[2]}|\lambda_2\mu_2 L_2\rangle$

Matrix elements of $[\alpha^{[2]}\times\alpha^{[2]}]^{[2]}$ are calculated also by means of the reduced Wigner coefficients

$$\langle \lambda_1\mu_1 L_1|[\alpha^{[2]}\times\alpha^{[2]}]^{[2]}|\lambda_2\mu_2 L_2\rangle = \sqrt{\frac{2}{9(2L_2+1)}}\frac{1}{N} \times \sum_{K=-K_s(2)}^{K_s}\sum_{K_1=-K_{1s}(2)}^{K_{1s}}\sum_{K_2=-K_{2s}(2)}^{K_{2s}}\langle L_1,K_1,2,K|L_2,-K_2\rangle \times \int_0^\pi \phi_{K_1}^{\lambda_1\mu_1 L_1}(\gamma)\phi_K^{\lambda=2\mu=0\,L=2}(\gamma)\phi_{K_2}^{\lambda_2\mu_2 L_2}(\gamma)\sin(3\gamma)d\gamma, \tag{38}$$

where $\phi_K^{\lambda=2\mu=0L=2}(\gamma)$ are the orthogonalized functions calculated from Eq. (19) at $\lambda=2,\mu=0,L=2$.

The selection rules for the matrix elements $\alpha^{[2]}$ and $[\alpha^{[2]}\times\alpha^{[2]}]^{[2]}$ are:

$$\lambda{+}\lambda_1{+}\lambda_2 \text{ even },\ \lambda{>}|\lambda_1{-}\lambda_2|,\ \lambda{<}\lambda_1{+}\lambda_2,\ L{>}|L_1{-}L_2|,\ L{<}L_1{+}L_2. \tag{39}$$

The columns of Table 8 are formed by the values of the angular momentum L_2, #MeT is the total number of matrix elements for given L_2 and $L_1=L_2-2,L_2-1,L_2$, except for the first row where the $L_1L_2=02,22,23$, #MeZ is the number of zero matrix elements that are calculated equal to 0 among the #MeT matrix elements, and the CPU time.

Table 8. The CPU time of calculation of the matrix elements $\langle\lambda_1\mu_1 L_1|\alpha^{[2]}|\lambda_2\mu_2 L_2\rangle$ and $\langle\lambda_1\mu_1 L_1|[\alpha^{[2]}\times\alpha^{[2]}]^{[2]}|\lambda_2\mu_2 L_2\rangle$ for a number of L_2 and fixed $\nu_{\max}=30$.

$\langle\lambda_1\mu_1 L_1\|\alpha^{[2]}\|\lambda_2\mu_2 L_2\rangle$				$\langle\lambda_1\mu_1 L_1\|[\alpha^{[2]}\times\alpha^{[2]}]^{[2]}\|\lambda_2\mu_2 L_2\rangle$			
L_2	#MeT	#MeZ	CPU time	L_2	#MeT	#MeZ	CPU time
3	59	0	1.80 s	3	77	0	2.56 s
4	113	0	7.86 s	4	167	0	12.06 s
5	72	0	5.80 s	5	105	0	8.16 s
6	213	8	24.42 s	6	317	0	35.66 s
7	152	9	20.33 s	7	225	0	28.64 s
8	333	40	56.45 s	8	490	8	1.34 min
9	253	30	48.70 s	9	377	7	1.14 min
10	466	100	1.91 min	10	690	36	2.74 min

Table 9. Values of the quadrupole moments $Q_n(L)$(in eb) of ^{186}Os for a number of L and fixed $\nu_{\max}=30$.

n, L	2	4	5	6
1	−1.51	−1.85	0.953	−1.95
2	1.46	−0.517	−0.912	−1.02
3	−0.929	2.13	0.421	0.915

3.6 An Example of Calculations of The $Q_n(L)$(in eb) of ^{186}Os

The required states are characterized by their angular momentum L and sequence number n for fixed angular momentum starting at the lowest state. The calculated values of the quadrupole moment $Q_n(L)$(in eb) of ^{186}Os from (33) shown in Table 9 are the same as may be produced by the FORTRAN program [20].

3.7 An Example of Calculations of the $B(E2)$ (in e^2b^2) of ^{186}Os

The states are characterized by their angular momentum L and sequence number n for fixed angular momentum starting at the lowest state. The transitions are indicated as $n_i \to n_j$. The calculated values $B(E2) = B_{n_2,n_1}(E2, L_2 \to L_1)$ (in e^2b^2) of ^{186}Os come from Eq. (34) for a number of (L_1L_2) transitions and fixed $\nu_{\max}=30$ shown in Table 10 are the same as may be produced by the FORTRAN program [20]. CPU time for calculation of all Q and $B(E2)$ for up to $L=6$ and with the number of states $n=3$ is 64 s. (with previously prepared data files for angular matrix elements and eigenvectors of Hamiltonian).

3.8 Finding the Optimal Basis Parameters [20]

As a basis in this code we use the eigenfunctions (13)–(20) of the five-dimensional harmonic oscillator (11), which are respectively parameterized in terms of the

Table 10. Values of the $B(E2) = B_{n_2,n_1}(E2, L_2 \to L_1)$ (in e^2b^2) of ^{186}Os for a number of (L_1L_2) transitions and fixed $\nu_{\max} = 30$.

transitions	(0,2)	(2,2)	(2,3)
$1 \to 1$	2.99	0.801	0.0207
$2 \to 1$	0.0228	0.0779	1.32
$3 \to 1$	0.00835	0.00182	0.151
$1 \to 2$	0.0389	0.0778	0.00000291
$2 \to 2$	0.249	0.746	0.00131
$3 \to 2$	0.000121	0.0000199	0.0000855
$1 \to 3$	0.00526	0.00182	0.000429
$2 \to 3$	0.248	0.0000199	0.0261
$3 \to 3$	0.0573	0.300	0.00386

Table 11. The values of the phenomenological potential parameters C_2, C_3, C_4, C_5, C_6, D_6, B_2, P_3, Eqs. (4), (5) for $N = 184$ isotones are determined by fitting [9].

	$^{298}114$	$^{300}116$	$^{302}118$	$^{304}120$	$^{306}122$	$^{308}124$
C_2	7579.22	7661.89	7744.29	7826.40	7908.23	7989.76
C_3	$3.25 \cdot 10^{-4}$	$-1.62 \cdot 10^{-3}$	$-1.61 \cdot 10^{-3}$	$-4.83 \cdot 10^{-4}$	$2.20 \cdot 10^{-3}$	$3.51 \cdot 10^{-4}$
C_4	$-2.93 \cdot 10^{-1}$	$1.98 \cdot 10^{-1}$	$1.84 \cdot 10^{-1}$	$-1.16 \cdot 10^{-1}$	$-8.39 \cdot 10^{-1}$	$-3.13 \cdot 10^{-1}$
C_5	$-4.11 \cdot 10^{-3}$	$2.05 \cdot 10^{-2}$	$2.04 \cdot 10^{-2}$	$6.10 \cdot 10^{-3}$	$-2.80 \cdot 10^{-2}$	$-4.44 \cdot 10^{-3}$
C_6	$1.65 \cdot 10^{-4}$	$-7.81 \cdot 10^{-4}$	$-7.72 \cdot 10^{-4}$	$-2.22 \cdot 10^{-4}$	$1.09 \cdot 10^{-3}$	$1.70 \cdot 10^{-4}$
D_6	1.79	−2.08	−1.98	$4.46 \cdot 10^{-1}$	6.15	1.96
B_2	226.573	226.573	226.573	226.573	226.573	226.573
P_3	0	0	0	0	0	0

basis parameters C_2' and B_2'. For a finite set of basic vectors, the parameters have to be chosen to get satisfactory convergence of the calculated energies and B(E2)-values. To find the best set of basis parameters one has to diagonalize a given Hamiltonian (23) and minimize the sum of (lowest) energy eigenvalues E_n^L by varying the basis parameters(see e.g. [16]). Since this procedure is quite time-consuming, we use another scheme that takes much less time and turned out to be also effective: we minimize only the sum of the first NUM diagonal matrix elements of the Hamiltonian for spin $I = 0$ and take B_2' fixed at B_2. The integer variable NUM should be equal to the number of the lowest $L = 0$ basis wave functions which contribute most to the first excited states. (Default: $NUM = 10$). The minimum is found by increasing a do–loop variable S, defined as $S = (C_2'B_2'/\hbar^2)^{1/4}$, successively by 0.5. In the case of failure to find reasonable basis parameters, the program is stopped and should be reruned with changed boundaries for S. In particular, for ^{186}Os: $S = 12.005370$, where $\hbar = 0.6582183$ (in 10^{-22}MeV s) , $B_2' = 90$(in 10^{-42}MeV s^2), $C_2' = 100$ (in MeV).

Table 12. The values of the phenomenological potential parameters, $C_2, C_3, C_4, C_5, C_6, D_6, B_2, P_3$, Eqs. (4), (5) for ^{152}Sm, ^{154}Sm,^{186}Os, ^{188}Os, ^{190}Os, ^{194}Pt and ^{196}Pt are determined by fitting [9].

	^{152}Sm	^{154}Sm	^{186}Os	^{188}Os	^{190}Os	^{194}Pt	^{196}Pt
C_2	−422.74	−464.74	−564.76	−398.83	−363.64	−161.58	−169.88
C_3	493.92	311.25	733.01	−380.74	−372.59	368.36	748.09
C_4	7983.60	6454.70	13546.	18295.43	19391.83	2610.08	5704.92
C_5	370.53	88.25	−8535.1	−17660.53	−19246.82	−130535.32	−315802.62
C_6	8279.78	3842.18	−41635.	74725.61	80003.64	583687.93	975896.18
D_6	−28041.74	−17430.86	0	−54507.20	−70794.69	997672.28	1841446.68
B_2	62.714	63.823	112.48	165.514	173.035	203.613	223.380
P_3	0	0	−0.0531	0	0	0	0

Table 13. The values of the phenomenological potential parameters, $C_2, C_3, C_4, C_5, C_6, D_6, B_2, P_3$, Eqs. (4), (5) for Nobelium isotopes ^{248}No, ^{250}No, ^{252}No, ^{254}No, ^{256}No, and ^{258}No are determined by fitting [9].

	^{248}No	^{250}No	^{252}No	^{254}No	^{256}No	^{258}No
C_2	−742.30	−740.31	−742.30	−820.82	−785.78	−755.83
C_3	308.99	308.17	183.87	307.77	220.57	172.21
C_4	19029.74	18978.78	17371.12	19240.37	18948.17	19152.27
C_5	6261.17	6244.40	8478.34	3008.90	4202.27	3693.95
C_6	6020.57	6004.45	15304.34	7515.07	4820.42	−20225.25
D_6	−39632.38	−39525.07	−11301.10	−58453.68	−42470.76	−20383.43
B_2	226.573	83.289	240.795	226.573	226.573	226.573
P_3	0	0	0	0	0	0

Table 14. The values of the phenomenological potential parameters for Seaborgium isotopes ^{258}Sg, ^{260}Sg, ^{262}Sg, ^{264}Sg, ^{266}Sg, ^{268}Sg, ^{270}Sg, ^{272}Sg are determined by fitting [9].

	^{258}Sg	^{260}Sg	^{262}Sg	^{264}Sg	^{266}Sg	^{268}Sg	^{270}Sg	^{272}Sg
C_2	−889.78	−862.28	−858.57	−707.00	−881.27	−953.97	−948.53	−816.63
C_3	302.98	273.96	156.35	−244.07	−191.92	−135.38	−236.13	−249.84
C_4	21572.37	21479.99	23326.53	15852.44	22306.53	24457.98	27362.39	29458.02
C_5	−181.54	−958.25	603.74	4107.14	1057.65	554.98	−106.83	1252.04
C_6	5756.03	4802.92	−15191.44	5714.98	2767.59	2200.10	7677.81	2858.93
D_6	−91050.30	−85406.47	−92394.99	−42886.06	−87378.21	−101284.80	−124100.10	−136456.34
B_2	226.573	226.573	226.573	226.573	226.573	226.573	226.573	226.573
P_3	0	0	0	0	0	0	0	0

Table 15. The values of the phenomenological potential parameters for Hassium isotopes ^{264}Hs, ^{266}Hs, ^{268}Hs , ^{270}Hs, ^{272}Hs, ^{274}Hs, ^{276}Hs are determined by fitting [9].

	^{264}Hs	^{266}Hs	^{268}Hs	^{270}Hs	^{272}Hs	^{274}Hs	^{276}Hs
C_2	−910.55	−960.16	−957.77	−974.18	−967.13	−892.06	−528.93
C_3	−237.56	−306.53	−305.77	−401.01	−293.31	−366.77	401.95
C_4	23771.37	25603.20	25539.27	25146.02	27982.38	28476.76	31704.06
C_5	870.21	530.39	529.12	465.71	−2668.59	1589.99	26.09
C_6	−8701.36	8602.71	8581.15	20760.67	39469.35	9918.38	27748.59
D_6	−90319.19	−114091.97	−113806.31	−105793.07	−140708.47	−134891.91	−156859.49
B_2	226.573	226.573	226.573	226.573	226.573	226.573	226.573
P_3	0	0	0	0	0	0	0

4 Conclusions

We have developed a symbolic method implemented as a code GCM in the Wolfram Mathematica to compute energy spectrum, quadrupole momentum, and electromagnetic transitions in Geometric Collective Model. The symbolic nature of the developed methods allows one to avoid the numerical round-off errors in the calculation of spectral characteristics (especially close to resonances) of quantum systems under consideration and to study their analytic properties for understanding the dominant symmetries. Efficiency of the elaborated procedures and the code is shown by benchmark calculations of ^{186}Os nucleus and demonstrate quick performance even on a laptop.

The GCM code can be applied to study the properties of super-heavy nuclei using an approach proposed in the papers [9,12]. Sets of the input parameters for some atomic nuclei and super–heavy nuclei are given in Appendix A.

To point out further investigations of the considered GCM model for atomic nuclei in the framework of the Computer Algebra System (CAS) of the boundary value problem (BVP) corresponding to quantum Hamiltonian Eq. (11) is presented in Appendix B. Solution of this problem by the finite element method (FEM) implemented in a suitable CAS code, for example, GCMFEM code [10] gives a possibility to compare GCM results with GCMFEM ones using the alternative FEM reduction of the BVP to algebraic problems and input parameters from Appendix A.

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A Appendix. Sets of Input Parameters for Atomic Nuclei

To denote approximately a range of applicability of the GCM code and to make it more friendly for users, we will accompany it by the sets of input files with the values of sets of parameters for atomic nuclei given in the papers [9,12,20].

For example, we present some of them in Tables 11, 12, 13, 14, 15, and 16. In Table 11 the macroscopic potential parameters are given. The value of C_2 is increased as we approach to double closed shell. Even the potential depends more on the quadratic term over β, it is not completely quadratic even if one approaches very close the double closed shell. Because of the great similarity, the authors only depict the PES of the $^{298}114$ and $^{304}120$ in Figs. 29 and 30 in Ref. [9]. The PES is perfectly spherical, thus, the spectrum will be that of a five-dimensional oscillator: The energy scales as $\hbar\sqrt{C_2/B_2}$. The first excited state is a 2^+ state at the energy $\hbar\sqrt{C_2/B_2}$ and at twice this energy, there are three degenerate states with spin and parity 0^+, 2^+ and 4^+. The first 3+ state is three times the energy of the first 2^+ state. For completeness, in Fig. 31 in Ref. [9], the authors depict the spectrum of the $^{298}114$ nucleus as predicted by the GCM [9].

Table 16. The values of the phenomenological potential parameters for ^{184}W are determined by fitting [12].

C_2	C_3	C_4	C_5	C_6	D_6	B_2	P_3
−521.77	−337.80	14306.01	−502.64	1902.26	−60439.94	112.697	0

The only parameter, which cannot be deduced is the collective mass B_2 of the geometrical model [8]. This parameter has to be adjusted to, e.g., a particular state in the ground state band. Also assuming for neighboring nuclei the same value of B_2 is in general far more accurate than using the Cranking Model. For the case of nuclei in the island of stability, one will use a generic value, i.e., results will scale with B_2 (as it is pointed out in page 128 in Ref. [9]).

B Appendix. Boundary Value Problem for GCM Model

The equation of geometric collective model (GCM) with respect to components $\Phi^L_{nK} = \Phi^L_{nK}(\beta,\gamma)$ and eigenvalue E^L_n (in MeV), $\bar{B}_2 = 2B_2/\sqrt{5}$ in (10^{-42}MeV s^2) and C_2 in (MeV) are mass and stiffness parameters, variable β in (fm), reads as

$$(T(\beta,\gamma)+T_K^L(\beta,\gamma)+\hat{V}(\beta,\gamma)-E_n^L)\Phi_{nK}^L(\beta,\gamma)=\sum_{K'=K\pm 2even}V_{KK'}^L(\beta,\gamma)\Phi_{vK'}^L(\beta,\gamma), \tag{40}$$

$$T(\beta,\gamma)=\frac{\hbar^2}{2\bar{B}_2}\left(-\frac{1}{\beta^4}\frac{\partial}{\partial\beta}\beta^4\frac{\partial}{\partial\beta}-\frac{1}{\beta^2\sin(3\gamma)}\frac{\partial}{\partial\gamma}\sin(3\gamma)\frac{\partial}{\partial\gamma}\right)+\mathcal{K}(\beta,\gamma),$$

$$T_K^L(\beta,\gamma)=+\frac{\hbar^2}{2\bar{B}_2}\left[(L(L+1)-K^2)\left(\frac{2\bar{B}_2}{4J_1}+\frac{2\bar{B}_2}{4J_2}\right)+\frac{K^2 2\bar{B}_2}{2J_3}\right],$$

$$V_{KK'}^L(\bar{\beta},\gamma)=-\frac{\hbar^2}{2\bar{B}_2}\left[\frac{2\bar{B}_2}{8J_1}-\frac{2\bar{B}_2}{8J_2}\right]C_{KK'}^L,\ C_{KK'}^L=\delta_{K'K-2}C_{KK-2}^L+\delta_{K'K+2}C_{KK+2}^L,$$

$$C_{KK-2}^L=(1+\delta_{K2})^{1/2}[(L+K)(L-K+1)(L+K-1)(L-K+2)]^{1/2},$$

$$C_{KK+2}^L=(1+\delta_{K0})^{1/2}[(L-K)(L+K+1)(L-K-1)(L+K+2)]^{1/2},$$

and the moments of the inertia denoted as $J_k=4\bar{B}_{(k)}\beta^2\sin^2(\gamma-\frac{2}{3}k\pi)$, where $k=1,2,3$ and $\bar{B}_{(k)}=\bar{B}_2$ is a mass parameter, with potential function $\hat{V}(\beta,\gamma)$ from (3), (4) and (5), and input set of parameters from Tables 11, 12, 13, 14, 15 and 16 in Appendix A, and additional kinetic function $\mathcal{K}(\beta,\gamma)$ determined in [11,14,17,20,23]. The bounded components ϕ_{vK}^L are subjected to homogeneous Neumann or Dirichlet boundary conditions at the boundary points of interval $\gamma=0$ and $\gamma=\pi/3$ for zero or odd values of L (for details of boundary conditions on interval of the β variable see [18,19,23]), and orthonormalization conditions (see Eq. (15))

$$\int_{\beta=0}^{\beta_{max}}\int_0^{\pi/3}\sum_{Keven}\Phi_{n'K}^L(\beta,\gamma)\Phi_{nK}^L(\beta,\gamma)\sin(3\gamma)d\gamma\beta^4 d\beta=\delta_{n'n}. \tag{41}$$

The BVP (40)–(41) will be solved by the FEM implemented in the CAS code.

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