Symbolic-Numeric Algorithm for Computing Orthonormal Basis of $O(5) \times SU(1,1)$ Group

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Abstract. We have developed a symbolic-numeric algorithm implemented in Wolfram Mathematica to compute the orthonormal non-canonical bases of symmetric irreducible representations of the $O(5) \times SU(1,1)$ and $\overline{O(5)} \times \overline{SU(1,1)}$ partner groups in the laboratory and intrinsic frames, respectively. The required orthonormal bases are labelled by the set of the number of bosons N, seniority λ, missing label μ denoting the maximal number of boson triplets coupled to the angular momentum $L = 0$, and the angular momentum (L, M) quantum numbers using the conventional representations of a five-dimensional harmonic oscillator in the laboratory and intrinsic frames. The proposed method uses a new symbolic-numeric orthonormalization procedure based on the Gram–Schmidt orthonormalization algorithm. Efficiency of the elaborated procedures and the code is shown by benchmark calculations of orthogonalization matrix $O(5)$ and $\overline{O(5)}$ bases, and direct product with irreducible representations of $SU(1,1)$ and $\overline{SU(1,1)}$ groups.

Keywords: Orthonormal non-canonical basis · Irreducible representations · Group $O(5) \times SU(1,1)$ · Gram–Schmidt orthonormalization · Wolfram Mathematica

1 Introduction

The Bohr–Mottelson collective model [1,2] has gained widespread acceptance in calculations of vibrational-rotational spectra and electromagnetic transitions in atomic nuclei [3–5]. For construction of basis functions of this model, different approaches were proposed, for example, [6–9], that lead only to nonorthogonal set of eigenfunctions needed in further orthonormalization, considered only in

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intrinsic frame [10–15]. However, until now, there are no sufficiently universal algorithms for evaluation of the required orthonormal bases needed for large-scale applied calculations in both intrinsic and laboratory frames used in modern models to revival point symmetries in specified degeneracy spectra [16,17]. Creation of such symbolic-numeric algorithm is a goal of the present paper.

In the present paper, we elaborate an universal effective symbolic-numeric algorithm implemented as the first version of `O5SU11` code in Wolfram Mathematica for computing the orthonormal bases of the Bohr–Mottelson(BM) collective model in both intrinsic and laboratory frames. It is done on the base of theoretical investigations for constructing the non-canonical bases for irreducible representations (IRs) of direct product groups $G = \mathrm{O}(5) \times \mathrm{SU}(1{,}1)$ in the laboratory frame [8] and $\bar{G} = \overline{\mathrm{O}(5)} \times \overline{\mathrm{SU}(1{,}1)}$ in the intrinsic frame [7]. We pay our attention to computing bases in both laboratory and intrinsic frames needed for construction of the algebraic models accounting symmetry group [18,19] based on anti-isomorphism between G and $\bar{G}$ partner groups [16,17], and point symmetries in modern calculations, for example, [20–23]. The required orthonormal bases are labelled by the set of the number of bosons N, seniority λ, missing label μ, denoting the maximal number of boson triplets coupled to the angular momentum $L = 0$, and the angular momentum (L, M) quantum numbers using the conventional representations of a five-dimensional harmonic oscillator in the laboratory and intrinsic frames. In the proposed method, the authors use a symbolic-numeric non-standard recursive and fast orthonormalization procedure based on the Gram–Schmidt (G–S) orthonormalization algorithm. Efficiency of the elaborated procedures and the code is shown by benchmark calculations of orthogonalization matrix $O(5)$ and $\overline{\mathrm{O}(5)}$ bases, and IRs of SU(1,1) group.

The structure of the paper is as follows. In the second section, we present characterization of group $G = \mathrm{O}(5) \times \mathrm{SU}(1{,}1)$ and characterization of states. In Subsects. 2.5 and 2.6, we give the explicit formulas needed for the construction of symmetric nonorthogonal bases for IRs of the O(5) and $G = \mathrm{O}(5) \otimes \mathrm{SU}(1{,}1)$ groups. In the third section, we present the construction of the orthonormal basis of the collective nuclear model in intrinsic frame corresponding IRs of the $\bar{G} = \overline{\mathrm{O}(5)} \times \overline{\mathrm{SU}(1{,}1)}$ group. In the fourth section, we present the algorithm and benchmark calculations of overlaps and orthogonalization upper triangular matrices applied for constructing the orthonormal basis vectors in the laboratory and intrinsic frames. In conclusion, we give a resumé and point out some important problems for further applications of proposed algorithms.

2 Characterization of Group O(5) × SU(1,1) and Characterization Of States in the Laboratory Frame

Quantum description of collective motions by using the deformation variables $\hat{\alpha}^{(l)}_m$ needs the Hilbert space $L_2(\hat{\alpha}^{(l)})$, which is the state space of $(2l+1)$-dimensional harmonic oscillator. The Hamiltonian of this harmonic oscillator has the form

$$H_l = \frac{1}{2} \sum_{\mu} \left(\hat{\pi}^{(l)}_{\mu} \hat{\pi}^{(l)\mu} + \hat{\alpha}^{(l)\mu} \hat{\alpha}^{(l)}_{\mu} \right), \tag{1}$$

where

$$\hat{\alpha}^{(l)}_m = \sum_\mu g_{m\mu}\hat{\alpha}^{(l)\mu} = (-1)^m \hat{\alpha}^{(l)-m} \tag{2}$$

denotes the multiplication operator by the variable $\hat{\alpha}^{(l)}_m$ and

$$\hat{\pi}^{(l)}_m = \sum_m g_{m\mu}\hat{\pi}^{(l)\mu} = -i\frac{\partial}{\partial\hat{\alpha}^{(l)m}} \tag{3}$$

denotes the conjugate momentum to the coordinate $\hat{\alpha}^{(l)}_\mu$.

The covariant metric tensor $g_{mm'}$ in the corresponding manifold has the form

$$g_{mm'} = g^{mm'} = (-1)^l\sqrt{2l+1}(lmlm'|00) = (-1)^m\delta_m^{-m'}. \tag{4}$$

The operators $\hat{\alpha}^{(l)}_m, \hat{\pi}^{(l)}_m$ fulfil the standard commutation relations

$$\left[\hat{\alpha}^{(l)}_m, \hat{\pi}^{(l)m'}\right] = i\delta_m^{m'}, \quad \left[\hat{\alpha}^{(l)}_m, \hat{\alpha}^{(l)}_{m'}\right] = 0, \quad \left[\hat{\pi}^{(l)m}, \hat{\pi}^{(l)m'}\right] = 0. \tag{5}$$

By using these operators one can build the creation and annihilation spinless boson operators $\eta^{(l)}_m$ and $\xi^{(l)}_m$ with the angular momentum l

$$\eta^{(l)}_m = \frac{1}{\sqrt{2}}\left(\hat{\alpha}^{(l)}_m - i\hat{\pi}^{(l)}_m\right), \quad \xi^{(l)}_m = \frac{1}{\sqrt{2}}\left(\hat{\alpha}^{(l)}_m + i\hat{\pi}^{(l)}_m\right). \tag{6}$$

Contravariant operators can be built in standard way

$$\eta^m = \sum_\mu g^{m\mu}\eta_\mu, \quad \xi^m = \sum_\mu g^{m\mu}\xi_\mu. \tag{7}$$

They satisfy the following commutation relations

$$[\xi^m, \eta_{m'}] = \delta^m_{m'}, \quad \left[\xi^m, \xi^{m'}\right] = [\eta_m, \eta_{m'}] = 0, \quad (\eta_m)^\dagger = \xi^m \quad (\xi_m)^\dagger = \eta^m. \tag{8}$$

2.1 Characterization of U(2l+1)

It can be shown that the bilinear forms

$$\begin{gathered}(\eta\otimes\eta)^{(L)}_M, \quad \left(\tilde{\xi}\otimes\tilde{\xi}\right)^{(L)}_M, \quad \left(\eta\otimes\tilde{\xi}\right)^{(L)}_M, \\ \text{where} \quad L = 0, 1\ldots 2l, \quad \tilde{\xi}_m = (-1)^m\xi_{-m}\end{gathered} \tag{9}$$

generate the non-compact symplectic group Sp(2(2l+1),R).

Group theory analysis leads to two classifications of boson states:

$$\begin{aligned}&\mathrm{Sp(2(2l+1),R)} \supset \mathrm{U(2l+1)}, \\ &\mathrm{Sp(2(2l+1),R)} \supset \mathrm{O(2l+1)} \times \mathrm{SU(1,1)}.\end{aligned} \tag{10}$$

The orthonormal group O(2l+1) and the non-compact unitary group SU(1,1) are complementary in two physical IRs of the symplectic group Sp(2(2l+1),R) (for odd and even number of bosons).

The unitary group U(2l+1) has $(2l{+}1)^2$ generators $E_{mm'}$ or bosons operators

$$(\eta\otimes\tilde{\xi})_M^{(L)}=\frac{1}{2}(-1)^l\sum_{mm'}(lmlm'|LM)E_{mm'},\quad \text{where}\quad L=0,1,\dots 2l, \tag{11}$$

$$E_{mm'}{=}\frac{1}{2}(N_{mm'}{+}\Lambda_{mm'}),\ N_{mm'}{=}\hat{\alpha}_m\hat{\alpha}_{m'}{+}\hat{\pi}_m\hat{\pi}_{m'},\ \Lambda_{mm'}{=}i(\hat{\alpha}_m\hat{\pi}_{m'}{-}\hat{\pi}_m\hat{\alpha}_{m'}).$$

The operators $(\eta\otimes\tilde{\xi})_M^{(L)}$ fulfil the following commutation relations

$$\begin{aligned}\left[(\eta\otimes\tilde{\xi})_{M_1}^{(L_1)},(\eta\otimes\tilde{\xi})_{M_2}^{(L_2)}\right] &= \sqrt{(2L_1+1)(2L_2+1)}\sum_{LM}[(-1)^L-(-1)^{L_1+L_2}]\\ &\times(L_1M_1L_2M_2|LM)\left\{\begin{matrix}L_1 & L_2 & L\\ l & l & l\end{matrix}\right\}(\eta\otimes\tilde{\xi})_M^{(L)}.\end{aligned}$$

The second order Casimir invariant of the group U(2l+1) is given by

$$C^2=\sum_{L=0}^{2l}A_L,\ A_L=(-1)^L\sqrt{2L+1}\left[(\eta\otimes\eta)^{(L)}\otimes(\tilde{\xi}\otimes\tilde{\xi})^{(L)}\right]_0^{(0)}. \tag{12}$$

It can be shown that

$$C^2=\hat{N}(\hat{N}-1),\quad \text{where}\quad \hat{N}=\sum_\mu\eta_\mu\xi^\mu=\sqrt{2l+1}(\eta\otimes\tilde{\xi})_0^{(0)}, \tag{13}$$

the operator $\hat{N}$ is the boson number operator.

The eigenvalues of C^2 depend only on the number of bosons in a given state. In the state which contains N bosons, the expectation value of C^2 is

$$\langle C^2\rangle_N=N(N-1). \tag{14}$$

At the same time, N uniquely labels symmetric IRs of $U(2l+1)$.

Arbitrary state of N bosons can be constructed by using the vectors:

$$|n_{-l},n_{-l+1}\dots n_l\rangle=\frac{1}{\sqrt{(n_{-l})!\,(n_{-l+1})!\,\dots(n_l)!}}(\eta_{-l})^{n_{-l}}\dots(\eta_l)^{n_l}|0\rangle. \tag{15}$$

According to this, to define uniquely the state of bosons, located on a level with angular momentum equal to l, one needs to have a set of $2l{+}1$ quantum numbers.

2.2 Characteristic of O(2l+1)

The orthogonal group O(2l+1) contains one-to-one transformations of linear spaces spanned by the tensors $\alpha^{(l)}=(\alpha_{-l}^{(l)},\dots,\alpha_l^{(l)})$ which do not change the quadratic form

$$\beta^2=\sum_\mu\alpha_\mu^{(l)}\alpha^{(l)\mu}. \tag{16}$$

Generators of this group are $l(2l{+}1)$ independent operators $\Lambda_{mm'}$ for $m > m'$. The commutation relation for these generators are

$$[\Lambda_{m_1m_2}, \Lambda_{m_3m_4}]{=}\delta_{m_2m_3}\Lambda_{m_1m_4}{+}\delta_{m_1m_4}\Lambda_{m_2m_3}{-}\delta_{m_1m_3}\Lambda_{m_3m_4}{-}\delta_{m_2m_4}\Lambda_{m_1m_3},$$
$$\text{where}\quad \delta_{mm'} = \sum_\mu g_{m\mu}\delta^\mu_{m'} = (-1)^m\delta^{-m}_{m'}. \tag{17}$$

It is possible to get a more useful form of these generators

$$\Lambda_{mm'} = \eta_m\xi_{m'} - \eta_{m'}\xi_m = (-1)^l\sum_{LM}[1-(-1)^L](lmlm'|LM)(\eta\otimes\tilde{\xi})^{(L)}_M. \tag{18}$$

This implies that the operators $(\eta\otimes\tilde{\xi})^{(L=1,\,3,\,5,\ldots,\,2l+1)}_M$ are the generators of the group O(2l+1).

The second-order Casimir invariant of the orthogonal group O(2l+1) is

$$\Lambda^2 = \sum_{L=0}^{2l}[1-(-1)^L]A_L. \tag{19}$$

For unique labelling of totally symmetric IRs of O(2l+1), one needs only one quantum number λ. Eigenvalues of operators Λ^2 are the numbers

$$\left\langle\Lambda^2\right\rangle_\lambda = \lambda(\lambda+2l-1). \tag{20}$$

The quantum number λ is called seniority and denotes the number of bosons which are not coupled to pairs with zero angular momentum.

2.3 Characteristic of SU(1,1)

The non-compact unitary group $SU(1,1)$ is the complementary group to the orthogonal group O(2l+1).

The group SU(1,1) has three generators:

$$S_+{=}\frac{\sqrt{2l+1}}{2}(\eta\otimes\eta)^{(0)}_0,\ S_-{=}\frac{\sqrt{2l+1}}{2}(\tilde{\xi}\otimes\tilde{\xi})^{(0)}_0,\ S_0{=}\frac{1}{2}\left(\hat{N}{+}\frac{2l+1}{2}\right). \tag{21}$$

The above generators satisfy the following commutation relations:

$$[S_+, S_-] = -2S_0, \quad [S_0, S_+] = S_+, \quad [S_0, S_-] = -S_-, \tag{22}$$

and the conjugation relation

$$(S_+)^\dagger = S_-. \tag{23}$$

The second-order Casimir invariant of the group SU(1,1) is the following operator

$$S^2 = S_0^2 - S_0 - S_+S_-. \tag{24}$$

One can show that the following relation is satisfied

$$\Lambda^2 = 4S^2 - \frac{1}{4}(2l-3)(2l+1). \tag{25}$$

So, the eigenvalues of S^2 are given by

$$\left\langle S^2\right\rangle = S(S-1),\ \text{where}\ S = \frac{1}{2}\left(\lambda+\frac{2l+1}{2}\right). \tag{26}$$

2.4 Construction of States with $N > \lambda$

Let the state

$$|\lambda, N = \lambda, \chi\rangle = |\lambda\lambda\chi\rangle \tag{27}$$

denote the state having the seniority number λ which is equal to the number of particles N in the system. Then it satisfies the conditions

$$S_{-}|\lambda\lambda\chi\rangle = 0,\ \ S_0|\lambda\lambda\chi\rangle = \frac{1}{2}(\lambda + \frac{2l+1}{2})|\lambda\lambda\chi\rangle. \tag{28}$$

In the above equations, χ denotes the set of quantum numbers which are needed for labelling the states of the boson system. One can construct the states having the number of bosons N greater than the seniority number λ $(N > \lambda)$ by using the action of creation operators of boson pairs coupled to zero angular momentum S_{+}:

$$|\lambda N\chi\rangle = \sqrt{\frac{\Gamma\left[\lambda + \frac{1}{2}(2l+1)\right]}{\left[\frac{1}{2}(N-\lambda)\right]!\ \Gamma\left[\frac{1}{2}(N+\lambda+2l+1)\right]}}\ (S_{+})^{\frac{1}{2}(N-\lambda)}|\lambda\lambda\chi\rangle. \tag{29}$$

Angular momentum is a good quantum number characterizing nuclear states. It implies that the rotation group O(3) generated by the operators

$$L_m^{(1)} = \sqrt{\frac{1}{3}l(l+1)(2l+1)}\ (\eta\otimes\tilde{\xi})_m^{(1)} \tag{30}$$

should be contained in the group chain which classifies these states.

The operator $\hat{L}^2$ of the squared angular momentum (the Casimir operator for SO(3)) can be constructed as follows:

$$\hat{L}^2 = \sum_{m=-1}^{1}(-1)^m L_m^{(1)}L_{-m}^{(1)} = l(l+1)(2l+1)\sum_{L=0}^{2l}\begin{Bmatrix} l & l & 1\\ l & l & L\end{Bmatrix} A_L + l(l+1)\hat{N}.$$

In conclusion, the quantum boson states for $l = 0, 1, 2, \ldots$ can be classified according to two group chains

$$\mathrm{U(2l{+}1)} \supset \mathrm{O(2l{+}1)} \supset \cdots \supset \mathrm{O(3)} \supset \mathrm{O(2)}, \tag{31}$$

$$\mathrm{O(2l{+}1)} \otimes \mathrm{SU(1,1)} \supset \cdots \supset, \mathrm{O(3)} \otimes \mathrm{U(1)} \supset \mathrm{O(2)}. \tag{32}$$

Unitary subgroup SU(1,1) $\supset$ U(1) is generated by the operator S_0, and the generator of rotation about the z-axis generating the subgroup O(3) $\supset$ O(2) is the operator $L_0^{(1)}$.

The states constructed according to the first group chain (31) will be denoted by

$$|N\lambda\xi LM\rangle, \tag{33}$$

and the states constructed according to the second group chain (32) will be denoted by replacing letters N and λ

$$|\lambda N\xi LM\rangle. \tag{34}$$

The vectors (33) and (34) though constructed in different way can be identified as the same vectors. In the following, we will treat them as identical.

But one has to stress that vectors (33) and (34) span IRs of different groups. The vectors (33) form a basis of IRs of the group U(2l+1), for given N. The vectors (34) span the basis of IRs of the group O(2l+1) $\otimes$ SU(1,1), for given λ. According to the above property, we can construct the states of N bosons by using the easier scheme (32).

Table 1. The set of values of dimensions of IRs O(5) group D^e_λ at even L and D^o_λ at odd L and their sum $D_\lambda = D^e_\lambda + D^o_\lambda$ vs λ

λ	10	20	30	40	50	60	70	80	90	100
D^e_λ	322	1892	5711	12782	24102	40671	63492	93562	131881	179452
D^o_λ	184	1419	4705	11039	21424	36860	58344	86879	123465	169099
D_λ	506	3311	10416	23821	45526	77531	121836	180441	255346	348551

2.5 Construction of the Nonorthogonal Basis for Symmetric IRs of the Group O(5)

As the first step, we start with the construction of a basis for the group O(5) from Subsect. 2.2 at $l = 2$. We start the construction with the state of maximal seniority λ and maximal angular momentum $L_0 = 2\lambda$:

$$|\lambda\rangle = (\eta^{(2)}_2)^\lambda |0\rangle \tag{35}$$

generated by the action of the creation spinless boson operator $\eta^{(2)}_2 \equiv \eta_2$ from (6) on the vacuum vector $|0\rangle$ in representation (15) of elementary boson basis of symmetric IR group U(5) from Subsect. 2.1 at $l = 2$. Next, we construct the operators $\hat{O}(\lambda, \mu, L, M)$ commuting with the Casimir operator $\hat{\Lambda}^2$ from (19) of group O(5) and with lowering the angular momentum to the required L

$$\hat{O}(\lambda, \mu, L, M) = \sum_{L \le m \le 2\lambda} \beta_m(\lambda, L)(L_-)^{m-M}(L_+)^{m+\lambda-3\mu} \left[(\eta \otimes \tilde{\xi})^{(3)}_{-3} \right]^{\lambda-\mu}, \tag{36}$$

where

$$\beta_m(\lambda, L) = \frac{(-1)^m}{(m-L)!(m+L+1)!}, \quad L_+ = -\frac{1}{\sqrt{2}} L^{(1)}_{+1}, \quad L_- = \frac{1}{\sqrt{2}} L^{(1)}_{-1}, \tag{37}$$

i.e., with commutator $[\hat{L}_i, \hat{L}_j] = +\imath\varepsilon_{ijk}\hat{L}_k,$ where ε_{ijk} is the totally antisymmetric symbol, $\varepsilon_{123} = +1$. The quantum number μ denotes the maximal number of boson triplets coupled to the angular momentum $L = 0$. It can be shown that if

$$(\lambda-3\mu) \le L \le 2(\lambda-3\mu)(\text{even L}), \; (\lambda-3\mu) \le (L+3) \le 2(\lambda-3\mu)L(\text{odd L}), \tag{38}$$

where $0 \le \mu \le [\lambda/3]$, and $[\frac{\lambda}{3}]$ denotes the integer part of $\frac{\lambda}{3}$, then the vectors $\hat{O}(\lambda, \mu, L, M)|\lambda\rangle$ are linearly independent and they form a basis for IRs of the group O(5), for given λ.

The dimension D_λ of this space is $D_\lambda = \frac{1}{6}(\lambda+1)(\lambda+2)(2\lambda+3)$ at fixed λ is determined by following [6]:

$$D_\lambda = D_\lambda^e + D_\lambda^o = \sum_{\mu=0}^{[\lambda/3]} \sum_{L=2[(\lambda+1-3\mu)/2]}^{[2\lambda-6\mu]\prime} (2L+1) + \sum_{\mu=0}^{[(\lambda-3)/3]} \sum_{L=2[(\lambda-3\mu)/2]+1}^{[2\lambda-6\mu-3]\prime} (2L+1), \quad (39)$$

where the prime means summation by step 2 and $[\mu] = \texttt{Floor}(\mu)$ is the largest integer not greater that μ. For example, see Table 1.

Table 2. The set of accessible values μ of the states $|\lambda\mu LL\rangle$ for $L = 0, \dots, 17$ and $\lambda = 0, \dots, 17$ in non empty square depending on accessible values of momentum L and seniority λ. Degeneracy $d_{\lambda L}$ is given by formula $d_{\lambda L} = \mu_{\max} - \mu_{\min} + 1$.

L, λ	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
0	0			1			2			3			4			5		
1																		
2		0	0		1	1		2	2		3	3		4	4		5	5
3				0			1			2			3			4		
4			0	0	0	1	1	1	2	2	2	3	3	3	4	4	4	5
5					0	0		1	1		2	2		3	3		4	4
6				0	0	0	0,1	1	1	1,2	2	2	2,3	3	3	3,4	4	4
7						0	0	0	1	1	1	2	2	2	3	3	3	4
8					0	0	0	0,1	0,1	1	1,2	1,2	2	2,3	2,3	3	3,4	3,4
9							0	0	0	0,1	1	1	1,2	2	2	2,3	3	3
10						0	0	0	0,1	0,1	0,1	1,2	1,2	1,2	2,3	2,3	2,3	3,4
11								0	0	0	0,1	0,1	1	1,2	1,2	2	2,3	2,3
12							0	0	0	0,1	0,1	0,1	0,1,2	1,2	1,2	1,2,3	2,3	2,3
13									0	0	0	0,1	0,1	0,1	1,2	1,2	1,2	2,3
14								0	0	0	0,1	0,1	0,1	0,1,2	0,1,2	1,2	1,2,3	1,2,3
15										0	0	0	0,1	0,1	0,1	0,1,2	1,2	1,2
16									0	0	0	0,1	0,1	0,1	0,1,2	0,1,2	0,1,2	1,2,3
17											0	0	0	0,1	0,1	0,1	0,1,2	0,1,2

The range of accessible values of μ at given accessible λ and L is determined by inequalities:

$$\mu_{\min} = \max(0, \texttt{Ceiling}\left(\frac{\lambda - L}{3}\right), \ \mu_{\max} = \texttt{Floor}\left(\frac{\lambda - (L + 3(L\bmod 2))/2}{3}\right), \quad (40)$$

where $\texttt{Ceiling}(\mu)$ is the lowest integer not lower that μ and $\texttt{Floor}(\mu)$ is the largest integer not greater that μ. The multiplicity $d_{\lambda L}$ is given by the value of $d_{\lambda L} = \mu_{\max} - \mu_{\min} + 1$. For example, the set of accessible values μ at the given accessible λ and L of states $|\lambda\mu LL\rangle$ is given in Tables 2 and 3. One can see that there is no degeneracy $d_{vL} = 1$ for the first few angular momenta L=0, 2, 3, 4, 5, 7, but not for L=6: $d_{\lambda L} = 2$. The range of angular moment L that corresponds to a given maximum d_{vL}^{max} of μ-degeneracy d_{vL} is [10]

$$6(d_{\lambda L}^{max} - 1) \leq L \leq 6(d_{\lambda L}^{max} - 1) + 5, \; d_{\lambda L}^{max} = 1, 2, \ldots.$$

For example, see Tables 2 and 3: $0 \leq L \leq 5$, $d_{\lambda L}^{max} = 1$, $6 \leq L \leq 11$, $d_{\lambda L}^{max} = 2$, $12 \leq L \leq 17$, $d_{\lambda L}^{max} = 3$.

Table 3. Continuation of Table 2 for $L = 0, \ldots, 17$ and $\lambda = 18, \ldots, 34$

L, λ	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34
0	6			7			8			9			10			11	
1																	
2		6	6		7	7		8	8		9	9		10	10		11
3	5			6			7			8			9			10	
4	5	5	6	6	6	7	7	7	8	8	8	9	9	9	10	10	10
5		5	5		6	6		7	7		8	8		9	9		10
6	4,5	5	5	5,6	6	6	6,7	7	7	7,8	8	8	8,9	9	9	9,10	10
7	4	4	5	5	5	6	6	6	7	7	7	8	8	8	9	9	9
8	4	4,5	4,5	5	5,6	5,6	6	6,7	6,7	7	7,8	7,8	8	8,9	8,9	9	9,10
9	3,4	4	4	4,5	5	5	5,6	6	6	6,7	7	7	7,8	8	8	8,9	9
10	3,4	3,4	4,5	4,5	4,5	5,6	5,6	5,6	6,7	6,7	6,7	7,8	7,8	7,8	8,9	8 9	8,9
11	3	3,4	3,4	4	4,5	4,5	5	5,6	5,6	6	6,7	6,7	7	7,8	7,8	8	8,9
12	2,3,4	3,4	3,4	3,4,5	4,5	4,5	4,5,6	5,6	5,6	5,6,7	6,7	6,7	6,7,8	7,8	7,8	7,8,9	8,9
13	2,3	2,3	3,4	3,4	3,4	4,5	4,5	4,5	5,6	5,6	5,6	6,7	6,7	6,7	7,8	7,8	7,8
14	2,3	2,3,4	2,3,4	3,4	3,4,5	3,4,5	4,5	4,5,6	4,5,6	5,6	5,6,7	5,6,7	6,7	6,7,8	6,7,8	7,8	7,8,9
15	1,2,3	2,3	2,3	2,3,4	3,4	3,4	3,4,5	4,5	4,5	4,5,6	5,6	5,6	5,6,7	6,7	6,7	6,7,8	7,8
16	1,2,3	1,2,3	2,3,4	2,3,4	2,3,4	3,4,5	3,4,5	3,4,5	4,5,6	4,5,6	4,5,6	5,6,7	5,6,7	5,6,7	6,7,8	6,7,8	6,7,8
17	1,2	1,2,3	1,2,3	2,3	2,3,4	2,3,4	3,4	3,4,5	3,4,5	4,5	4,5,6	4,5,6	5,6	5,6,7	5,6,7	6,7	6,7,8

As conclusion of this analysis, we get the non-orthogonal basis for the totally symmetric IRs of the group O(5) which is denoted by four quantum numbers λ, μ, L, M

$$|\lambda\mu LM\rangle_{no} = \sum_{L \leq m \leq 2\lambda} \beta_m(\lambda, L)(L_-)^{m-M}(L_+)^{m+\lambda-3\mu}(\eta_{-1})^{\lambda-\mu}(\eta_2)^{\mu}|0\rangle, \quad (41)$$

where λ denotes the seniority number, μ can be interpreted as the maximal number of boson triplets coupled to the angular momentum $L = 0$.

These results can be rewritten in representation (15) of elementary boson basis of symmetric IRs group U(5) from Subsect. 2.1 at $l = 2$. For this purpose, let us assume that the third component of the angular momentum has its maximal value $M = L$

$$|\lambda\mu L\; M = L\rangle = \sum_{n_{-2}\ldots n_2} \langle n_{-2}\, n_{-1} \ldots n_2 | \lambda\mu L\; M = L\rangle_{no} |n_{-2} \ldots n_2\rangle. \quad (42)$$

Here the vectors $\langle n'_{-2}\dots n'_2|\lambda\mu' LM = L\rangle_{no}$ in the representation of the five-dimensional harmonic oscillator $\langle n'_{-2}\dots n'_2|$ have the form

$$\langle n_{-2}\dots n_2|\lambda\mu LM = L\rangle{=}(2L+1)\sqrt{\frac{6^{n_0}\,(n_{-2})!\,(n_{-1})!\dots(n_2)!\,(2L)!}{(L+\lambda-3\mu)!\,(L{-}\lambda{+}3\mu)!}} \tag{43}$$
$$\times\sum_{p_1\dots p_8\;q_1\dots q_5}(-1)^{p_1+p_3+p_5+p_7+q_2+q_4}\;2^{p_1+2p_3+2p_6+p_8+q_2+q_4}$$
$$\times\frac{(\lambda{-}\mu)!\;\mu!\;(p_2{+}p_3{+}2p_5{+}2p_6{+}2p_7{+}3p_8)!\;(p_2{+}p_6{+}p_8{+}q_2{+}2q_3{+}3q_4{+}4q_5)!}{(p_1)!\,(p_2)!\dots(p_8)!\,(q_1)!\,(q_2)!\dots(q_5)!\,(L+2\lambda-p_4-p_5+1)!},$$

where the following conditions are satisfied

$$\sum_i n_i=\lambda,\quad \sum_i in_i=L,\quad \sum_i p_i=\lambda-\mu,\quad \sum_i q_i=\mu, \tag{44}$$
$$p_1{+}q_1{=}n_{-2},\;\; p_3{+}p_4{+}q_2{=}n_{-1},\;\; p_2{+}p_7{+}q_3{=}n_0,\;\; p_5{+}p_6{+}q_4{=}n_1,\;\; p_8{+}q_5{=}n_2.$$

Vectors $\langle n_{-2}\dots n_2|\lambda\mu LM\rangle$ at $-L{\le}M{<}L$ are calculated from recurrence relations

$$\begin{aligned}&\langle n_{-2}\dots n_2|\lambda\mu LM-1\rangle=((L{-}M{+}1)(L{+}M))^{-1/2}\langle n_{-2}\dots n_2|\hat{L}_-|\lambda\mu LM\rangle=\\&((L{-}M{+}1)(L{+}M))^{-1/2}\Big[2\sqrt{n_{-2}(n_{-1}{+}1)}\langle n_{-2}{-}1,n_{-1}{+}1,n_0,n_1,n_2|\lambda\mu LM\rangle\\&+\sqrt{6n_{-1}(n_0{+}1)}\langle n_{-2},n_{-1}{-}1,n_0{+}1,n_1,n_2|\lambda\mu LM\rangle\\&+\sqrt{6n_0(n_1{+}1)}\langle n_{-2},n_{-1},n_0{-}1,n_1{+}1,n_2|\lambda\mu LM\rangle\\&+2\sqrt{n_1(n_2{+}1)}\langle n_{-2},n_{-1},n_0,n_1{-}1,n_2{+}1|\lambda\mu LM\rangle\Big],\end{aligned} \tag{45}$$

where summation is performed over $n_i\ge 0$ subjected to the following conditions: $\sum_i n_i=\lambda, \sum_i in_i=M$.

Calculating the above coefficients one gets the vectors of the non-orthogonal basis for the totally symmetric IRs of the group O(5) which is denoted by four quantum numbers λ, μ, L, M for given λ:

$$|\lambda\lambda\mu LM\rangle=\sum_{n_{-2}\dots n_2}\langle n_{-2}\dots n_2|\lambda\lambda\mu LM\rangle|n_{-2}\dots n_2\rangle. \tag{46}$$

2.6 Basis of IRs for Groups O(5) ⊗ SU(1,1)

In this part, we construct the states with an arbitrary number of bosons equal to N, greater than seniority number $N>\lambda$. At this point, we use the construction described in Sect. 2.4. By using Eq. (29) for $l=2$ one gets

$$|\lambda N\mu LM\rangle=\sqrt{\frac{2^{\frac{N-\lambda}{2}}(2\lambda+3)!!}{\left(\frac{N-\lambda}{2}\right)!\,(N+\lambda+3)!!}}(S_+)^{\frac{N-\lambda}{2}}|\lambda\mu LM\rangle, \tag{47}$$

where $(N-\lambda)/2 = 1, 2, \dots$ is integer. Next we can rewrite operator $(S_+)^{\frac{N-\lambda}{2}}$ in a polynomial form:

$$
\begin{aligned}
(S_+)^{\frac{N-\lambda}{2}} &= \left(\eta_{-2}\eta_2 - \eta_{-1}\eta_1 + \frac{1}{2}\eta_0\eta_0\right)^{\frac{N-\lambda}{2}} \\
&= \sum_{k_1k_2k_3} (-1)^{k_2} \left(\frac{1}{2}\right)^{k_3} \binom{\frac{N-\lambda}{2}}{k_1k_2k_3} (\eta_{-2}\eta_2)^{k_1} (\eta_{-1}\eta_1)^{k_2} (\eta_0)^{2k_3}, \\
\binom{k}{k_1\dots k_N} &= \delta^k_{\sum_{i=1}^N k_i} \frac{k!}{k_1!\dots k_N!}.
\end{aligned}
$$

After easy transformations one gets

$$
\begin{aligned}
&\langle n_{-2}\dots n_2|\lambda N\mu LM\rangle = \sqrt{\frac{2^{\frac{N-\lambda}{2}}(2\lambda+3)!!}{\left(\frac{N-\lambda}{2}\right)!\,(N+\lambda+3)!!}} \\
&\times \sum_{k_1k_2k_3} \frac{(-1)^{k_2}}{2^{k_3}} \binom{\frac{N-\lambda}{2}}{k_1k_2k_3} \sqrt{\frac{n_{-2}!\,n_{-1}!\,n_0!\,n_1!\,n_2!}{(n_{-2}-k_1)!(n_{-1}-k_2)!(n_0-2k_3)!(n_1-k_2)!(n_2-k_1)!}} \\
&\times \langle n_{-2}-k_1,\, n_{-1}-k_2,\, n_0-2k_3,\, n_1-k_2,\, n_2-k_1|\lambda\mu LM\rangle. \qquad (48)
\end{aligned}
$$

Calculating the above coefficients one gets the vectors of the non-orthogonal symmetric basis of IRs of the group O(5) $\otimes$ SU(1,1) which is denoted by five quantum numbers λ, N, μ, L, and M for given λ and N:

$$
|\lambda N\mu LM\rangle = \sum_{n_{-2}\dots n_2} \langle n_{-2}\dots n_2|\lambda N\mu LM\rangle |n_{-2}\dots n_2\rangle, \qquad (49)
$$

$$
\Psi^{\text{lab}}_{\lambda N\mu LM}(\alpha_m) = \sum_{n_{-2}\dots n_2} \langle \alpha_m|n_{-2}\dots n_2\rangle \langle n_{-2}\dots n_2|\lambda N\mu LM\rangle, \qquad (50)
$$

where $\langle \alpha_m|n_{-2}\dots n_2\rangle$ is the orthonormal basis from (15) $\langle n_{-2}\dots n_2|n'_{-2}\dots n'_2\rangle$ $=\delta_{n_{-2}n'_{-2}}\dots\delta_{n_2n'_2}$, the following conditions are fulfilled: $\sum_i n_i = N$, $\sum_i in_i = M$. The effective algorithm for calculation of the required orthonormal basis is given in Sect. 4.

3 Nonorthogonal Basis of the IRs $\overline{\text{O(5)}} \times \overline{\text{SU(1,1)}}$ Group in the Intrinsic Frame

The collective variables α_m at $m = -2, -1, 0, 1, 2$ in the laboratory frame are expressed through variables $a_{m'} = a_{m'}(\beta, \gamma)$ in the intrinsic frame by the relations

$$
\alpha_m = \sum_{m'} D^{2*}_{mm'}(\Omega) a_{m'},\; a_{-2} = a_2 = \beta\sin\gamma/\sqrt{2},\; a_{-1} = a_1 = 0,\; a_0 = \beta\cos\gamma, \qquad (51)
$$

where $D^{2*}_{mm'}(\Omega)$ is the Wigner function of IRs of $\overline{\text{O(3)}}$ group in the intrinsic frame [24] (marker * is complex conjugate). The five-dimensional equation of the

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

$$\{H^{(BM)}{-}E^{BM}_n\}\Psi_{\lambda N\mu LM}{=}0,\ H^{(BM)}{=}\frac{1}{2}\left(-\frac{1}{\beta^4}\frac{\partial}{\partial\beta}\beta^4\frac{\partial}{\partial\beta}{+}\frac{\hat{\Lambda}^2}{\beta^2}{+}\beta^2\right). \quad (52)$$

Here $E^{BM}_N = (N+\frac{5}{2})$ are eigenvalues, $\hat{\Lambda}^2$ is the quadratic Casimir operator of $\overline{\text{O(5)}}$ in $L_2(S^4(\gamma,\Omega))$ at nonnegative integers $N = 2n_\beta + \lambda$, i.e., at even and nonnegative integers $N - \lambda$ determined as

$$(\hat{\Lambda}^2{-}\lambda(\lambda{+}3))\Psi_{\lambda N\mu LM}{=}0, \hat{\Lambda}^2{=}{-}\frac{1}{\sin(3\gamma)}\frac{\partial}{\partial\gamma}\sin(3\gamma)\frac{\partial}{\partial\gamma}{+}\sum_{k=1}^{3}\frac{(\hat{\bar{L}}_k)^2}{4\sin^2(\gamma{-}\frac{2}{3}k\pi)}, \quad (53)$$

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

Eigenfunctions $\Psi^{int}_{\lambda N\mu LM}$ of the five-dimensional oscillator have the form

$$\Psi^{int}_{\lambda N\mu LM}(\beta,\gamma,\Omega){=}\sum_{Keven}\Phi^{int}_{\lambda N\mu LK}(\beta,\gamma)\mathcal{D}^{(L)*}_{MK}(\Omega), \quad (54)$$

where $\Phi^{int}_{\lambda N\mu LK}(\beta,\gamma){=}F_{N\lambda}(\beta)C^{\lambda\mu}_L\hat{\phi}^{\lambda\mu L}_K(\gamma)$ are the components in the intrinsic frame, $\mathcal{D}^{(L)*}_{MK}(\Omega) = \sqrt{\frac{2L+1}{8\pi^2}}\frac{D^{(L)*}_{MK}(\Omega)+(-1)^L D^{(L)*}_{M,-K}(\Omega)}{1+\delta_{K0}}$ are the orthonormal Wigner functions with measure $d\Omega$, summation over K runs even values K in range:

$$K = 0, 2, \ldots, L \ \text{ for even integer } L : 0 \le L \le L_{max}, \quad (55)$$
$$K = 2, \ldots, L-1 \ \text{ for odd integer } L : 3 \le L \le L_{max}.$$

The orthonormal components $F_{N\lambda}(\beta) \in L_2(R^1_+)$ corresponding to reduced functions $\beta^{-2}\mathfrak{F}_{N\lambda}(\beta)$ with measure $d\beta$ of IRs of $\overline{\text{SU(1,1)}}$ group [25] are as follows:

$$F_{N\lambda}(\beta){=}\sqrt{\frac{2(\frac{1}{2}(N{-}\lambda))!}{\Gamma(\frac{1}{2}(N{+}\lambda{+}5))}}\beta^\lambda L^{\lambda+\frac{3}{2}}_{(N-\lambda)/2}(\beta^2)\exp\Big(-\frac{1}{2}\beta^2\Big), \quad (56)$$

where $L^{\lambda+\frac{3}{2}}_{(N-\lambda)/2}(\beta^2)$ is the associated Laguerre polynomial with the number of nodes $n_\beta = (N-\lambda)/2$ [26]. The overlap of the eigenfunctions (54) characterized their nonorthogonality with respect to the missing label μ reads as

$$\langle\Psi^{int}_{\lambda N\mu LM}|\Psi^{int}_{\lambda' N'\mu' L'M'}\rangle = \int d\tau \Psi^{int*}_{\lambda N\mu LM}(\beta,\gamma,\Omega)\Psi^{int}_{\lambda N\mu LM}(\beta,\gamma,\Omega) \quad (57)$$
$$={\delta_{N,N'}\delta_{\lambda,\lambda'}\delta_{L,L'}\delta_{M,M'}}\langle\phi^{\lambda\mu L}|\phi^{\lambda\mu' L}\rangle,$$

where $\langle\phi^{\lambda\mu L}|\phi^{\lambda\mu' L}\rangle$ is the reduced overlap: scalar product with integration by γ

$$\langle\phi^{\lambda\mu L}|\phi^{\lambda\mu' L}\rangle = C^{\lambda\mu}_L C^{\lambda\mu'}_L \int_0^\pi d\gamma \sin(3\gamma)\sum\nolimits_{Keven}\frac{2(\hat{\phi}^{\lambda\mu L}_K(\gamma)\hat{\phi}^{\lambda\mu' L}_K(\gamma))}{1+\delta_{K0}}, \quad (58)$$

and $C_L^{\lambda\mu}$ is the corresponding normalization factor of $\phi_K^{\lambda\mu L}(\gamma) = C_L^{\lambda\mu}\hat{\phi}_K^{\lambda\mu L}(\gamma)$

$$(C_L^{\lambda\mu})^{-2}=\int_0^\pi d\gamma \sin(3\gamma) \sum_{K\mathrm{even}} \frac{2(\hat{\phi}_K^{\lambda\mu L}(\gamma))^2}{1+\delta_{K0}}. \tag{59}$$

The reduced Wigner coefficients in the chain $\overline{\mathrm{O}(5)} \supset \overline{\mathrm{O}(3)}$ read as [13]

$$(\lambda\mu L, \lambda'\mu' L', \lambda\mu L'')=\int_0^\pi d\gamma \sin(3\gamma) \sum_{KK'K''} (-1)^{L-L'}(L, L', K, K'|L'', -K'') \times\phi_K^{\lambda\mu L}(\gamma)\phi_{K'}^{\lambda'\mu' L'}(\gamma)\phi_{K'}^{\lambda'\mu' L'}(\gamma), \tag{60}$$

where $\phi_K^{\lambda\mu L}(\gamma)$ are the orthonormalized eigenfunctions calculated in the section 4 with respect to the overlap (58)corresponds to the orthonormalized eigenfunctions (54) with respect to the overlap (57) with the set of quantum numbers λ, μ, L, and M.

The components $\hat{\phi}_K^{\lambda\mu L}(\gamma)=(-1)^L\hat{\phi}_{-K}^{\lambda\mu L}(\gamma)$ for even K and $\hat{\phi}_K^{\lambda\mu L}(\gamma) = 0$ for odd L and $K = 0$ as well as for odd K are determined below according to [5–7,12]. It should be noted that for these components, $L \neq 1$, $|K| \leq L$ for $L =$ even and $|K| \leq L-1$ for $L =$ odd:

$$\hat{\phi}_K^{\lambda\mu L}(\gamma)=\sum_{n=0}^{n_{\max}} F_{n\lambda L}^{\sigma\tau\mu}(\gamma)\left[G_{|K|}^{nL}(\gamma)\delta_{L,\mathrm{even}} + \bar{G}_{|K|}^{nL}(\gamma)\delta_{L,\mathrm{odd}}\right]; \tag{61}$$

$$K = K_{\min}, K_{\min}+2, \ldots, K_{\max};$$

$$K_{\min} = \begin{cases} 0\ , L = \mathrm{even}, \\ 2\ , L = \mathrm{odd}; \end{cases} \quad K_{\max} = \begin{cases} L \quad\ \ , L = \mathrm{even}, \\ L-1\ , L = \mathrm{odd}; \end{cases}$$

$$n_{\max} = \begin{cases} L/2 \qquad\quad , L = \mathrm{even}, \\ (L-3)/2\ , L = \mathrm{odd}; \end{cases}$$

$$\delta_{L,\mathrm{even}} = \begin{cases} 1\ , L = \mathrm{even}, \\ 0\ , L = \mathrm{odd}; \end{cases} \quad \delta_{L,\mathrm{odd}} = \begin{cases} 0\ , L = \mathrm{even}, \\ 1\ , L = \mathrm{odd}; \end{cases}$$

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

$$\bar{G}_K^{nL}(\gamma)=\sum_{k=3-L,2}^{L-3} \langle L-3, 3, k, K-k|LK\rangle G_{|k|}^{nL-3}(\gamma)\sin 3\gamma(\delta_{K-k,2}-\delta_{K-k,-2}); \tag{62}$$

$$G_K^{nL}(\gamma)=(-\sqrt{2})^n \sum_{k=2n-L,2}^{L-2n} \langle L-2n, 2n, k, K-k|LK\rangle S_{|k|}^{(L-2n)/2}(\gamma)S_{|K-k|}^{n}(-2\gamma); \tag{63}$$

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

$$F^{\sigma\tau\mu}_{n\lambda L}(\gamma) = (-1)^{\mu+\tau-n}2^{-n/2}\sum_{r=0}^{[(\mu+\tau-n)/2]} C^{\sigma\tau\mu}_{rn\lambda L}2^{-r}(\cos 3\gamma)^{\mu+\tau-n-2r}; \qquad (64)$$

$$\tau = \begin{cases} \lambda-3\mu-L/2 & , L=\text{even}, \\ \lambda-3-3\mu-(L-3)/2 & , L=\text{odd}. \end{cases} \quad \sigma = L-\lambda+3\mu;$$
$$C^{\sigma\tau\mu}_{rn\lambda L} = \frac{3^n\sigma!\lambda!(-1)^r 2^r(2\mu+2\tau-2r+\delta_{L,\text{odd}})!(3r)!}{2^{\mu+n}n!(2\lambda+1)!r!(\mu+\tau-r)!(\mu+\tau-n-2r)!} \qquad (65)$$
$$\times \sum_{s=\max(n-\tau,0)}^{\min(\sigma,\lambda,3r-\tau+n)} \frac{(-1)^s4^s(\tau+s)!(2\lambda+1-2s)!}{s!(\sigma-s)!(\tau-n+s)!(3r-\tau+n-s)!(\lambda-s)!};$$

where $S^r_K(\gamma)$ is taken to be equal 0, if $\sin 3\gamma{=}0$ or $\cos 3\gamma{=}0$, $F^{\sigma\tau\mu}_{n\lambda L}(\gamma)$ 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 $\mu{+}\tau{-}n{-}2r{<}0$.

For example, at $\lambda = 3\mu$ and $L = 0, M = 0$, and $\lambda = 3\mu{+}3$ and $L = 3, M = 3$, the eigenfunctions are known:

$$\Psi_{\lambda N\mu LM}(\beta,\gamma,\Omega) = C^0_\mu\beta^{3\mu}\exp(-\beta^2/2)P_\mu(\cos(3\gamma)), \qquad (66)$$

$$\Psi_{\lambda N\mu LM}(\beta,\gamma,\Omega){=}C^3_\mu\beta^{3\mu+3}\exp(-\beta^2/2)P^1_{\mu+1}(\cos(3\gamma))(D^{(3)*}_{32}(\Omega){-}D^{(3)*}_{3,-2}(\Omega)),$$

where $P^1_{\mu+1}(\cos(3\gamma))$ are associated Legendre polynomials [26].

The eigenfunctions $\Psi_{\lambda N\mu LM}(\beta,\gamma,\Omega)$ at $L{\le}6$ were calculated in [27,28]. However, for calculation of the required orthogonal basis including large values of λ and L for large-scale calculations of eigenvalue BM problem (52) for Hamiltonian $\mathcal{H}{=}H^{BM}(\beta,\gamma,\Omega){+}V(\beta,\gamma){+}\mathcal{K}(\beta,\gamma)$ with potential function $V(\beta,\gamma)$ and additional kinetic function $\mathcal{K}(\beta,\gamma)$ determined in [5,7,10,11], one needs to have a fast algorithm for calculation and orthonormalization of nonorthogonal eigenfunctions $\Psi_{\lambda N\mu LM}(\beta,\gamma,\Omega)$ from (54) at accessible degeneracy characterized by the missing label $\mu_{\min} \le \mu \le \mu_{\max}$ from (40) and also Tables 2 and 3. The effective algorithm for calculation of the required orthonormal basis is given in the Sect. 4.

4 Algorithm and Benchmark Calculations of Overlaps and Orthogonalization Matrices

In the laboratory frame, the overlaps $\langle\hat u_\mu|\hat u_{\mu'}\rangle{\equiv}\langle\lambda N\mu LM|\lambda N\mu' LM\rangle$ are calculated by the formula

$$\langle\hat u_\mu|\hat u_{\mu'}\rangle{=}\sum_{n'_{-2}\ldots n'_2}\langle\lambda N\mu LM|n'_{-2}\ldots n'_2\rangle\langle n'_{-2}\ldots n'_2|\lambda N\mu' LM\rangle. \qquad (67)$$

Here vectors $\langle\alpha_m|\hat u_{\mu'}\rangle{=}\langle\alpha_m|\lambda N\mu' LM\rangle$ in the representation of the orthonormal basis $\langle n'_{-2}\ldots n'_2|$ of the five-dimensional harmonic oscillator (15) are determined by Eqs. (49) and (50) through the unnormalized and non-orthogonal μ' components $\langle n'_{-2}\ldots n'_2|\lambda N\mu' LM\rangle$ of the reduced vectors $|\hat{u}'_{\mu}\rangle$ from Eqs. (43, 45, 48).

In the intrinsic frame, the overlap $\langle \hat{u}_{\mu}|\hat{u}_{\mu'}\rangle \equiv \langle \lambda N\mu LM|\lambda N\mu' LM\rangle$ reads as:

$$\langle \hat{u}_{\mu}|\hat{u}_{\mu'}\rangle = \int_0^{\pi} \sin(3\gamma)d\gamma \sum_{K\geq 0, even} \frac{2\hat{\phi}_K^{\lambda\mu L}(\gamma)\hat{\phi}_K^{\lambda\mu' L}(\gamma)}{1+\delta_{K0}}. \tag{68}$$

Here vectors $\langle \beta,\gamma,\Omega|\hat{u}_{\mu'}\rangle = \langle \beta,\gamma,\Omega|\lambda N\mu' LM\rangle$ in the representation of the orthonormal Wigner functions $\mathcal{D}_{MK}^{(L)*}(\Omega)$ and components $F_{N\lambda}(\beta)$ are determined by Eqs. (54)-(59) through the unnormalized and non-orthogonal by μ' components $\hat{\phi}_K^{\lambda\mu' L}(\gamma)$ of the reduced vectors $|\hat{u}_{\mu'}\rangle = \langle \gamma|\hat{\phi}^{\lambda\mu' L}\rangle$ from (61)–(65).

The numerical calculations performed in the program `SO5U11` use the floating-point arithmetics. In this case, we use instead of the unnormalized nonorthogonal $|\hat{u}_{\mu}\rangle$ the normalized but nonorthogonal eigenvectors $|u_{\mu}\rangle$:

$$|u_{\mu}\rangle = \hat{N}_{\mu\mu}^{-1}|\hat{u}_{\mu}\rangle,\ \hat{N}_{\mu\mu} = (\langle \hat{u}_{\mu}|\hat{u}_{\mu}\rangle)^{1/2}\ , \tag{69}$$

where the normalization matrix is equal to $\hat{N}_{\mu\mu'} = \hat{N}_{\mu\mu}\delta_{\mu\mu'}$, and the normalized overlaps are

$$\langle u_{\mu}|u_{\mu'}\rangle = \langle \hat{u}_{\mu}|\hat{N}_{\mu\mu}^{-1}\hat{N}_{\mu'\mu'}^{-1}|\hat{u}_{\mu'}\rangle,\ \langle u_{\mu}|u_{\mu}\rangle = 1. \tag{70}$$

We orthonormalize these normalized nonorthogonal BM states $|u_{\mu}\rangle$:

$$|\phi_{\mu}\rangle = \sum_{\mu'=\mu_{\min}}^{\mu_{\max}} |u_{\mu'}\rangle A_{\mu',\mu} = \sum_{\mu'=\mu_{\min}}^{\mu_{\max}} |\hat{u}_{\mu'}\rangle \hat{A}_{\mu',\mu}, \qquad \mathbf{A} = \hat{\mathbf{N}}\hat{\mathbf{A}}. \tag{71}$$

Below the hat symbol over some vectors and matrices is used to label calculations with unnormalized BM vectors. The symbols $A_{\mu',\mu}$ denote the matrix elements of the upper triangular matrix of the BM basis orthonormalization coefficients. These coefficients satisfy the following condition

$$A_{\mu',\mu} = 0, \quad \text{if } \mu' > \mu, \quad \mu,\mu' = \mu_{\min},\ldots,\mu_{\max}. \tag{72}$$

The matrix $\mathbf{A}$ is constructed to satisfy the orthonormalization conditions

$$\langle \phi_{\mu}|\phi_{\mu'}\rangle = \delta_{\mu\mu'},\ \sum_{i',k'=1}^{d_{\lambda L}} A_{i',i}\langle u_{i'}|u_{k'}\rangle A_{k',k} = \delta_{i,k},\ \langle u_i|u_{k'}\rangle = \sum_{k'=1}^{d_{\lambda L}} A_{k',i}^{-1}A_{k',k}^{-1}. \tag{73}$$

Here the multiplicity index i or internal index $k,k' = 1,\ldots,d_{\lambda L}$ is recalculated by formula $d_{\lambda L} = \mu_{\max} - \mu_{\min} + 1$ to external index $\mu,\mu' = \mu_{\min},\ldots,\mu_{\max}$ and vice versa was introduced to distinguish the orthonormalized BM states at given values of quantum numbers λ, N, L, M and takes the same number of values as μ. Note the last relation in (73) is a decomposition of the overlap matrix to a product of the low and upper triangular inverse matrices $(\mathbf{A}^{-1})^T\mathbf{A}^{-1}$.

Table 4. *Algorithm* for calculation of elements of the upper triangular matrix $A_{\mu,\mu'}$ which is used for the generation of an orthonormal basis $|\phi_\mu\rangle = \sum_{\mu'=\mu_{\min}}^{\mu_{\max}} |u_{\mu'}\rangle A_{\mu',\mu}$ starting from $|u_{\mu_{\min}}\rangle$ till $|u_{\mu_{\max}}\rangle$, where the external index $\mu, \mu' = \mu_{\min}, \ldots, \mu_{\max}$ is recalculated by formula $k = \mu - \mu_{\min} + 1$ to internal index $k, k' = 1, \ldots, d_{\lambda L}$, $d_{\lambda L} = \mu_{\max} - \mu_{\min} + 1$ and vice versa

Input:	Overlap matrix $\langle u_k \| u_{k'}\rangle$;	
Output:	Orthogonalization of the upper triangular matrix $A_{k',k}$;	
1.1	$A_{k',k} = \delta_{k'k}, \quad k = 1, \ldots, d_{\lambda L}, k' = k, \ldots, d_{\lambda L}$;	
1.2	$f_{k,k'} = \langle u_k \| u_{k'}\rangle, \quad k = 1, \ldots, d_{\lambda L}, k' = k, \ldots, d_{\lambda L}$;	
	for $n = 1$ to $d_{\lambda L}$ do	
2.1	$u_k = -f_{k,n}/f_{k,k}, \ k = 1, \ldots, n-1$;	$u_k \equiv u_{k,n}$;
2.2	$f_{n,n} = f_{n,n} + \sum_{k=1}^{n-1} u_k^2 f_{k,k} + 2\sum_{k=1}^{n-1} u_k f_{k,n}$;	
2.3	$f_{n,k} = f_{n,k} + \sum_{k'=1}^{n-1} u_{k'} f_{k',k}, \quad k = n+1, \ldots, d_{vL}$;	
2.4	$A_{k,n} = \sum_{k'=k}^{n-1} A_{k,k'} u_{k'}, \quad k = 1, \ldots, n-1$;	
	end for	
3.1	$A_{k',k} = A_{k',k}/\sqrt{f_{kk}}, \quad k = 1, \ldots, n, k' = 1, \ldots, k$;	
test:	$\sum_{n',k'=1}^{d_{\lambda L}} A_{n',n} \langle u_{n'} \| u_{k'}\rangle A_{k',k} = \delta_{n,k}$	

Below we present the analytical orthonormalization algorithm (see Table 4) based on the G-S orthonormalization procedure of a set of non-orthogonal linear independent vectors: $\hat{u}_1, \ldots, \hat{u}_{i_{max}}$ unnormalized or $u_1, \ldots, u_{i_{max}}$ normalized [29]

$$\hat{\phi}_i = u_i - \frac{\langle \hat{\phi}_1 | u_i \rangle}{\langle u_1 | u_1 \rangle} - \cdots - \frac{\langle \hat{\phi}_{i-1} | u_i \rangle}{\langle u_{i-1} | u_{i-1} \rangle}, \ i = 1, \ldots, i_{\max}. \tag{74}$$

Here for the intrinsic frame, the scalar product $\langle \hat{\phi}_i | \hat{\phi}_i \rangle$ is determined by (68) while for laboratory frame $\langle \hat{\phi}_i | \hat{\phi}_i \rangle = \hat{\phi}_i^T \hat{\phi}_i$. After calculation of a set of orthogonal but as yet *unnormalized* vectors $\hat{\phi}_i$ starting from $i = 1$ till $i_{\max}$, one calculates the set of orthogonal and *normalized* vectors ϕ_i: $\phi_i = \hat{\phi}_i / \sqrt{\langle \hat{\phi}_i | \hat{\phi}_i \rangle}$ at $i = 1, \ldots, i_{\max}$. It is important that here the normalization of calculated orthogonal *unnormalized* vectors $\hat{\phi}_i$ is realized after orthogonalization with respect to conventional realization G-S procedure [30]. It gives important possibility to avoid the source of numerical round-off errors in floating-point calculations or if necessary to use the integer arithmetic or symbolic calculations of the recursive algorithm given below. The essential part of the proposed algorithm consists in factorization of the recursive relations (74) by extracting the required orthogonalization upper triangular matrix $A_{\mu'\mu}$ acting on the initial set of non-orthogonal vectors $|u_{\mu'}\rangle$: $|\phi_\mu\rangle = \sum_{\mu'=\mu_{\min}}^{\mu_{\max}} |u_{\mu'}\rangle A_{\mu',\mu}$. It means that the calculated matrix $A_{\mu'\mu} \equiv A^{lab}_{\mu',\mu}(N, M)$ in the laboratory frame is the same on all components $|u_\mu\rangle = \langle n_{-2}, n_{-1}, n_0, n_1, n_2 | u_\mu \rangle$ of the initial set of the non-orthogonal reduced vectors $|u_{\mu'}\rangle$; action of calculated matrix $A_{\mu'\mu} \equiv A^{int}_{\mu',\mu}(\lambda, N, L, M)$ in the intrinsic frame is the same on all components $\phi_K^{\lambda\mu' L}(\gamma) = C_L^{\lambda\mu'} \hat{\phi}_K^{\lambda\mu' L}(\gamma)$ of the initial set of the non-orthogonal reduced vectors $|u_{\mu'}\rangle = \langle \gamma | \phi^{\lambda\mu' L} \rangle$. The accuracy of its calculation is automatically checked by means of orthogonality relations (73) without preliminary calculation of required orthogonal normalized vectors ϕ_i.

Remark. A direct calculation of the overlap of the orthogonal bases $\Psi^{lab}_{\lambda N\mu LM}(\alpha_m)$ in the laboratory frame (50) and $\Phi^{int}_{\lambda N\mu LK}(\beta,\gamma)$ in the intrinsic frame (54) is the tutorial task. Using Eq. (1.16) of Ref. [7] one can check that the following relations hold:

$$\Psi^{lab}_{\lambda N\mu LM}(\alpha_m) = \sum_{K=0,even}^{L} \Phi^{int}_{\lambda N\mu LK}(\beta,\gamma)\mathcal{D}^{L*}_{MK}(\Omega), \tag{75}$$

$$\Phi^{int}_{\lambda N\mu LK}(\beta,\gamma) = \sum_{M=0}^{L} \Psi^{lab}_{\lambda N\mu LM}(\alpha_m)\mathcal{D}^{L}_{MK}(\Omega), \tag{76}$$

where the variables α_m in the laboratory frame are expressed through the ones $a_m = a_m(\beta,\gamma)$ in the intrinsic frame by relations (51).

The presented Algorithm (see Table 4) can be realized in any Computer Algebra System. It has been realized here as the function `NormOverlapa` of the first version of `O5SU11` code implemented in Mathematica 11.1 [31].

```
NormOverlapa[Overlap_] :=Module[{},
  For[x = 1, x <= Length[Overlap], x++,
    A[x, x]=1;
    For[xx = x, xx <= Length[Overlap], xx++,
      fover[x, xx] = Part[Overlap, x, xx];
    ]
  ];
  For[n = 1, n <= Length[Overlap], n++,
    For[k = 1, k <= n-1, k++,
      ui[k]=-fover[k, n]/fover[k, k];
    ]
    fover[n, n]=fover[n, n]+Sum[ui[k]*ui[k]*fover[k, k],{k,1,n-1}]
       +Sum[2*ui[k]*fover[k, n],{k,1,n-1}];
    For[k = n+1, k <= Length[Overlap], k++,
     fover[n, k]=fover[n, k]+Sum[ui[kk]*fover[kk, k],{kk,1,n-1}];
    ];
    For[k = 1, k <= n-1, k++,
     A[k, n]=Sum[A[k,kk]*ui[kk],{kk,k,n-1}];
    ]
  ];
   Return[
    Table[
     If[x > xx, 0, A[x, xx]/Sqrt[fover[xx, xx]] ]
     , {x, 1,   Length[Overlap]}, {xx, 1, Length[Overlap]}]]
   ];
(*test: *)
    A=NormOverlapa[Overlap]
      Transpose[A]*Overlap*A    (*gives identity matrix*)
```

Below we present benchmark calculations of the overlap matrices $\langle\hat{u}_\mu|\hat{u}_{\mu'}\rangle$ or $\langle u_\mu|u_{\mu'}\rangle$ and orthogonalization matrices $\hat{A}_{\mu'\mu}$ or $A_{\mu'\mu}$ executed with help of the `O5SU11` code.

In the laboratory frame, the unnormalized overlap $\langle\hat{u}_\mu|\hat{u}_{\mu'}\rangle$ from (67) and orthogonalization matrix $\hat{A}_{\mu'\mu}$ from (71) at λ=12, $N = 12$, μ=0, 1, 2, L=12, M=12 are as follows:

$$\langle\hat{u}_\mu|\hat{u}_{\mu'}\rangle=\begin{pmatrix} 159549545.26713809 & 213803.08882591313 & 57637.968478797638 \\ 213803.08882591313 & 4988824.1342315109 & -422776.94375296634 \\ 57637.968478797638 & -422776.94375296634 & 744945.4277113013 \end{pmatrix},$$

$$\hat{A}_{\mu'\mu}=\begin{pmatrix} 0.0000791684632054189660 & -5.999558704952660*10^{-7} & -5.501511852913287*10^{-7} \\ 0 & 0.000447714234829464325 & 0.0000982042323533844462 \\ 0 & 0 & 0.00115861132845170549 \end{pmatrix}.$$

The normalized overlap $\langle u_\mu|u_{\mu'}\rangle_{no}$ from (67) and orthogonalization matrix $A_{\mu'\mu}$ from (71) at λ=12, $N = 12$, μ=0, 1, 2, L=12, M=12:

$$\langle u_\mu|u_{\mu'}\rangle=\begin{pmatrix} 1.0000000000000000000 & 0.00757821796968012826 & 0.00528687022845146168 \\ 0.00757821796968012826 & 1.0000000000000000000 & -0.2193057245440392052 \\ 0.00528687022845146168 & -0.2193057245440392052 & 1.0000000000000000000 \end{pmatrix},$$

$$A_{\mu'\mu}=\begin{pmatrix} 1.0000000000000000000 & -0.00757821796968012826 & -0.00694912043276433934 \\ 0 & 1.0000000000000000000 & 0.2193457895990078230 \\ 0 & 0 & 1.0000000000000000000 \end{pmatrix}.$$

The unnormalized overlap $\langle\hat{u}_\mu|\hat{u}_{\mu'}\rangle$ from (67) and orthogonalization matrix $\hat{A}_{\mu'\mu}$ from (71) at λ=12, N=14, μ=0, 1, 2, L=12, M=12:

$$\langle\hat{u}_\mu|\hat{u}_{\mu'}\rangle=\begin{pmatrix} 4.62693681274700*10^{9} & 6.200289575951*10^{6} & 1.671501085885*10^{6} \\ 6.200289575951*10^{6} & 1.44675899892714*10^{8} & -1.22605313688360*10^{7} \\ 1.671501085885*10^{6} & -1.22605313688360*10^{7} & 2.16034174036277*10^{7} \end{pmatrix},$$

$$\hat{A}_{\mu'\mu}=\begin{pmatrix} 0.0000147012145478877 6 & -1.1140900826293*10^{-7} & -1.021605104012*10^{-7} \\ 0 & 0.0000831384462433374 & 0.0000182360681372795 \\ 0 & 0 & 0.0002151487224526028 \end{pmatrix}.$$

The normalized overlap $\langle u_\mu|u_{\mu'}\rangle_{no}$ from (67) and orthogonalization matrix $A_{\mu'\mu}$ from (71) at λ=12, N=14, μ=0, 1, 2, L=12, M=12:

$$\langle u_\mu|u_{\mu'}\rangle=\begin{pmatrix} 1.0000000000000000000 & 0.00757821796968012826 & 0.00528687022845146168 \\ 0.00757821796968012826 & 1.0000000000000000000 & -0.2193057245440392052 \\ 0.00528687022845146168 & -0.2193057245440392052 & 1.0000000000000000000 \end{pmatrix},$$

$$A_{\mu'\mu}=\begin{pmatrix} 1.0000000000000000000 & -0.00757821796968012826 & -0.00694912043276433934 \\ 0 & 1.0000000000000000000 & 0.2193457895990078230 \\ 0 & 0 & 1.0000000000000000000 \end{pmatrix}.$$

Note that the overlaps $\langle\hat{u}_\mu|\hat{u}_{\mu'}\rangle$ calculated in the laboratory frame and defined by Eqs. (43), (45) at fixed values of λ and L are independent of M, i.e., they are equal for different values of the quantum number M. This is due to the Wigner–Eckart theorem for spherical tensors in respect to SO(3) group. It means that the corresponding orthogonalization matrices $A_{\mu',\mu}$ defined by Eq. (73) at fixed values of λ and L with different values of quantum number M are equal too. These facts give essential optimization of the computer resources in the large-scale calculations with increasing seniority number λ determined by eigenvalues of the Casimir operator of the group O(5), see Table 1 and Eq. (39).

One can see also that the overlaps of orthogonalization matrices at fixed L for the case of $N > \lambda$ differ only by an integer multiplier from the case $N = \lambda$, for example, in the above cases, this multiplier is equal to 29.

In intrinsic frame, the unnormalized overlap $\langle \hat{u}_\mu | \hat{u}_{\mu'} \rangle$ is determined by (68) and orthogonalization matrix $\hat{A}_{\mu'\mu}$ from (71) at λ=6, N=6, μ=0, 1, L=6, with summation over K=0, 2, 4, 6:

$$\langle \hat{u}_\mu | \hat{u}_{\mu'} \rangle = \begin{pmatrix} 7572204\pi/385 & -301113\pi/40040 \\ -301113\pi/40040 & 1699\pi/65065 \end{pmatrix} = \begin{pmatrix} 61789.0401503461 & -23.6257339835260 \\ -23.6257339835260 & 0.0820343643809891 \end{pmatrix},$$

$$\hat{A}_{\mu'\mu} = \begin{pmatrix} 0.004022946671779255 & 0.001334983666487966 \\ 0 & 3.491419967151016 \end{pmatrix}.$$

The following normalized overlap $\langle u_\mu | u_{\mu'} \rangle$ and matrix $A_{\mu'\mu}$ are

$$\langle u_\mu | u_{\mu'} \rangle = \begin{pmatrix} 1.000000000000000 & -0.3318422478360953 \\ -0.3318422478360953, & 1.000000000000000 \end{pmatrix},$$

$$A_{\mu'\mu} = \begin{pmatrix} 1.000000000000000 & 0.3318422478360953 \\ 0 & 1.000000000000000 \end{pmatrix}.$$

The unnormalized overlap $\langle \hat{u}_\mu | \hat{u}_{\mu'} \rangle$ from (68) and the orthogonalization matrix $\hat{A}_{\mu'\mu}$ from (71) at λ=12, N=12, μ=0, 1, 2, L=12, with summation over K=0, 2, ..., 12:

$$\langle \hat{u}_\mu | \hat{u}_{\mu'} \rangle = \begin{pmatrix} 1116847934437.424 & -48516553.06697824 & 7016.562464786226 \\ -48516553.06697824 & 5966.500516763265 & -0.9790521939740782 \\ 7016.562464786226 & -0.9790521939740782 & 0.0008802758859593768 \end{pmatrix},$$

$$\hat{A}_{\mu'\mu} = \begin{pmatrix} 9.462436483745545e-7 & 5.623880080711865e-7 & -4.629117698040114e-8 \\ 0 & 0.01294613581264879 & 0.003808823740956861 \\ 0 & 0 & 33.70471020973709 \end{pmatrix}.$$

The following normalized overlap $\langle u_\mu | u_{\mu'} \rangle$ and matrix $A_{\mu'\mu}$ are

$$\langle u_\mu | u_{\mu'} \rangle = \begin{pmatrix} 1.000000000000000 & -0.5943374193710569 & 0.2237783001963385 \\ -0.5943374193710569 & 1.000000000000000 & -0.4272052696463735 \\ 0.2237783001963385 & -0.4272052696463735 & 1.000000000000000 \end{pmatrix},$$

$$A_{\mu'\mu} = \begin{pmatrix} 1.000000000000000 & 0.5943374193710569 & -0.04892099097301160 \\ 0 & 1.000000000000000 & 0.2942054521964399 \\ 0 & 0 & 1.000000000000000 \end{pmatrix}.$$

As an example, in Fig. 1 we show the CPU time and MaxMemoryUsed during of calculations of overlap integrals (67) and (68) and execution of the G-S orthonormalization procedure (71)-(72) in the laboratory and intrinsic frames by the above *symbolic algorithm* versus parameter λ with help of the `O5SU11` code using the PC Intel Celeron CPU 2.16 GHz 4GB 64bit Windows 8.1. The computations were evaluated numerically to 20-digit precision that have been confirmed by the calculated values of the diagonal matrices from the last arrow `test` of Algorithm in Table 4 to 20-digit precision. One can see that the CPU time (in logarithmic scale) of execution of the overlap integrals is linearly growing. However, the G–S orthonormalization procedure in the intrinsic frame has reduced the computer resources in comparison with one in the laboratory frame.

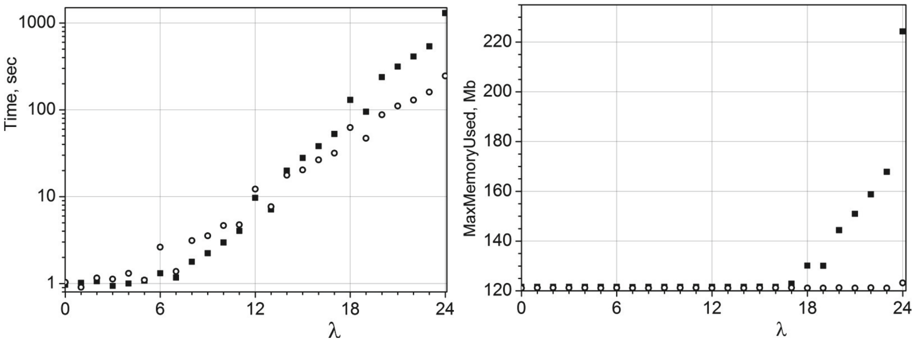

Fig. 1. The CPU time in s. (on the left) and the maximum memory in Mb used to store intermediate data for the current Mathematica session in computation of the overlap integrals and orthogonalization matrices (on the right). Both values are given versus the parameter λ at $L = \lambda$ in the laboratory (marked by squares) and intrinsic (marked by cycles) frames.

5 Conclusion

In present paper, we have elaborated a new universal effective symbolic-numeric algorithm implemented as the first version of O5SU11 code in the Wolfram Mathematica for computing the orthonormal basis of the Bohr–Mottelson(BM) collective model in the both intrinsic and laboratory frames, which can be implemented in any computer algebra system. This kind of basis is widely used for calculating the spectra and electromagnetic transitions in solid, molecular, and nuclear physics. The new symbolic algorithm for orthonormalization of the obtained BM basis based on the Gram–Schmidt orthonormalization procedure has been developed.

The distinct advantage of this method is that it does not involve any square root operation on the expressions coming from the previous steps for computation of the orthonormalization coefficients for this basis. This makes the proposed method very suitable for calculations using computer algebra systems. The symbolic nature of the developed algorithms allows one to avoid the numerical round-off errors in calculation of spectral characteristics (especially close to resonances) of quantum systems under consideration and to study their analytical properties for understanding the dominant symmetries [19].

The program SO5U11 in the Mathematica language for the orthonormalization of the non-canonical basis using the overlap integrals in the laboratory and intrinsic frames (Eqs. (67) and (68)) given by the analytical formula is now prepared and will be published as an open code elsewhere. The great advantage of the program SO5U11 is the possibility to specify an arbitrary precision of calculations which is especially important for large-scale calculations of physical quantities that involve procedures of matrices inversion in eigenvalue problems with degenerated spectra or similar one [32].

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