Symbolic-Numerical Algorithm for Large Scale Calculations the Orthonormal SU(3) BM Basis

A. Deveikis[1], A. A. Gusev[2(✉)], V. P. Gerdt[2], S. I. Vinitsky[2,3], A. Góźdź[4], A. Pędrak[5], and Č. Burdik[6]

[1] Department of Applied Informatics, Vytautas Magnus University, Kaunas, Lithuania
algirdas.deveikis@vdu.lt
[2] Joint Institute for Nuclear Research, Dubna, Russia
gooseff@jinr.ru
[3] RUDN University, 6 Miklukho-Maklaya, 117198 Moscow, Russia
[4] Institute of Physics, Maria Curie-Skłodowska University, Lublin, Poland
[5] National Centre for Nuclear Research, Warsaw, Poland
[6] Department of Mathematics, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University, Prague, Czech Republic

Abstract. In this paper we proposed a new symbolic, non-standard recursive and fast orthonormalization procedure of linearly independent vectors but as in other approaches not orthonormal based on the Gram-Schmidt orthonormalization algorithm. Our adaptation of the Gram-Schmidt orthonormalization procedure provide simple analytic formulas for the SU(3) Bargmann-Moshinsky basis orthonormalization coefficients and do not involve any square root operation on the expressions coming from the previous iterative computation steps. This distinct features of the proposed orthonormalization algorithm may make the large scale symbolic calculations feasible. We demonstrate efficiency of our procedure by benchmark large-scale calculations of the non-canonical BM basis with the highest weight vectors of SO(3) irreducible representations.

1 Introduction

Despite the significant number of works on the development of algorithms and construction programs in both analytical and numerical form of the orthonormalized Bargman-Moshinsky basis, there are still no efficient and cost-effective algorithms and programs for its construction and calculation with its help, tensor operators necessary for constructing Hamiltonians by a collective of a model of a nucleus with tetrahedral symmetry under study by modern experiments [1]. Creation of such algorithms and programs is an actual problem in the field of Computer Algebra in Scientific Computing.

In our previous papers [2,3] noted below as I and II, we started to study optimal ways of building up fast versions of Gram-Schmidt orthonormalization

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procedure of the non-canonical BM basis in computer algebra systems and its application to scientific computing of a spectrum of the SU(3) collective nuclei models [4].

In this paper we developed the new symbolic, non-standard recursive and fast orthonormalization procedure of linearly independent vectors but as in other approaches not orthonormal, based on the Gram-Schmidt orthonormalization algorithm. Our adaptation of Gram-Schmidt orthonormalization procedure provide simple analytic formulas for BM basis orthonormalization coefficients and do not involve any square root operation on expressions coming from the previous iterative computation steps. This distinct features of the proposed orthonormalization algorithm may make the large scale symbolic calculations feasible. We demonstrate efficiency of our procedure by benchmark large-scale calculations of the non-canonical SU(3) BM basis [5–7] with the highest weight vectors of SO(3) irreducible representations(irreps). Note, the SU(3) irreps. presented in the form of expansions over the BM basis [6] have a wide range of applications in nuclei physics and quantum optics.

The structure of the paper is following. In the first section we present new *symbolic-numerical algorithm* of the Gram-Schmidt orthonormalization realized on example of non-canonical BM basis in a form of the program implemented in the computer algebra system Wolfram Mathematica 10.1. In the second section we present the best economical algorithm for generation of matrix of tensor operators and algebraic eigenvalue problem using calculated orthonormal BM basis as input and show final results of calculation of a spectrum of the SU(3) collective nuclear models. In conclusion we give a resume and point out some important problems for further applications of proposed algorithms.

2 Symbolic-Numerical Orthonormalization Algorithm

We start from the BM states constructed in the papers I and II:

$$|u_\alpha\rangle \equiv \left| \begin{matrix} (\lambda,\mu)_B \\ \alpha, L, L \end{matrix} \right\rangle, \tag{1}$$

which are linearly independent but as in other approaches not orthonormal. The quantum numbers $\lambda, \mu = 0, 1, 2, \ldots$ label irreducible representations of the SU(3) group. We assume that $\lambda \geq \mu$. The labels L, M are the quantum numbers of angular momentum and its projection (in our case $M = L$); α is the additional index required to distinguish equivalent irreducible representations of SO(3) appearing in a given irreducible representation of SU(3), the problem is not multiplicity free.

The orthogonalized BM states $|\psi_\alpha\rangle$ may be expressed in terms of the orthonormalized BM states $|\phi_\alpha\rangle$ as [7]:

$$|\psi_\alpha\rangle = -|u_\alpha\rangle + \sum_{\alpha'=\alpha+1}^{\alpha_{\max}} c_{\alpha\alpha'} |\phi_{\alpha'}\rangle, \text{ when } 0 \leq \alpha < \alpha_{\max}, \tag{2}$$

here $\alpha_{\max}$ is a number of linearly independent BM states $|u_\alpha\rangle$, and $c_{\alpha\alpha'}$ are linear coefficients. The orthonormalization process (2) starts (somewhat deliberately) by taking $|\psi_{\alpha_{\max}}\rangle = |u_{\alpha_{\max}}\rangle$.

The goal of this paper is to perform orthonormalization of the BM states $|u_\alpha\rangle$:

$$|\phi_i\rangle = \sum_{\alpha=0}^{\alpha_{\max}} A_{i,\alpha}|u_\alpha\rangle. \tag{3}$$

Here multiplicity index i is introduced to differentiate the orthonormalized BM states and takes the same range of values as α. The symbols $A_{i,\alpha}$ denotes matrix elements of the upper triangular matrix of the BM basis orthonormalization coefficients. These coefficients fulfill the following condition

$$A_{i,\alpha} = 0, \quad \text{if } i > \alpha. \tag{4}$$

In this paper we developed an analytical orthonormalization procedure based on the Gram-Schmidt orthonormalization algorithm (GSOA). For explicit construction of the orthonormalized BM basis let us consider step by step the *symbolic algorithm*.

Step 1. First step needs to perform initial setup and check the consistency of the input. The maximum possible value of α for a given μ is $\alpha_{\max}$. It is given by

$$\alpha_{\max} = \begin{cases} \frac{\mu}{2}, & \mu \text{ even}, \\ \frac{\mu-1}{2}, & \mu \text{ odd}. \end{cases} \tag{5}$$

The maximum value of L of the BM state is defined by the expression

$$L_{\max} = \mu - 2\alpha + \lambda - \beta, \tag{6}$$

where

$$\beta = \begin{cases} 0, & \lambda + \mu - L \text{ even}, \\ 1, & \lambda + \mu - L \text{ odd}. \end{cases} \tag{7}$$

To have a consistent input $L \leq L_{\max}$. From the expressions (6) and (7) it follows, that for some L values sufficiently close to the $L_{\max}$, the α values may be less than $\alpha_{\max}$ or even not exist. So, for every particular L value the expressions (6) and (7) allows to find the maximum value of α for which there exist the BM state i.e. $\alpha_{\max K}$.

At the same time there exists the lower boundary condition $L_{\min} \leq L$ that should be evaluated for every particular value of α. If $\alpha = 0$ and $\mu = 0$ the $L_{\min}$ is defined by

$$L_{\min} = \begin{cases} 0, & \lambda \text{ even}, \\ 1, & \lambda \text{ odd}. \end{cases} \tag{8}$$

In case of $\alpha = 0$ and $\mu \neq 0$ the minimum value of L will be $L_{\min} = \mu$. When $0 < \alpha < \alpha_{\max}$ then $L_{\min} = \mu - 2\alpha$. If $\alpha = \alpha_{\max}$ and μ is even then $L_{\min} = 1$. Finally, when $\alpha = \alpha_{\max}$ and μ is odd the $L_{\min}$ takes value given by expression (8). There may exist only the BM states for which the condition $L_{\min} \leq L$ is

satisfied. So, the presented $L_{\min}$ calculation procedure allows to find for every particular L the minimum value of α for which there exists the BM state i.e. $\alpha_{\min K}$. So, for actual calculations of the BM basis orthonormalization coefficients $\alpha = \alpha_{\min K}, \alpha_{\min K} + 1, \ldots, \alpha_{\max K}$. An illustrative example for calculation of $\alpha_{\min K}$ and $\alpha_{\max K}$ for $\mu = 4$ when $\lambda = 0, \ldots, 6$ is presented in Table 1.

Table 1. The values of $\alpha_{\min K}$ and $\alpha_{\max K}$ for $\mu = 4$ when $\lambda = 0, \ldots, 6$.

L												
λ	α	0	1	2	3	4	5	6	7	8	9	10
0	$\alpha_{\min K}$	2		1		0						
	$\alpha_{\max K}$	2		1		0						
1	$\alpha_{\min K}$		2	1	1	0	0					
	$\alpha_{\max K}$		2	1	1	0	0					
2	$\alpha_{\min K}$	2	0	1	1	0	0	0				
	$\alpha_{\max K}$	2	1	2	1	1	0	0				
3	$\alpha_{\min K}$		2	1	1	0	0	0	0			
	$\alpha_{\max K}$		2	1	2	1	1	0	0			
4	$\alpha_{\min K}$	2		1	1	0	0	0	0	0		
	$\alpha_{\max K}$	2		2	1	2	1	1	0	0		
5	$\alpha_{\min K}$		2	1	1	0	0	0	0	0	0	
	$\alpha_{\max K}$		2	1	2	1	2	1	1	0	0	
6	$\alpha_{\min K}$	2	0	1	1	0	0	0	0	0	0	0
	$\alpha_{\max K}$	2	1	2	1	2	1	2	1	1	0	0

For practical calculation there may be useful the condition that allows to find such minimal value of L ($L_{\min}^{\text{total}}$) for which all the BM basis orthonormalization coefficients that forms the matrix A and as consequence the matrix A itself do not exist. For definition of this condition one should start with calculation of the quantity $K = \mu - 2\alpha_{\max K}$. If $K = 0$ then

$$L_{\min}^{\text{total}} = \begin{cases} 0, & \lambda \text{ even}, \\ 1, & \lambda \text{ odd}. \end{cases} \tag{9}$$

If $K \neq 0$ then $L_{\min}^{\text{total}} = K$.

Step 2. Second step needs to introduce and iteratively calculate the convenient intermediate quantities $f_{\alpha,\alpha'}^{(n)}$, here $n = 0, 1, \ldots, \alpha_{\max K} - 1$ indicates a number of iteration. The iteration starts at $n = 0$ by calculation of all $f_{\alpha,\alpha'}^{(0)}$ that are defined by the overlap integrals $\langle u_\alpha | u_{\alpha'} \rangle$ given in the paper I:

$$f_{\alpha,\alpha'}^{(0)} = \langle u_\alpha | u_{\alpha'} \rangle, \tag{10}$$

where $\alpha = \alpha_{\min K}, \alpha_{\min K} + 1, \ldots, \alpha_{\max K} - 1$ and $\alpha < \alpha' \leq \alpha_{\max K}$.

The above overlap was applied in symbolic calculations to test our procedure in paper I with analytical results of [7].

At the next iteration step $n = 1$ the calculation of $f^{(1)}_{\alpha,\alpha'}$ is defined by the formula

$$f^{(1)}_{\alpha,\alpha'} = -f^{(0)}_{\alpha,\alpha'} + \frac{f^{(0)}_{\alpha,\alpha_{\max K}} f^{(0)}_{\alpha',\alpha_{\max K}}}{\langle u_{\alpha_{\max K}} | u_{\alpha_{\max K}} \rangle}, \tag{11}$$

where $\alpha = \alpha_{\min K}, \alpha_{\min K} + 1, \ldots, \alpha_{\max K} - 2$ and $\alpha < \alpha' \leq \alpha_{\max K} - 1$. For all next iteration steps $n > 1$, the $f^{(n)}_{\alpha,\alpha'}$ are defined by the formula

$$f^{(n)}_{\alpha,\alpha'} = f^{(n-1)}_{\alpha,\alpha'} + \frac{f^{(n-1)}_{\alpha,\alpha_{\max K-n+1}} f^{(n-1)}_{\alpha',\alpha_{\max K-n+1}}}{\langle \psi_{\alpha_{\max K-n+1}} | \psi_{\alpha_{\max K-n+1}} \rangle}, \tag{12}$$

where $\alpha = \alpha_{\min K}, \alpha_{\min K} + 1, \ldots, \alpha_{\max K} - n - 1$ and $\alpha < \alpha' \leq \alpha_{\max K} - n$. Here the normalization integral is defined as

$$\langle \psi_\alpha | \psi_\alpha \rangle = \langle u_\alpha | u_\alpha \rangle - \sum_{\alpha'=\alpha+1}^{\alpha_{\max}} \frac{\left(f^{(\alpha_{\max K}-\alpha')}_{\alpha,\alpha'} \right)^2}{\langle \psi_{\alpha'} | \psi_{\alpha'} \rangle}. \tag{13}$$

It should be noted, that all quantities $f^{(n)}_{\alpha,\alpha'}$ at iteration step n may be calculated solely from the quantities $f^{(n-1)}_{\alpha,\alpha'}$ and normalization integrals $\langle \psi_\alpha | \psi_\alpha \rangle$ obtained at the previous iteration step $n - 1$. So, at the every iteration step (except the $n = 0$) the corresponding quantities: $f^{(n)}_{\alpha,\alpha'}$ and the normalization integrals $\langle \psi_\alpha | \psi_\alpha \rangle$, are calculated and put into the storage.

For the linear storage of the quantities $f^{(n)}_{\alpha,\alpha'}$ the corresponding sequence number s may be introduced. It depends on the quantities $n, \alpha, \alpha', \alpha_{\max}$ by the formula

$$\begin{aligned} s = {} & \frac{1}{6} \left(\left(2 + 6\alpha_{\max} + 3\alpha_{\max}^2 \right) n - 3 \left(1 + \alpha_{\max} \right) n^2 + n^3 \right) \\ & + \left(\alpha_{\max} - n \right) \alpha + \frac{1}{2} \left(1 - \alpha \right) \alpha - \alpha + \alpha'. \end{aligned}$$

Step 3. Finally, having calculated the quantities $f^{(n)}_{\alpha,\alpha'}$ and the normalization integrals $\langle \psi_\alpha | \psi_\alpha \rangle$, one may straightforwardly compute the required orthonormalization coefficients $A_{\alpha,\alpha'}$ of the expansion (3). In the case when $\alpha = \alpha' = \alpha_{\max K}$ the formula for calculation of $A_{\alpha,\alpha'}$ is

$$A_{\alpha_{\max K},\alpha_{\max K}} = \langle u_{\alpha_{\max K}} | u_{\alpha_{\max K}} \rangle^{-1/2}. \tag{14}$$

In case when $\alpha = \alpha'$ and $\alpha = \alpha_{\min K}, \alpha_{\min K} + 1, \ldots, \alpha_{\max K} - 1$ the formula for calculation of $A_{\alpha,\alpha'}$ is

$$A_{\alpha,\alpha} = -\langle \psi_\alpha | \psi_\alpha \rangle^{-1/2}. \tag{15}$$

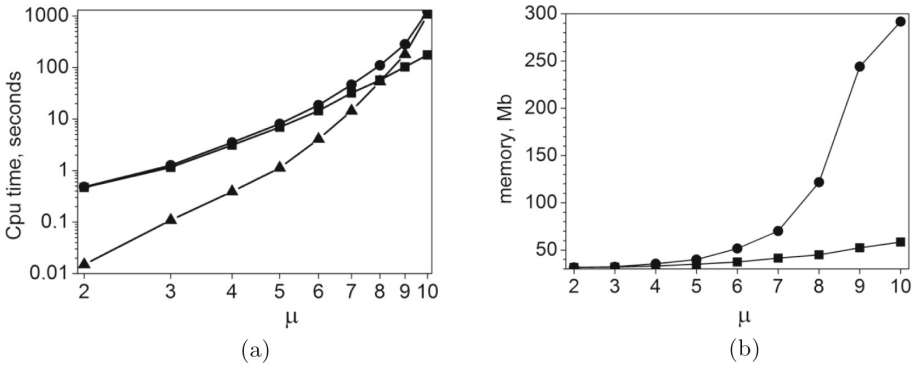

Fig. 1. The CPU time versus parameter μ (a) and MaxMemoryUsed versus parameter μ (b): maximum number of Megabytes (Mb) used to store all data for the current Wolfram System session during the calculations of the orthogonal BM basis (circles) consisted of calculation of the overlap integrals (10) (squares) and execution of the othonormalization Gram–Schmidt procedure (11)–(17) (triangles).

In the case when $\alpha < \alpha' < \alpha_{\max K}$ the formula for calculation of $A_{\alpha,\alpha'}$ is

$$A_{\alpha,\alpha'} = \frac{1}{\langle\psi_{\alpha'}|\psi_{\alpha'}\rangle} \sum_{\alpha''=\alpha}^{\alpha'-1} A_{\alpha,\alpha''} f_{\alpha'',\alpha'}^{(\alpha_{\max K}-\alpha')}. \tag{16}$$

In the case when $\alpha = \alpha_{\min K}, \alpha_{\min K}+1, \ldots, \alpha_{\max K}-1$ and $\alpha' = \alpha_{\max K}$ the formula for calculation of $A_{\alpha,\alpha'}$ is

$$A_{\alpha,\alpha_{\max K}} = -\frac{1}{\langle\psi_{\alpha_{\max K}}|\psi_{\alpha_{\max K}}\rangle} \sum_{\alpha''=\alpha}^{\alpha_{\max K}-1} A_{\alpha,\alpha''} f_{\alpha'',\alpha_{\max K}}^{(0)}. \tag{17}$$

The above *algorithm* was realized in the form of the program implemented in the computer algebra system Wolfram Mathematica 10.1.

Remark 1. The two advantages of the proposed *algorithm*. First of all its simplicity: at any iterative step n the quantities $f_{\alpha,\alpha'}^{(n)}$ are composed of fragments that are not more complicated than that defined in the right hand side of Eq. (12) and the normalization integrals (13). Secondly, iterative calculation of the quantities $f_{\alpha,\alpha'}^{(n)}$ (12) and the normalization integrals (13) do not involve any square root operation in contradistinction to the conventional one [14]. This distinct features of the proposed orthonormalization algorithm make the large scale symbolic calculations *in principle* feasible.

In the case of the subset of three independent BM vectors (1) indicated by the displayed values of labels, expansion (3) demonstrated execution of the othonormalization Gram–Schmidt procedure (OGSP) (11)–(17) takes the form ($\mu = 4$, $\lambda - L$ even))

$$\left|\begin{matrix}(\lambda,\mu)\\ f_2,L,L\end{matrix}\right\rangle = A_{2,2}^{(\lambda,\mu)}(L)\left|\begin{matrix}(\lambda,\mu)_B\\ 2,L,L\end{matrix}\right\rangle,$$
$$\left|\begin{matrix}(\lambda,\mu)\\ f_1,L,L\end{matrix}\right\rangle = A_{1,1}^{(\lambda,\mu)}(L)\left|\begin{matrix}(\lambda,\mu)_B\\ 1,L,L\end{matrix}\right\rangle + A_{1,2}^{(\lambda,\mu)}(L)\left|\begin{matrix}(\lambda,\mu)_B\\ 2,L,L\end{matrix}\right\rangle,$$
$$\left|\begin{matrix}(\lambda,\mu)\\ f_0,L,L\end{matrix}\right\rangle = A_{0,0}^{(\lambda,\mu)}(L)\left|\begin{matrix}(\lambda,\mu)_B\\ 0,L,L\end{matrix}\right\rangle + A_{0,1}^{(\lambda,\mu)}(L)\left|\begin{matrix}(\lambda,\mu)_B\\ 1,L,L\end{matrix}\right\rangle + A_{0,2}^{(\lambda,\mu)}(L)\left|\begin{matrix}(\lambda,\mu)_B\\ 2,L,L\end{matrix}\right\rangle,$$

$$A_{2,2}^{(\lambda,4)}(L) = (\langle u_2|u_2\rangle)^{-1/2},$$
$$A_{1,1}^{(\lambda,4)}(L) = -\langle\psi_1|\psi_1\rangle^{-1/2}, \qquad A_{1,2}^{(\lambda,4)}(L) = \langle\psi_1|\psi_1\rangle^{-1/2}\frac{\langle u_2|u_1\rangle}{\langle u_2|u_2\rangle},$$
$$A_{0,0}^{(\lambda,4)}(L) = -\langle\psi_0|\psi_0\rangle^{-1/2},$$
$$A_{0,1}^{(\lambda,4)}(L) = -\frac{\langle\psi_0|\psi_0\rangle^{-1/2}}{\langle\psi_1|\psi_1\rangle}\left(-\langle u_1|u_0\rangle + \frac{\langle u_2|u_1\rangle\langle u_2|u_0\rangle}{\langle u_2|u_2\rangle}\right),$$
$$A_{0,2}^{(\lambda,4)}(L) = \langle\psi_0|\psi_0\rangle^{-1/2}\left[\frac{\langle u_2|u_0\rangle}{\langle u_2|u_2\rangle} + \frac{1}{\langle\psi_1|\psi_1\rangle}\left(-\langle u_1|u_0\rangle + \frac{\langle u_2|u_1\rangle\langle u_2|u_0\rangle}{\langle u_2|u_2\rangle}\right)\frac{\langle u_2|u_1\rangle}{\langle u_2|u_2\rangle}\right],$$
$$\langle\psi_0|\psi_0\rangle = \langle u_0|u_0\rangle - \frac{\langle u_2|u_0\rangle^2}{\langle u_2|u_2\rangle} - \frac{1}{\langle\psi_1|\psi_1\rangle}\left(-\langle u_1|u_0\rangle + \frac{\langle u_2|u_1\rangle\langle u_2|u_0\rangle}{\langle u_2|u_2\rangle}\right)^2,$$
$$\langle\psi_1|\psi_1\rangle = \langle u_1|u_1\rangle - \frac{\langle u_2|u_1\rangle^2}{\langle u_2|u_2\rangle}.$$

As an example, in Fig. 1 we show the CPU time and MaxMemoryUsed during of calculations of overlap integrals (13) and execution of the othonormalization Gram–Schmidt procedure (OGSP) (11)–(17) by the above *symbolic algorithm* versus parameter μ using the PC Intel Pentium CPU 1.50 GHz 4 GB 64bit Windows 8. One can see that the CPU time (in double logarithmic scale) of execution of the overlap integrals is linearly growing in contradistinction to the OGSP, whose execution time is growing faster than linearly due to manipulations with rational expressions.

3 Benchmark for Symbolic Numerical Algorithm

Because the BM vectors $|u_\alpha\rangle$ are linearly independent, one can require the orthonormalization properties for the vectors $|\phi_i\rangle$

$$\langle\phi_i|\phi_j\rangle = \delta_{ij}. \tag{18}$$

From Eq. (18) there may be derived the orthonormalization property of the orthonormalization coefficients $A_{\alpha,\alpha'}$ matrix $\boldsymbol{\mathcal{A}}$

$$\boldsymbol{\mathcal{A}}\boldsymbol{\mathcal{U}}\tilde{\boldsymbol{\mathcal{A}}} = \boldsymbol{\mathcal{I}}. \tag{19}$$

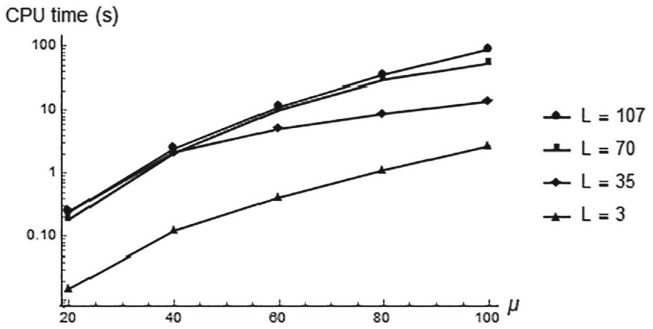

Fig. 2. The CPU time versus parameter μ for calculations of the A matrix with $\lambda = 119$ for $L = 3, 35, 70, 107$.

Here matrices $\boldsymbol{\mathcal{A}}, \boldsymbol{\mathcal{U}}$ and $\boldsymbol{\mathcal{I}}$ have dimension $\alpha_{\max}+1$. The matrix $\tilde{\boldsymbol{\mathcal{A}}}$ is transposed of $\boldsymbol{\mathcal{A}}$. In general case, when $\alpha_{\max K} < \alpha_{\max}$ and $\alpha_{\min K} > 0$, these matrices have the following block structure

$$\boldsymbol{\mathcal{A}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \boldsymbol{A} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \boldsymbol{\mathcal{U}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \boldsymbol{U} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \boldsymbol{\mathcal{I}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \boldsymbol{I} & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Here the matrices $\boldsymbol{A}$, $\boldsymbol{U}$ and $\boldsymbol{I}$ have the dimension $\alpha_{\max K} - \alpha_{\min K} + 1$. The zeroes represents the sub-blocks with the appropriate dimensions that are filled with zeroes. The $\boldsymbol{I}$ is the unity matrix.

Let as display a structure of indices of the matrix $\boldsymbol{A}$

$$\boldsymbol{A} = \begin{pmatrix} A_{\alpha_{\min K},\alpha_{\min K}} & \cdots & A_{\alpha_{\min K},\alpha_{\max K}} \\ \vdots & \ddots & \vdots \\ A_{\alpha_{\max K},\alpha_{\min K}} & \cdots & A_{\alpha_{\max K},\alpha_{\max K}} \end{pmatrix}. \tag{20}$$

Finally, the entries of the matrix $\boldsymbol{U}$ are the overlap integrals $\langle u_\alpha | u_{\alpha'} \rangle$

$$\boldsymbol{U} = \begin{pmatrix} \langle u_{\alpha_{\min K}} | u_{\alpha_{\min K}} \rangle & \cdots & \langle u_{\alpha_{\min K}} | u_{\alpha_{\max K}} \rangle \\ \vdots & \ddots & \vdots \\ \langle u_{\alpha_{\max K}} | u_{\alpha_{\min K}} \rangle & \cdots & \langle u_{\alpha_{\max K}} | u_{\alpha_{\max K}} \rangle \end{pmatrix}. \tag{21}$$

The Eq. (19) may be used for control of consistency and accuracy of calculations.

The efficiency of **A** matrix calculations for different values of the quantum number L is illustrated in Fig. 2. The computations were evaluated numerically to 150-digit precision. Such high precision was taken in order to compare these calculations with fuhrer calculations of $q_{ijk}^{(\lambda\mu)}(L)$ presented in Sect. 4.

Remark 2. From a conventional point of view the proposed symbolic orthonormalisation algorithm can be called as a non-standard recursive, or actually iterative, since it traverses the computation graph not from top to bottom, but from

bottom to top. It has been organized in such a way, to have one to one correspondence of obtained results with definition of the orthonormalisation coefficients A assumed in Ref. [7]. This algorithm allows one to find the analytical expressions of the orthonormalized basis, if it is implemented in any computer algebra system, in particular, Wolfram Mathematica 10.1. It is given in the present paper and tested in the paper I with analytical results at small values λ and μ obtained in [7]. However, to perform the really fast large scale calculations with characteristics of computer time shown in Fig. 2, it has been implemented in the multi-precision arithmetics as a *symbolic-numerical algorithm*.

Table 2. The values of $(\alpha_{\min K}, \alpha_{\max K})\dim(\boldsymbol{A})$ and $\alpha_{\max}$ for $\mu = 60, 85, 100, 115$ and $\lambda = 120, 125$ when $L = 2, 31, 70, 120, 180$.

			L				
μ	λ	$\alpha_{\max}$	2	31	70	120	180
60	120	30	(29,30)2	(15,29)15	(0,30)31	(0,30)31	(0,0)1
	125		(29,29)1	(15,30)16	(0,29)30	(0,29)30	(0,2)3
85	120	42	(42,42)1	(27,42)16	(8,42)35	(0,42)43	(0,12)13
	125		(42,42)1	(27,42)16	(8,42)35	(0,42)43	(0,15)16
100	120	50	(49,50)2	(35,49)15	(15,50)36	(0,50)51	(0,20)21
	125		(49,49)1	(35,50)16	(15,49)35	(0,49)50	(0,22)23
115	120	57	(57,57)1	(42,57)16	(23,57)35	(0,57)58	(0,27)28
	125		(57,57)1	(42,57)16	(23,57)35	(0,57)58	(0,30)31

In numerical benchmark calculations given below we will demonstrate also the results of execution of the same OGSP (11)–(17) but with the normalized nonorthogonal eigenvectors $|\check{u}_\alpha\rangle = N^{-1}_{\alpha\alpha}|u_\alpha\rangle$ and normalized overlap $\langle\check{u}_\alpha|\check{u}_{\alpha'}\rangle = \langle u_\alpha|N^{-1}_{\alpha\alpha}N^{-1}_{\alpha'\alpha'}|u_{\alpha'}\rangle$, $N_{\alpha\alpha} = (\langle u_\alpha|u_\alpha\rangle)^{1/2}$, respectively, i.e. $\langle\check{u}_\alpha|\check{u}_\alpha\rangle = 1$.

The examples of the output ($\alpha_{\min K}$, $\alpha_{\max K}$, `dim(A)`) of the program `Abound.nb` for some values of μ, λ, and L are presented in Table 2.

The orthonormalization of the BM basis, i.e. the calculation of the matrix $\boldsymbol{\mathcal{A}}$ for given values of μ, λ, L and precision is provided by the program `BMOrthonorm.nb`. The calculation of the orthonormalized BM basis is based on the overlap integrals $\langle u_\alpha|u_{\alpha'}\rangle$. In case if that quantities are needed one may call the function `overlapIntegral[`μ`, `α`, `α'`, L, `λ`]`. As an example, we consider a case with $\mu = 10$, $\lambda = 11$ and $L = 6$ for $\alpha = 2$ and $\alpha' = 3$. In this case calling the function `overlapIntegral` produces the output $\langle u_\alpha|u_{\alpha'}\rangle$ `= 59566465014885384192000000`, i.e. the function `overlapIntegral` computes the *exact numerical* value of the overlap integral $\langle u_\alpha|u_{\alpha'}\rangle$.

Let us consider an example of the orthonormalization of the BM basis and take for it a case with $\mu = 10$, $\lambda = 11$ and $L = 6$. In this case $\alpha_{\max} = 5$, $\alpha_{\min K} = 2$, $\alpha_{\max K} = 4$, and precision was taken to be equal to `prec` $= 15$. For calculation of $\boldsymbol{\mathcal{A}}$ matrix one may call the function `Amatrix[`μ`, L, `λ`, prec]`.

In this case the matrix $\boldsymbol{\mathcal{A}}$ acting on unnormalized vector $\boldsymbol{u}$ prints as

$$\boldsymbol{\mathcal{A}}^{\mu\lambda}(L) = \begin{pmatrix} 0\,0 & 0 & 0 & 0 & 0 \\ 0\,0 & 0 & 0 & 0 & 0 \\ 0\,0 & -5.268 \times 10^{-14} & 4.324 \times 10^{-14} & -5.671 \times 10^{-15} & 0 \\ 0\,0 & 0 & -1.271 \times 10^{-13} & 4.782 \times 10^{-14} & 0 \\ 0\,0 & 0 & 0 & 9.304 \times 10^{-14} & 0 \\ 0\,0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

while $\check{\boldsymbol{\mathcal{A}}} = \boldsymbol{\mathcal{A}}\mathbf{N}$ acting on normalized vector $\check{\boldsymbol{u}}$ prints as

$$\check{\boldsymbol{\mathcal{A}}}^{\mu\lambda}(L) = \begin{pmatrix} 0\,0 & 0 & 0 & 0 & 0 \\ 0\,0 & 0 & 0 & 0 & 0 \\ 0\,0 & -1.06241748771592 & 0.382535950822453 & -0.060953283607289 & 0 \\ 0\,0 & 0 & -1.12436060747693 & 0.513991026814558 & 0 \\ 0\,0 & 0 & 0 & 1.00000000000000 & 0 \\ 0\,0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

The accuracy of calculations of the matrix $\boldsymbol{\mathcal{A}}$ may be evaluated by the function `TestOrthonormalization[`μ`, L,` λ`, base, prec]` that use for this purpose the orthonormalization property Eq. (19). At first, the function `TestOrthonormalization[`μ`, L,` λ`, base, prec]` calculates the left hand side of the Eq. (19), i.e. the product of three matices $\boldsymbol{\mathcal{A}}\,\boldsymbol{\mathcal{U}}\tilde{\boldsymbol{\mathcal{A}}}$. The result may be printed as the matrix `test` to ensure that its diagonal elements in the submatrix $\alpha_{\min K} \ldots \alpha_{\max K}$ are actually equal to one and other elements are equal to zero. Finally this submatrix is taken off (as matrix `testK`), printed and used to evaluate the accuracy of orthonormalization coefficients using the condition:

$$|10^{-\mathtt{prec}} - \|\mathtt{testK} - \boldsymbol{I}\|| < \mathtt{base}^{-\mathtt{prec}}, \tag{22}$$

here the norm $\|...\|$ is defined as giving the maximum singular value of a matrix, and parameter `base` defines the accuracy of calculations of the matrix $\boldsymbol{\mathcal{A}}^{\mu\lambda}(L)$ - in this case `base` is taken equal to `9.5`. In the case under consideration the function `TestOrthonormalization[`μ`, L,` λ`, base, prec]` prints the following matrix for unnormalized $\boldsymbol{\mathcal{U}}^{\mu\lambda}(L)$:

$$\boldsymbol{\mathcal{U}}^{\mu\lambda}(L) = \begin{pmatrix} 0\,0 & 0 & 0 & 0 & 0 \\ 0\,0 & 0 & 0 & 0 & 0 \\ 0\,0 & 4.068 \times 10^{26} & 5.957 \times 10^{25} & 2.325 \times 10^{25} & 0 \\ 0\,0 & 5.957 \times 10^{25} & 7.826 \times 10^{25} & 4.347 \times 10^{25} & 0 \\ 0\,0 & 2.325 \times 10^{25} & 4.347 \times 10^{25} & 1.155 \times 10^{26} & 0 \\ 0\,0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

while for normalized $\check{\boldsymbol{\mathcal{U}}}^{\mu\lambda}(L)$

$$\check{\boldsymbol{\mathcal{U}}}^{\mu\lambda}(L) = \begin{pmatrix} 0\,0 & 0 & 0 & 0 & 0 \\ 0\,0 & 0 & 0 & 0 & 0 \\ 0\,0 & 1.00000000000000 & 0.333834605013026 & 0.107226660720115 & 0 \\ 0\,0 & 0.333834605013026 & 1.00000000000000 & 0.457140728158342 & 0 \\ 0\,0 & 0.107226660720115 & 0.457140728158342 & 1.00000000000000 & 0 \\ 0\,0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

In this case the matrix product $\boldsymbol{\mathcal{A}}\boldsymbol{\mathcal{U}}\tilde{\boldsymbol{\mathcal{A}}}$ will be printed as the matrix `test`: for the unnormalized overlap $\boldsymbol{\mathcal{U}}$

$$\left(\boldsymbol{\mathcal{A}}\boldsymbol{\mathcal{U}}\tilde{\boldsymbol{\mathcal{A}}}\right)^{\mu\lambda}(L) = \begin{pmatrix} 0\,0 & 0 & 0 & 0 & 0 \\ 0\,0 & 0 & 0 & 0 & 0 \\ 0\,0 & 1.0000000000 & 1.\times 10^{-15} & 1.\times 10^{-16} & 0 \\ 0\,0 & 1.\times 10^{-15} & 1.0000000000 & 1.\times 10^{-15} & 0 \\ 0\,0 & 1.\times 10^{-15} & 1.\times 10^{-15} & 1.0000000000 & 0 \\ 0\,0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

and the matrix product $\check{\boldsymbol{\mathcal{A}}}\check{\boldsymbol{\mathcal{U}}}\tilde{\check{\boldsymbol{\mathcal{A}}}}$ for the normalized overlap $\check{\boldsymbol{\mathcal{U}}}$

$$\left(\check{\boldsymbol{\mathcal{A}}}\check{\boldsymbol{\mathcal{U}}}\tilde{\check{\boldsymbol{\mathcal{A}}}}\right)^{\mu\lambda}(L) = \begin{pmatrix} 0\,0 & 0 & 0 & 0 & 0 \\ 0\,0 & 0 & 0 & 0 & 0 \\ 0\,0 & 1.0000000000 & 1.\times 10^{-15} & 1.\times 10^{-15} & 0 \\ 0\,0 & 1.\times 10^{-15} & 1.0000000000 & 1.\times 10^{-15} & 0 \\ 0\,0 & 1.\times 10^{-15} & 1.\times 10^{-15} & 1.0000000000 & 0 \\ 0\,0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

here for saving the space we do not present last 4 zeroes after the decimal point for the diagonal matrix elements.

The efficiency of $\boldsymbol{A}$ matrix calculations for different values of parameter L is illustrated in Fig. 2. The computations were evaluated numerically to 15-digit precision. It should be pointed out that the CPU time for calculations of the $\boldsymbol{A}$ matrix less depend on the values of λ, L and the taken precision but more on the dimension of the matrix $\boldsymbol{A}$. The apparent dependency of CPU time on the value of L reflects actually the changing of dimension of the matrix $\boldsymbol{A}$ depending on the value of L but not the change of the time for calculation of overlap integrals.

Remark 3. As shown by our benchmark calculation it would be appropriate in the future numerical calculation to provide scaling: the use of non-orthogonal normalized basis similar to Ref. [13] and the corresponding input matrix elements of scalar products – overlap integrals and intermediate output coefficients of orthogonalization and intermediate input matrix elements of tensor operators. Naturally, with such scaling, the result of calculating the orthonormal basis and the final values of the matrix elements of the tensor operators do not change. In this case, the desired numerical values coincide with the analytical values, but the intermediate values will remain within 16 significant figures, which corresponds to the accepted accuracy of the final results of $2 \cdot 10^{-16}$. Meanwhile, the principal problem of calculation exact numerical value of overlap integral in nonnormalized nonorthogonal BM basis at extremely large value of λ and μ will be solved using Wolfram Mathematica. The corresponding study of an efficiency of such adaptation of our code implemented in Wolfram Mathematica 10.1 and comparison with code implemented in Fortran are subject of a separate paper published elsewhere.

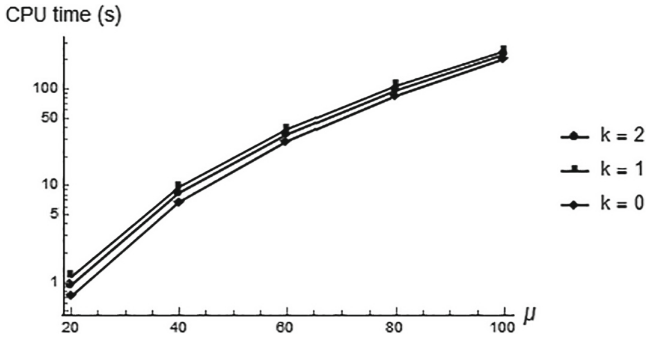

Fig. 3. The CPU time versus parameter μ for calculations of the $q_{ijk}^{(\lambda\mu)}(L)$ with $\lambda = 119$ and $L = 107$ for $k = 0, 1, 2$.

4 Generation and Solution of SU(3) algebraic problem

The Casimir operator of SO(3) irreducible representations corresponding to the group chain $SU(3) \supset O(3) \supset O(2)$ have the form:

$$C_2(SU(3)) = Q \cdot Q + 3L \cdot L = 4(\lambda^2 + \mu^2 + \lambda\mu + 3\lambda + 3\mu). \tag{23}$$

The dimension of the subspace for given λ, μ can be calculated by using the following formula:

$$D_{\lambda\mu} = \frac{1}{2}(\lambda + 1)(\mu + 1)(\lambda + \mu + 2). \tag{24}$$

As a benchmark example we consider a perturbation operator announced in Ref. [4]

$$H''_{4Q} = \sqrt{\frac{14}{5}}(\bar{Q} \otimes \bar{Q})^4_0 + (\bar{Q} \otimes \bar{Q})^4_{-4} + (\bar{Q} \otimes \bar{Q})^4_4, \tag{25}$$

where $(T_{\lambda'} \otimes T_\lambda)^L_M$ denotes the tensor product of two spherical tensors [8]. The matrix elements of the Hamiltonian (25) can be calculated by using the following formula:

$$(H''_{4Q})^{(\lambda\mu)}_{\alpha LM,\alpha' L' M'} = \frac{1}{\sqrt{(2L+1)}} \sum_{L''=|L'-2|}^{L'+2} \frac{1}{\sqrt{(2L''+1)}} \sum_{\alpha''=0}^{\alpha_{\max}}$$
$$\sum_{M''=-L''}^{L''} \left(H''^{(1)}_{LL'L''M''} + H''^{(2)}_{LL'L''M''} \right) R^{(\lambda\mu)}_{\alpha L,\alpha'' L''} R^{(\lambda\mu)}_{\alpha'' L'',\alpha' L'}. \tag{26}$$

Matrix elements $H''^{(1)}_{LL'L''M''}$ and $H''^{(2)}_{LL'L''M''}$ read as

$$H''^{(1)}_{LL'L''M''} = \sqrt{\frac{14}{5}} \sum_{\eta=-2}^{2} \begin{bmatrix} 2 & 2 & 4 \\ \eta & -\eta & 0 \end{bmatrix} \begin{bmatrix} L'' & 2 & L \\ M'' & \eta & M \end{bmatrix} \begin{bmatrix} L' & 2 & L'' \\ M' & -\eta & M'' \end{bmatrix}, \tag{27}$$

Table 3. The example of spectrum E of Hamiltonian (32) for $\gamma = 1.5$ and $h_{4Q} = 10$. The pair (λ, μ) labels the irreducible representations of the group SU(3) and the label ν denote degeneration of eigenvalues due to the intrinsic tetrahedral/octahedral symmetry.

(λ, μ)	$D_{\lambda\mu}$	$\gamma C_2(SU(3))$	E	ν	CPU time, s.
$(0,0)$	1	0	0	1	0.016
$(1,0)$	3	24	24	3	0.656
$(2,0)$	6	60	61.44	2	3.547
			60	1	
			59.04	3	
$(2,1)$	15	96	98.5042	3	28.531
			97.6949	3	
			96.96	1	
			95.52	2	
			93.9758	3	
			93.8251	3	

$$H''^{(2)}_{LL'L''M''} = \begin{bmatrix} L'' & 2 & L \\ M'' & -2 & M \end{bmatrix} \begin{bmatrix} L' & 2 & L'' \\ M' & -2 & M'' \end{bmatrix} + \begin{bmatrix} L'' & 2 & L \\ M'' & 2 & M \end{bmatrix} \begin{bmatrix} L' & 2 & L'' \\ M' & 2 & M'' \end{bmatrix}. \quad (28)$$

Here the notation of the Clebsh-Gordan coefficients [8] by the square brackets is introduced. The reduced matrix elements of the quadrupole operator have the form

$$R^{(\lambda\mu)}_{\alpha L,\alpha' L'} = \sqrt{2L'+1} \begin{bmatrix} L & 2 & L' \\ -L' & 0 & -L' \end{bmatrix}^{(-1)} q^{(\lambda\mu)}_{\alpha\alpha'(L-L')}(L). \quad (29)$$

If $L < L'$ then primed parameters should be interchanged with not primed parameters on the right hand side of the formula (29) and the overall sign should be changed as well if the $L - L'$ is the odd number. Matrix elements $q^{(\lambda\mu)}_{ijk}(L)$ read as

$$q^{(\lambda\mu)}_{ijk}(L) = \sum_{\substack{\alpha=0,\ldots,\alpha_{\max} \\ s=0,\pm 1}} A^{(\lambda\mu)}_{i,\alpha}(L) a^{(k)}_s \tilde{A}^{(\lambda\mu)}_{j,(\alpha+s)}(L+k), \quad (30)$$

where coefficients $a^{(k)}_s$ are given in II: and $\tilde{A}^{(\lambda,\mu)}_{i,\alpha}(L)$ are elements of the inverse and the transpose of the matrix $\mathbf{A}$

$$\tilde{A}^{(\lambda,\mu)}_{i,\alpha}(L) = (A^{-1})^{(\lambda,\mu)}_{\alpha,i}(L). \quad (31)$$

The above formula was applied in symbolic calculations to test our procedure in paper II with analytical results of [9]. In present paper the efficiency of $q^{(\lambda\mu)}_{ijk}(L)$ calculations for different values of parameter k is illustrated in Fig. 3. The computations were evaluated numerically to 150-digit precision. Such high precision is necessary for accurate calculation of inverse matrix $\mathbf{A}^{-1}$.

Remark 4. If we wish to calculate $q_{ijk}^{(\lambda\mu)}(L)$ with help of the normalized matrix $\check{\mathbf{A}}$ then we will scale matrix $\mathbf{a}$ by such a way $\check{\mathbf{a}} = \mathbf{N}^{-1}\mathbf{a}\mathbf{N}$ which corresponds to action of $\check{\mathbf{a}}$ on normalized vector $\check{\boldsymbol{u}}$.

Let us calculate for example the low lying energy levels $E_n \equiv E_{\lambda,\mu,\nu}$ of the Hamiltonian:

$$H \equiv H/h_{4Q} = \gamma C_2(SU(3)) + H''_{4Q}/h_{4Q},\ H|\lambda,\mu,\nu>= E_n|\lambda,\mu,\nu> . \quad (32)$$

The computational results for an example of spectrum of the Hamiltonian (32) are presented in Table 3. The columns of the table are: (λ,μ) labels the irreducible representations of the group SU(3); $D_{\lambda\mu}$ is the dimension of the (λ,μ) irrep from Eq. (24) determining a complexity of the above algorithm; $C_2(SU(3))$ marks the eigenvalues of the second order Casimir operator (23); E presents the energy levels that results after diagonalization of the Hamiltonian (32); ν is the degeneration of the corresponding energy spectrum E; CPU time is the H_{4Q} matrix calculation time in seconds. The computations were evaluated numerically to 10-digit precision.

The computations was performed on Intel i7-3630QM 2.40 GHz CPU with 8 GB RAM running 64-bit Windows 8.

5 Conclusion

We present the effective and fast symbolic algorithm for constructing of the non-canonical Bargmann–Moshinsky (BM) basis with the highest weight vectors of SO(3) irreps which can be implemented in any computer algebra system. This kind of basis is widely used for calculating spectra and electromagnetic transitions in molecular and nuclear physics. The new symbolic algorithm for orthonormalisation of the obtained BM basis based on the Gram-Schmidt orthonormalisation procedure is developed.

To avoid misunderstanding we recall that from a conventional view point the proposed symbolic orthonormalisation algorithm can be called as a non-standard recursive, or 'actually iterative', since it traverses the computation graph not from top to bottom, but from bottom to top. It has been organized in such a way, to have one to one correspondence of obtained results with definition of the orthonormalisation coefficients of matrix $\mathbf{A}$ from Eqs. (3) and (20) assumed in Ref. [7].

This algorithm allows one to find the analytical expressions of the orthonormalized basis, if it is implemented in any computer algebra system, in particular, Wolfram Mathematica 10.1. It has been given in the present paper and tested explicitly on analytical results at small values λ and μ Refs. [7,9] in our previous papers I and II. However, to realized the really fast large scale calculations with characteristics of computer time shown in Figs. 2 and 3, it has been implemented in the multi-precision arithmetics as a symbolic-numerical algorithm. It can be also implemented in Fortran to apply in the fast large scale calculations like in Ref. [10].

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 orthonormalisation coefficients for this basis. This makes the proposed method very suitable for calculations on 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 [4]. The program in the Mathematica language for orthonormalisation of the non-canonical BM basis using the overlap integrals in Eq. (21) given by the analytical formula [2,7] is now prepared and will be published as an open code elsewhere. The great advantage of the program 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. The high efficiency of the developed program was illustrated by orthonormalisation of BM basis up to extremely high quantum numbers (λ, μ), which is not given by other symbolic algorithms known in the literature [11,12].

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