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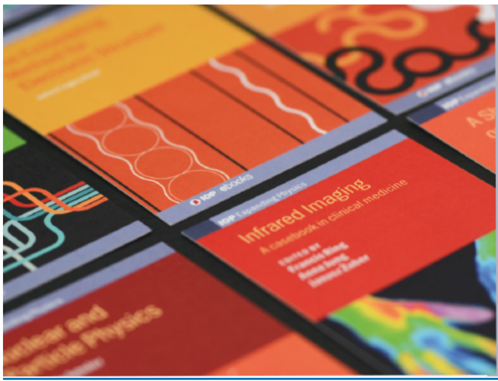

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On generation of the Bargmann-Moshinsky basis of $\mathrm{SU}(3)$ group

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Abstract. An efficient procedure of orthonormalisation of the Bargmann–Moshinsky (BM) basis is examined using analytical formulas of the overlap integrals of the BM basis. Calculations of components of the quadrupole operator between the both BM and the orthonormalised bases needed for construction of the nuclear models are tested. The proposed procedure is also implemented as the Fortran program.

1. Introduction

The formalism of SU(3) group provides a comprehensive theoretical foundation for understanding this symmetry in nuclear structure [1, 2, 3, 4, 5]. However, the construction of the SU(3) bases usually can be performed analytically only for some special cases. In this respect, because of mathematical simplicity of its definition, the Bargmann–Moshinsky (BM) basis [6, 7] is especially convenient for calculation. However, the necessity to introduce the physically relevant angular momentum observable gives rise to the non-canonical group reduction SU(3) ⊃ SO(3) ⊃ SO(2). The BM vectors may be calculated from the simplest vectors which correspond to the highest angular momentum projection $M = L$, i.e. the highest weight basis vectors with respect to the SO(3) group that was proved in [7]. It should be stressed, that the analytical and what is very important an effective algorithm for construction of this basis is required for analysis of some quantum systems.

As an example one can consider the quadrupole vibrational and rotational motions which are the most important low energy nuclear motions. The simplest SU(3) model Hamiltonian consists of the quadrupole-quadrupole interaction, the rotational term and potentially the other terms constructed from generators of the partner groups $G = \mathrm{SU(3)} \times \overline{\mathrm{SU(3)}}$, see [4] and references therein. A possible Hamiltonian H used in this schematic nuclear model can be written as:

$$\begin{aligned} H &= \gamma C_2(\mathrm{SU(3)}) - \kappa Q \cdot Q + \beta L \cdot L + H''(\bar{Q}, \bar{L}) \\ &= (\gamma - \kappa) C_2(\mathrm{SU(3)}) + (3\kappa + \beta) L^2 + H''(\bar{Q}, \bar{L}), \end{aligned} \tag{1}$$

where the second order Casimir operator $C_2(\mathrm{SU(3)}) = Q \cdot Q + 3L \cdot L$, Q and L are generators of SU(3), i.e. quadrupole and angular momentum, respectively. $\bar{Q}$ and $\bar{L}$ are generators of the intrinsic group $\overline{\mathrm{SU(3)}}$. Some examples of physically interesting forms of the interaction H'' can be written as

$$H_{3Q} = h_{3Q} \left((\bar{Q} \otimes \bar{Q})^3_2 - (\bar{Q} \otimes \bar{Q})^3_{-2} \right) , \tag{2}$$

$$H_{3LQ} = h_{3LQ} \left((\bar{L} \otimes \bar{Q})^3_2 - (\bar{L} \otimes \bar{Q})^3_{-2} \right) , \tag{3}$$

$$H_{4Q} = h_{4Q} \Big(\sqrt{\frac{14}{5}} (\bar{Q} \otimes \bar{Q})^4_0 + (\bar{Q} \otimes \bar{Q})^4_{-4} + (\bar{Q} \otimes \bar{Q})^4_4 \Big), \tag{4}$$

where $(T_{\lambda'} \otimes T_{\lambda})^L_M$ denotes the tensor product of two spherical tensors [8]. For, example, these interaction terms can simulate either the tetrahedral or octahedral nuclear symmetry now widely considered in nuclear physics [9]. To find the corresponding energies and quantum nuclear states one needs to solve the eigenvalue problem of the Hamiltonian (1).

To solve the eigenvalue problem for H the appropriate basis constructed according to the group chain SU(3) ⊃ SO(3) ⊃ SO(2) is required. There were several attempts to construct such bases. They were based on different group theoretical technics, for a short review see the introduction in the paper [10, 11]. In all those cases one obtains the non-orthogonal basis. This increases a complexity of calculations of the reduced matrix elements of different operators, Clebsch-Gordan coefficients, etc. It requires an adaptation of the Gram-Schmidt like orthogonalization procedure to be more effective in symbolic calculations.

We start from the BM states which are linearly independent but as in other approaches not orthonormal. We developed an effective symbolic algorithm suitable for implementation in computer algebra systems [12]. It is based on the adapted Gram-Schmidt orthonormalization procedure but using the overlap integrals calculated in an analytical form [11]. It provides the analytic construction of the desirable orthonormalized basis. Our adaptation of Gram-Schmidt orthonormalization procedure consists in construction of recursive calculation of the required quantities and the normalization integrals. These calculations do not involve any square root operation. This distinct features of the proposed orthonormalization algorithm allows for a large scale symbolic calculations [12].

Then one can calculate in this orthonormalized basis the zero component of the quadrupole operator Q_0 in the analytical form using its simpler form given in the non-canonical BM basis [13, 14]. The other components of the quadrupole operator Q_k written in the analytical form can be obtained by making use of the Wigner-Eckart theorem with conventional SO(3) Clebsch-Gordan coefficients [8]. This is required theorem for a final construction of the above Hamiltonian (1) also in an analytical form.

Meanwhile, to organize a real large scale calculations of the required matrix elements of the quadrupole operator with $\lambda, \mu > 5$, where (λ, μ) are Elliot labels denoting the irreducible representations (irrep.) of SU(3), one needs to have a quick algorithm implemented in Fortran that reduces computer resources. The construction and testing of such algorithm is given in the present paper.

The paper is organized as follows. In Section 2, the *procedure 1* for calculation of overlap integrals of BM vectors is shown. In Section 3, the *procedure 2* for orthonormalization of BM basis is given. In Section 4, the *procedure 3* of an action of the quadrupole operator Q_0 onto the constructed basis is presented. In Conclusions further applications of the elaborated *procedures* are outlined.

2. Calculations of the overlap integrals of the BM basis

The effective method for constructing a non-canonical BM basis with the highest weight vectors of SO(3) irreducible representations corresponding to the group chain $SU(3) \supset O(3) \supset O(2)$ with commutation relations of the spherical tensors $L_\nu(\nu = \pm 1, 0)$, $Q_\nu(\nu = \pm 2, \pm 1, 0)$:

$$\begin{aligned} [L_\nu, L_{\nu'}] &= -\sqrt{2} C_{1\nu 1\nu'}^{1\nu+\nu'} L_{\nu+\nu'}, \\ [L_\nu, Q_{\nu'}] &= -\sqrt{6} C_{1\nu 2\nu'}^{2\nu+\nu'} Q_{\nu+\nu'}, \\ [Q_\nu, Q_{\nu'}] &= -3\sqrt{10} C_{2\nu 2\nu'}^{1\nu+\nu'} L_{\nu+\nu'}, \end{aligned} \tag{5}$$

and the Casimir operator

$$C_2(SU(3)) = Q \cdot Q + 3L \cdot L = 4(\lambda^2 + \mu^2 + \lambda\mu + 3\lambda + 3\mu)$$

was described in [11] and implemented as a symbolic algorithm in [12]. Let us introduce the notation for overlaps of the vectors of this basis:

$$\left\langle u_\alpha \middle| u_{\alpha'} \right\rangle = \left\langle \begin{array}{c} (\lambda, \mu)_B \\ \alpha, L, M \end{array} \middle| \begin{array}{c} (\lambda, \mu)_B \\ \alpha', L, M \end{array} \right\rangle \tag{6}$$

Here the quantum numbers λ, μ which label the irreducible representations (irreps), $\lambda, \mu = 0, 1, 2, \ldots$ and $\lambda > \mu$; L, M are the quantum numbers of angular momentum $L \cdot L$ and its projection L_0 (in our case, $M = L$); α is the additional index that is used for unambiguously distinguishing the equivalent SO(3) irreps (L) in a given SU(3) irrep (λ, μ). The dimension of an irrep of SU(3) for a given λ, μ can be calculated by using the following formula:

$$D_{\lambda\mu} = \frac{1}{2}(\lambda + 1)(\mu + 1)(\lambda + \mu + 2). \tag{7}$$

In order to perform classification of the BM states (6) one should determine a set of allowed values of α and L. It is well known that the ranges of quantum numbers α and L are determined by the values of quantum numbers λ and μ. However, the determination of the former quantities is rather cumbersome.

The easiest way to get the allowed values of α and L is by using the following *procedures*:

Step 1. Firstly we start with choosing some particular value of the quantum number μ. For the following consideration, it is convenient to introduce auxiliary label K [3] which varies within the range

$$K = \mu, \mu - 2, \mu - 4, ..., 1 \text{ or } 0, \quad \text{for } \lambda > \mu. \tag{8}$$

The label K is related to α by

$$\alpha = \frac{1}{2}(\mu - K). \tag{9}$$

So, for every fixed μ, the set of possible values of K can be obtained directly from Ref. (8). Now, the set of allowed values of α may be determined from these K values using relation (9).

Step 2. In the case $K = 0$, that may occur only for even values of μ, the allowed values of L are determined by the label λ:

$$L = \lambda, \lambda - 2, \lambda - 4, ..., 1 \text{ or } 0. \tag{10}$$

Step 3. In the case $K \neq 0$ the $L_{\min} = K$. Since for every particular μ, there is a number of possible K numbers, according to (8) there exists a number of the corresponding numbers α. It means that for every particular μ, there will be a number of pairs $(\alpha, L_{\min})$. The maximal value of L is defined by the expression $L_{\max} = \mu - 2\alpha + \lambda - \beta$, where

$$\beta = \begin{cases} 0, & \lambda + \mu - L \text{ even}, \\ 1, & \lambda + \mu - L \text{ odd}. \end{cases} \tag{11}$$

To determine $L_{\max}$ it is convenient to consider two alternatives: $\lambda - L$ is even and $\lambda - L$ is odd. In both cases, the label β is defined by the given value μ value. The number $L_{\max}$ is determined in a similar manner. An illustrative example for calculation of allowed values of α and L is presented in Table 1 of ref [12]. It should be noted that the set of allowed values of L for overlap integrals is given by intersection of these sets for the corresponding $< bra|$ and $|ket >$ vectors.

The highest-weight vector of the BM basis of the SO(3) multiplets for all kinds of irreducible representation of SU(3) can be written in the form [11]

$$\left| \begin{array}{c} (\lambda, \mu)_B \\ \alpha \; L \; L \end{array} \right\rangle \equiv |\beta n_0 n_1 n_2 \alpha\rangle = w^\beta (\xi_1)^{n_0} (x_{10})^{n_1} (\boldsymbol{\xi}^2)^{n_2} A^\alpha |0\rangle, \tag{12}$$

that differ from the states Eq. (3.8) given in [7] in the definition of the number α and coincide up to a phase factor $(-1)^\alpha$. Here the set of numbers n_0, n_1, n_2 is given in terms of the above defined λ, μ, α, L and β

$$n_0 = L - \mu + 2\alpha, \quad n_1 = \mu - 2\alpha - \beta, \quad n_2 = (\lambda + \mu - L - 2\alpha - \beta)/2. \tag{13}$$

The corresponding operators are determined by the following relations:

$$\begin{aligned} &x_{10} = \xi_1\eta_0 - \xi_0\eta_1, \quad x_{1-1} = \xi_1\eta_{-1} - \xi_{-1}\eta_1, \quad x_{0-1} = \xi_0\eta_{-1} - \xi_{-1}\eta_0, \\ &w = \xi_1 x_{1-1} - \xi_0 x_{10} = \xi_1^2\eta_{-1} - \xi_{-1}\xi_1\eta_1 - \xi_0\xi_1\eta_0 + \xi_0^2\eta_1, \quad \boldsymbol{\xi}^2 = \xi_0^2 - 2\xi_{-1}\xi_1, \\ &A = (2x_{10}x_{0-1} - x_{1-1}^2) \\ &= 2\xi_0\xi_1\eta_0\eta_{-1} - 2\xi_{-1}\xi_1\eta_0^2 - 2\xi_0^2\eta_{-1}\eta_1 + 2\xi_0\xi_{-1}\eta_0\eta_1 - \xi_1^2\eta_{-1}^2 + 2\xi_{-1}\xi_1\eta_{-1}\eta_1 - \xi_{-1}^2\eta_1^2, \end{aligned} \tag{14}$$

via two SO(3) spherical vectors belong to two independent SU(3) representations [8]

$$\xi_\pm = \mp\frac{1}{\sqrt{2}}(\xi_x \pm \imath\xi_y), \quad \xi_0 = \xi_z, \tag{15}$$

which we consider as the vector-boson creation operators ξ_m and η_m with $(L, M) = (1, M = 1, 0, -1)$. Then the states (12) are polynomials constructed from these operators which act on the vacuum state denoted by $|0\rangle$. The pairs of creation ξ_m and η_m, and annihilation ξ_m^+ and η_m^+ vector-boson operators are defined by relations

$$\xi_m^+|0\rangle = \eta_m^+|0\rangle = 0, \quad [\xi_m^+, \xi_n] = [\eta_m^+, \eta_n] = (-1)^m \delta_{-m,n}. \tag{16}$$

With the help of $\boldsymbol{\xi}$ and $\boldsymbol{\eta}$ one can construct the irreducible tensor operators

$$F_M^L = \sum_{\mu\nu} C_{1\mu 1\nu}^{LM} (\xi_\mu \xi_\nu^+ + \eta_\mu \eta_\nu^+),$$

where $C_{1\mu 1\nu}^{LM}$ are Clebsch–Gordan coefficients [8]. The vectors $\boldsymbol{\xi}^+$ and $\boldsymbol{\eta}^+$ can be chosen in the form

$$\xi_\nu^+ = (-1)^\nu \partial/\partial\xi_{-\nu}, \quad \eta_\nu^+ = (-1)^\nu \partial/\partial\eta_{-\nu},$$

i.e. the vectors $\boldsymbol{\xi}$, $\boldsymbol{\eta}$ and $\boldsymbol{\xi}^+$, $\boldsymbol{\eta}^+$ can be considered as creation and annihilation operators of two distinct kinds of vector-boson in Fock representation.

The tensor operators satisfy the following commutation relations

$$[F_{M_1}^{L_1}, F_{M_2}^{L_2}] = \sqrt{(2L_1+1)(2L_2+1)} \sum_L ((-1)^{L_1+L_2} - (-1)^L) C_{L_1 M_1 L_2 M_2}^{LM_1+M_2} \left\{ \begin{array}{ccc} L_1 & L_2 & 1 \\ 1 & 1 & 1 \end{array} \right\} F_{M_1+M_2}^L,$$

where $\{...\}$ is the 6j–Wigner symbol [8]. If we introduce $L_m = -\sqrt{2}F_m^1$ and $Q_k = -\sqrt{6}F_k^2$, we can see that operators L_m $(m = 0, \pm 1)$ and Q_k $(k = 0, \pm 1, \pm 2)$ satisfy the standard commutation relations of SU(3)group (5). It is evident that the operators L_m $(m = 0, \pm 1)$ define the algebra of angular momentum SO(3) and the operators Q_k $(k = 0, \pm 1, \pm 2)$ extend this algebra to SU(3) algebra.

Using the above definitions (15) and (16), we determine the standard boson basis

$$|k_1, k_2, k_3, k_4, k_5, k_6\rangle = (k_1!k_2!k_3!k_4!k_5!k_6!)^{-1/2} (\xi_{-1})^{k_1} (\xi_0)^{k_2} (\xi_1)^{k_3} (\eta_{-1})^{k_4} (\eta_0)^{k_5} (\eta_1)^{k_6} |0\rangle, \tag{17}$$

which is orthonormal

$$\langle k'_1, k'_2, k'_3, k'_4, k'_5, k'_6 | k_1, k_2, k_3, k_4, k_5, k_6\rangle = \delta_{k'_1 k_1} \delta_{k'_2 k_2} \delta_{k'_3 k_3} \delta_{k'_4 k_4} \delta_{k'_5 k_5} \delta_{k'_6 k_6}. \tag{18}$$

Then we expand the vectors (12) in the terms of basis (17). As the first step we apply the multipliers of (12) in the variables ξ_{-1}, ξ_0, ξ_1, η_{-1}, η_0, η_1. In fact we use only operator expansion. Because $\beta = 0$ or $\beta = 1$, we write

$$w^\beta = \sum_\nu b_\nu^\beta (\xi_{-1})^{\nu_1} (\xi_0)^{\nu_2} (\xi_1)^{\nu_3} (\eta_{-1})^{\nu_4} (\eta_0)^{\nu_5} (\eta_1)^{\nu_6}, \quad \nu \equiv (\nu_1, \nu_2, \nu_3, \nu_4, \nu_5, \nu_6). \tag{19}$$

By comparing (14) and (19), we obtain that the sum in (19) contains one term for $\beta = 0$ and four terms for $\beta = 1$:

$$b^0_{(0,0,0,0,0,0)}{=}1,\ b^1_{(0,0,2,1,0,0)}{=}1,\ b^1_{(1,0,1,0,0,1)}{=}-1,\ b^1_{(0,1,1,0,1,0)}{=}-1,\ b^1_{(0,2,0,0,0,1)}{=}1.$$

From (14) using the multinomial theorem, we also calculate the needed powers of the operators

$$(x_{10})^{n_1} = \sum_{k_1=0}^{n_1} \left(\begin{array}{c} n_1 \\ k_1 \end{array} \right) (-1)^{k_1} \xi_0^{k_1} \xi_1^{n_1-k_1} \eta_0^{n_1-k_1} \eta_1^{k_1}, \tag{20}$$

$$(\boldsymbol{\xi}^2)^{n_2} = \sum_{k_2=0}^{n_2} \left(\begin{array}{c} n_2 \\ k_2 \end{array} \right) (-1)^{k_2} 2^{k_2} \xi_{-1}^{k_2} \xi_0^{2(n_2-k_2)} \xi_1^{k_2} \eta_0^{n_1-k_1},$$

$$A^\alpha = \sum_{s\in\Omega_{s,\alpha}} \left(\begin{array}{c} \alpha \\ s_1 s_2 s_3 s_4 s_5 s_6 s_7 \end{array} \right) (-1)^{s_1+s_3+s_5+s_7} \xi_{-1}^{s_2+s_4+s_6+2s_7} \xi_0^{s_1+2s_3+s_4}$$
$$\times \xi_1^{s_1+s_2+2s_5+s_6} \eta_{-1}^{s_1+s_3+2s_5+s_6} \eta_0^{s_1+2s_2+s_4} \eta_1^{s_3+s_4+s_6+2s_7},$$

where a set of indices runs within the range $\Omega_{s,\alpha} = \{s_1, ..., s_7 | s_1 \geq 0, ..., s_7 \geq 0, s_1 + ... + s_7 = \alpha\}$.

So, we have the highest-weight vector of the BM basis

$$|\beta n_0 n_1 n_2 \alpha\rangle = \sum_{\nu} \sum_{k_1=0}^{n_1} \sum_{k_2=0}^{n_2} \sum_{s\in\Omega_{s,\alpha}} b_\nu^\beta (-1)^{k_1+k_2+s_1+s_3+s_5+s_7} 2^{k_2+s_1+s_2+s_3+s_4+s_6} \tag{21}$$
$$\times \begin{pmatrix} n_1 \\ k_1 \end{pmatrix} \begin{pmatrix} n_2 \\ k_2 \end{pmatrix} \begin{pmatrix} \alpha \\ s_1 s_2 s_3 s_4 s_5 s_6 s_7 \end{pmatrix} (\xi_{-1})^{\gamma_1} (\xi_0)^{\gamma_2} (\xi_1)^{\gamma_3} (\eta_{-1})^{\gamma_4} (\eta_0)^{\gamma_5} (\eta_1)^{\gamma_6} |0\rangle,$$

where the set multi-indices γ_1,...,γ_6 is determined by the relations

$$\gamma_1 = \nu_1 + k_2 + s_2 + s_4 + s_6 + 2s_7, \quad \gamma_2 = \nu_2 + k_1 + 2(n_2 - k_2) + s_1 + 2s_3 + s_4, \tag{22}$$
$$\gamma_3 = \nu_3 + n_0 + n_1 - k_1 + k_2 + s_1 + s_2 + 2s_5 + s_6, \quad \gamma_4 = \nu_4 + s_1 + s_3 + 2s_5 + s_6,$$
$$\gamma_5 = \nu_5 + n_1 - k_1 + s_1 + 2s_2 + s_4, \quad \gamma_6 = \nu_6 + k_1 + s_3 + s_4 + s_6 + 2s_7.$$

From (21) in the boson representation (17) we obtain the required BM states

$$|\beta n_0 n_1 n_2 \alpha\rangle = \sum_{\nu} \sum_{k_1=0}^{n_1} \sum_{k_2=0}^{n_2} \sum_{s\in\Omega_{s,\alpha}} B(\beta, n_0, n_1, n_2, \alpha, \nu, k_1, k_2, s) |\gamma_1, \gamma_2, \gamma_3, \gamma_4, \gamma_5, \gamma_6\rangle, \tag{23}$$

where the coefficients $B(\beta, n_0, n_1, n_2, \alpha, \nu, k_1, k_2, s)$ have the following form

$$B(\beta, n_0, n_1, n_2, \alpha, \nu, k_1, k_2, s) = b_\nu^\beta (-1)^{k_1+k_2+s_1+s_3+s_5+s_7} 2^{k_2+s_1+s_2+s_3+s_4+s_6}$$
$$\times \begin{pmatrix} n_1 \\ k_1 \end{pmatrix} \begin{pmatrix} n_2 \\ k_2 \end{pmatrix} \begin{pmatrix} \alpha \\ s_1 s_2 s_3 s_4 s_5 s_6 s_7 \end{pmatrix} \sqrt{\gamma_1! \gamma_2! \gamma_3! \gamma_4! \gamma_5! \gamma_6!}.$$

Step 4. The overlap integrals are determined by the relation

$$\langle \beta' n_0' n_1' n_2' \alpha' | \beta n_0 n_1 n_2 \alpha\rangle = \delta_{\beta'\beta} \sum_{\nu', k_1', k_2', s'} \sum_{\nu, k_1, k_2, s} B(\beta', n_0', n_1', n_2', \alpha', \nu', k_1', k_2', s') \tag{24}$$
$$\times B(\beta, n_0, n_1, n_2, \alpha, \nu, k_1, k_2, s) \delta_{\gamma_1\gamma_1'} \delta_{\gamma_2\gamma_2'} \delta_{\gamma_3\gamma_3'} \delta_{\gamma_4\gamma_4'} \delta_{\gamma_5\gamma_5'} \delta_{\gamma_6\gamma_6'},$$

where domains of summation are determined by the definitions (19) and (20).

Output of Step 4. The overlap integral (24) has been calculated with algorithm implemented in Fortran. The obtained results for $\lambda = 0, ..., 10$ and $\mu = 1, ..., 10$ for $\lambda \geq \mu$ and corresponding sets of values α and L (for example, see Table 1 of ref. [12]) coincide up to 10 digits with results of calculations obtained with help of symbolic algorithm [12] implemented in Wolfram Mathematica.

3. Orthogonalisation of the BM basis

Let us construct the orthonormal basis in the space spanned by the non-canonical BM vectors (6), $(M = L)$. For this purpose, we propose a bit more efficient form of the Gram–Schmidt orthonormalisation procedure

$$|z_i\rangle \equiv \left| \begin{array}{c} (\lambda, \mu) \\ f_i, L, L \end{array} \right\rangle = \sum_{\alpha=0}^{\alpha_{\max}} A_{i,\alpha}^{(\lambda,\mu)}(L) \left| \begin{array}{c} (\lambda, \mu)_B \\ \alpha, L, L \end{array} \right\rangle \equiv \sum_{\alpha=0}^{\alpha_{\max}} A_{i,\alpha}^{(\lambda,\mu)}(L) |u_\alpha\rangle. \tag{25}$$

Here multiplicity index i is introduced to distinguish the orthonormalized states. The symbols $A_{i,\alpha}^{(\lambda,\mu)}(L)$ denotes the matrix elements of the upper triangular matrix of the BM basis orthonormalization coefficients. These coefficients fulfill the following condition

$$A_{i,\alpha}^{(\lambda,\mu)}(L) = 0, \quad \text{if } i > \alpha. \tag{26}$$

Because the BM vectors (6) are linearly independent, one can require the orthonormalization properties for the vectors (25)

$$\left\langle \begin{matrix} (\lambda,\mu) \\ f_i, L, L \end{matrix} \middle| \begin{matrix} (\lambda,\mu) \\ f_k, L, L \end{matrix} \right\rangle = \delta_{ik}. \tag{27}$$

Step 5. Gramian of a set of BM eigenvectors $u_{\alpha_{\max}}, ..., u_0$ from r.h.s. of (25) in notations (6)

$$G(u_{\alpha_{\max}}, ..., u_0) = \begin{vmatrix} \langle u_{\alpha_{\max}}|u_{\alpha_{\max}}\rangle & \dots & \langle u_{\alpha_{\max}}|u_1\rangle & \langle u_{\alpha_{\max}}|u_0\rangle \\ \langle u_{\alpha_{\max}-1}|u_{\alpha_{\max}}\rangle & \dots & \langle u_{\alpha_{\max}-1}|u_1\rangle & \langle u_{\alpha_{\max}-1}|u_0\rangle \\ \vdots & \ddots & \vdots & \vdots \\ \langle u_1|u_{\alpha_{\max}}\rangle & \dots & \langle u_1|u_1\rangle & \langle u_1|u_0\rangle \\ \langle u_0|u_{\alpha_{\max}}\rangle & \dots & \langle u_0|u_1\rangle & \langle u_0|u_0\rangle \end{vmatrix}.$$

Set of orthogonal (not orthonormal) vectors are calculated in the following way [15]:

$$|y_{\alpha_{\max}}\rangle = |u_{\alpha_{\max}}\rangle, \qquad \bar{A}^{(\lambda,\mu)}_{\alpha_{\max},\alpha_{\max}}(L) = 1,$$

$$\bar{A}^{(\lambda,\mu)}_{\alpha_{\max},s}(L) = 0, \qquad s = 0, ..., \alpha_{\max} - 1,$$

$$|y_{\alpha_{\max}-1}\rangle = \begin{vmatrix} \langle u_{\alpha_{\max}}|u_{\alpha_{\max}}\rangle & |u_{\alpha_{\max}}\rangle \\ \langle u_{\alpha_{\max}-1}|u_{\alpha_{\max}}\rangle & |u_{\alpha_{\max}-1}\rangle \end{vmatrix},$$

$$\bar{A}^{(\lambda,\mu)}_{\alpha_{\max}-1,\alpha_{\max}-1}(L) = \langle u_{\alpha_{\max}}|u_{\alpha_{\max}}\rangle,$$

$$\bar{A}^{(\lambda,\mu)}_{\alpha_{\max}-1,\alpha_{\max}}(L) = -\langle u_{\alpha_{\max}-1}|u_{\alpha_{\max}}\rangle,$$

$$\bar{A}^{(\lambda,\mu)}_{\alpha_{\max}-1,s}(L) = 0, \qquad s = 0, ..., \alpha_{\max} - 2,$$

$$...,$$

$$|y_{\alpha_{\max}-t}\rangle = \begin{vmatrix} \langle u_{\alpha_{\max}}|u_{\alpha_{\max}}\rangle & \dots & \langle u_{\alpha_{\max}}|u_{\alpha_{\max}-t+1}\rangle & |u_{\alpha_{\max}}\rangle \\ \langle u_{\alpha_{\max}-1}|u_{\alpha_{\max}}\rangle & \dots & \langle u_{\alpha_{\max}-1}|u_{\alpha_{\max}-t+1}\rangle & |u_{\alpha_{\max}-1}\rangle \\ \vdots & \ddots & \vdots & \vdots \\ \langle u_{\alpha_{\max}-t+1}|u_{\alpha_{\max}}\rangle & \dots & \langle u_{\alpha_{\max}-t+1}|u_{\alpha_{\max}-t+1}\rangle & |u_{\alpha_{\max}-t+1}\rangle \\ \langle u_{\alpha_{\max}-t}|u_{\alpha_{\max}}\rangle & \dots & \langle u_{\alpha_{\max}-t}|u_{\alpha_{\max}-t+1}\rangle & |u_{\alpha_{\max}-t}\rangle \end{vmatrix},$$

$$\bar{A}^{(\lambda,\mu)}_{\alpha_{\max}-t,\alpha_{\max}-t'}(L) = (-1)^{t+t'+1} \begin{vmatrix} \langle u_{\alpha_{\max}}|u_{\alpha_{\max}}\rangle & \dots & \langle u_{\alpha_{\max}}|u_{\alpha_{\max}-t+1}\rangle \\ \langle u_{\alpha_{\max}-1}|u_{\alpha_{\max}}\rangle & \dots & \langle u_{\alpha_{\max}-1}|u_{\alpha_{\max}-t+1}\rangle \\ \vdots & \ddots & \vdots \\ \langle u_{\alpha_{\max}-t'-1}|u_{\alpha_{\max}}\rangle & \dots & \langle u_{\alpha_{\max}-t'-1}|u_{\alpha_{\max}-t+1}\rangle \\ \langle u_{\alpha_{\max}-t'+1}|u_{\alpha_{\max}}\rangle & \dots & \langle u_{\alpha_{\max}-t'+1}|u_{\alpha_{\max}-t+1}\rangle \\ \vdots & \ddots & \vdots \\ \langle u_{\alpha_{\max}-t+1}|u_{\alpha_{\max}}\rangle & \dots & \langle u_{\alpha_{\max}-t+1}|u_{\alpha_{\max}-t+1}\rangle \\ \langle u_{\alpha_{\max}-t}|u_{\alpha_{\max}}\rangle & \dots & \langle u_{\alpha_{\max}-t}|u_{\alpha_{\max}-t+1}\rangle \end{vmatrix},$$

$$t' = 0, ..., t,$$

$$\bar{A}^{(\lambda,\mu)}_{\alpha_{\max}-t,s}(L) = 0, \qquad s = 0, ..., \alpha_{\max} - t - 1,$$

where $t = 0, 1, ..., \alpha_{\max}$. In result we have a set of the orthonormal vectors and coefficients:

$$|z_i\rangle = \frac{|y_i\rangle}{\sqrt{\langle y_i|y_i\rangle}} = \frac{|y_i\rangle}{\sqrt{G_{i+1}G_i}}, \quad \langle y_i|y_i\rangle = G_{i+1}G_i, \quad i = \alpha_{\max}, ..., 0, \quad G_{\alpha_{\max}+1} = 1,$$

$$A^{(\lambda,\mu)}_{\alpha_{\max}-t,s'}(L) = \frac{\bar{A}^{(\lambda,\mu)}_{\alpha_{\max}-t,s'}(L)}{\sqrt{G_{\alpha_{\max}-t+1}G_{\alpha_{\max}-t'}}}.$$

Output of Step 5. The required set of the coefficients $A^{(\lambda,\mu)}_{i,\alpha}(L)$ are the components of the orthonormal vector $|z_i\rangle$, at $i=\alpha_{\max},\alpha_{\max}-1,...,0$ has been calculated with the above algorithm implemented in Fortran. Note, the orthonormalization procedure is performed in the reverse order with respect to the one adopted in [15], that allows us to obtain the same orthonormal basis as in the papers [11, 12]. The obtained results for $\lambda,\mu=0,...,10$, where $\lambda\geq\mu$ coincide up to 10 digits with results of calculations obtained by the symbolic algorithm [12] implemented in Wolfram Mathematica.

4. Action of the the quadrupole operator onto the orthonormal basis

Step 6. Following the paper [14], we determine the action of the zero component Q_0 of the second order generator of SU(3) group onto the BM basis vectors

$$Q_0\left|\begin{array}{c}(\lambda,\mu)_B\\ \alpha,L,L\end{array}\right\rangle=\sum_{\substack{k=0,1,2\\ s=0,\pm1}}a^{(k)}_s\left|\begin{array}{c}(\lambda,\mu)_B\\ \alpha+s,L+k,L\end{array}\right\rangle. \tag{28}$$

The coefficients $a^{(k)}_s$ can be calculated as in [13] and in [14]. To calculate action of Q_0 onto the orthogonal BM basis vectors (25), we determine the inverse transformation $\tilde{A}^{(\lambda,\mu)}_{i,\alpha}(L)$ taken from the formula (25)

$$\left|\begin{array}{c}(\lambda,\mu)_B\\ \alpha,L,L\end{array}\right\rangle=\sum_{i=0}^{\alpha}\tilde{A}^{(\lambda,\mu)}_{i,\alpha}(L)\left|\begin{array}{c}(\lambda,\mu)\\ f_i,L,L\end{array}\right\rangle, \tag{29}$$

where the following relations take place

$$\sum_i\tilde{A}^{(\lambda,\mu)}_{i,\alpha'}(L)A^{(\lambda,\mu)}_{i,\alpha}(L)=\delta_{\alpha',\alpha}\quad\text{and}\quad\sum_\alpha\tilde{A}^{(\lambda,\mu)}_{i',\alpha}(L)A^{(\lambda,\mu)}_{i,\alpha}(L)=\delta_{i',i}. \tag{30}$$

Using (28), (29), and (30), we obtain the action of the zero component Q_0 of the quadrupole operator onto the orthogonal BM basis vectors as

$$Q_0\left|\begin{array}{c}(\lambda,\mu)\\ f_i,L,L\end{array}\right\rangle=\sum_{\substack{j=0,...,\alpha_{\max}\\ k=0,1,2}}q^{(\lambda,\mu)}_{i,j,k}(L)\left|\begin{array}{c}(\lambda,\mu)\\ f_j,L+k,L\end{array}\right\rangle, \tag{31}$$

where the coefficients $q^{(\lambda,\mu)}_{i,j,k}(L)$ are calculated by the formula

$$q^{(\lambda,\mu)}_{i,j,k}(L)=\sum_{\substack{\alpha=0,...,\alpha_{\max}\\ s=0,\pm1}}A^{(\lambda,\mu)}_{i,\alpha}(L)a^{(k)}_s\tilde{A}^{(\lambda,\mu)}_{j,(\alpha+s)}(L+k), \tag{32}$$

and $\tilde{A}^{(\lambda,\mu)}_{i,\alpha}(L)$ are elements of the inverse and the transpose of the matrix $A^{(\lambda,\mu)}$

$$\tilde{A}^{(\lambda,\mu)}_{i,\alpha}(L)=(A^{-1})^{(\lambda,\mu)}_{\alpha,i}(L). \tag{33}$$

4.1. Calculations of the action of the quadrupole operator zero component onto the BM basis

Let us calculate action of the operator Q_0 according Eq. (28)

$$Q_0\left|\begin{array}{c}(\lambda,\mu)_B\\ \alpha\ L\ L\end{array}\right\rangle=\sum_{s=0,\pm1}\left\{\tilde{a}^{(0)}_s\left|\begin{array}{c}(\lambda,\mu)_B\\ \alpha{+}s\ L\ L\end{array}\right\rangle+\tilde{a}^{(1)}_s\left|\begin{array}{c}(\lambda,\mu)_B\\ \alpha{+}s\ L{+}1\ L\end{array}\right\rangle+\tilde{a}^{(2)}_s\left|\begin{array}{c}(\lambda,\mu)_B\\ \alpha{+}s\ L{+}2\ L\end{array}\right\rangle\right\} \tag{34}$$

$$=\sum_{s=0,\pm1}\left\{\tilde{a}^{(0)}_s\left|\begin{array}{c}(\lambda,\mu)_B\\ \alpha{+}s\ L\ L\end{array}\right\rangle+\tilde{a}^{(1)}_sL_{-1}\left|\begin{array}{c}(\lambda,\mu)_B\\ \alpha{+}s\ L{+}1\ L{+}1\end{array}\right\rangle+\tilde{a}^{(2)}_s(L_{-1})^2\left|\begin{array}{c}(\lambda,\mu)_B\\ \alpha{+}s\ L{+}2\ L{+}2\end{array}\right\rangle\right\},$$

where the coefficients $\tilde{a}_s^{(k)} \equiv \tilde{a}_s^{(k)}(L)$ are related to $a_s^{(k)} \equiv a_s^{(k)}(L)$ by the factors:

$$\tilde{a}_s^{(2)} = a_s^{(2)}\sqrt{L+2}\sqrt{2L+3}, \qquad \tilde{a}_s^{(1)} = a_s^{(1)}\sqrt{L+1}, \qquad \tilde{a}_s^{(0)} = a_s^{(0)}. \tag{35}$$

We rewrite the BM basis vectors (12) in the form

$$\left| \begin{array}{c} (\lambda,\mu)_B \\ \alpha\ L\ L \end{array} \right\rangle \equiv |\beta n_0 n_1 n_2 \alpha\rangle = c_1^{\beta} c_2^{n_0} c_3^{n_1} c_4^{n_2} c_5^{\alpha}|0\rangle, \tag{36}$$

where $c_1 = w$, $c_2 = \xi_1$, $c_3 = x_{10}$, $c_4 = \boldsymbol{\xi}^2$, $c_5 = A$, and the powers $n_0 = L-\mu+2\alpha$, $n_1 = \mu-2\alpha-\beta$, $n_2 = (\lambda+\mu-L-2\alpha-\beta)/2$, and β are defined by relations (14) and (11). The expression $\xi_{-1}, \xi_1, \eta_{-1}, \eta_0$ in terms of $c_1, ..., c_5$ give us the formal expressions: $\xi_1 = c_2$, $\eta_0 = c_3/c_2 + \xi_0\eta_1/c_2$, $\xi_{-1} = -c_4/2/c_2 + \xi_0^2/2/c_2$, $\eta_{-1} = (c_1 - (-\xi_0 c_3 - (1/2)\xi_0^2\eta_1 + (1/2)\eta_1 c_4))/c_2^2$, and the following relation among the components $c_1, ..., c_5$:

$$c_1^2 = -c_5 c_2^2 + c_4 c_3^2.$$

Firstly, we calculate action of operators Q_0, L_{-1} and L_{-1}^2 over eigenvectors (36) and express them in terms of components $c_1, ..., c_5$. Using the above relations, implemented in REDUCE we obtain action of operators Q_0, L_{-1} and L_{-1}^2 onto eigenvectors (36). For even $\lambda+\mu-L$ we get:

$$Q_0\left| \begin{array}{c} (\lambda,\mu)_B \\ \alpha\ L\ L \end{array} \right\rangle = [6\alpha c_2^{n_0-2} c_3^{n_1+2} c_4^{n_2+1} c_5^{\alpha-1} + 6\alpha\xi_0^2 c_2^{n_0-2} c_3^{n_1+2} c_4^{n_2} c_5^{\alpha-1} + 6n_2\xi_0^2 c_2^{n_0} c_3^{n_1} c_4^{n_2-1} c_5^{\alpha}$$
$$+(-4\alpha - n_0 + n_1 - 2n_2) c_2^{n_0} c_3^{n_1} c_4^{n_2} c_5^{\alpha} + 12\alpha\xi_0 c_1 c_2^{n_0-2} c_3^{n_1+1} c_4^{n_2} c_5^{\alpha-1}]|0\rangle$$
$$L_{-1}\left| \begin{array}{c} (\lambda,\mu)_B \\ \alpha{+}s\ L{+}1\ L{+}1 \end{array} \right\rangle = [(-n_1+1) c_2^{n_0+2} c_3^{n_1-2} c_4^{n_2-1} c_5^{\alpha+1} + n_1 c_2^{n_0} c_3^{n_1} c_4^{n_2} c_5^{\alpha}$$
$$+(n_0+n_1+1)\xi_0 c_1 c_2^{n_0} c_3^{n_1-1} c_4^{n_2-1} c_5^{\alpha}]|0\rangle$$
$$(L_{-1})^2\left| \begin{array}{c} (\lambda,\mu)_B \\ \alpha{+}s\ L{+}2\ L{+}2 \end{array} \right\rangle = [(2n_0^2 + 4n_0 n_1 + 7n_0 + 2n_1^2 + 7n_1 + 6)/2\xi_0^2 c_2^{n_0} c_3^{n_1} c_4^{n_2-1} c_5^{\alpha}$$
$$+(-n_1^2 + n_1) c_2^{n_0+2} c_3^{n_1-2} c_4^{n_2-1} c_5^{\alpha+1} + (-n_0 + 2n_1^2 - n_1 - 2)/2 c_2^{n_0} c_3^{n_1} c_4^{n_2} c_5^{\alpha}$$
$$+(2n_0 n_1 + 2n_1^2 + 3n_1)\xi_0 c_1 c_2^{n_0} c_3^{n_1-1} c_4^{n_2-1} c_5^{\alpha}]|0\rangle$$

and for odd $\lambda+\mu-L$ we get:

$$Q_0\left| \begin{array}{c} (\lambda,\mu)_B \\ \alpha\ L\ L \end{array} \right\rangle = [12\alpha\xi_0 c_2^{n_0-2} c_3^{n_1+3} c_4^{n_2+1} c_5^{\alpha-1} + (-12\alpha - 6)\xi_0 c_2^{n_0} c_3^{n_1+1} c_4^{n_2} c_5^{\alpha}$$
$$+6\alpha c_1 c_2^{n_0-2} c_3^{n_1+2} c_4^{n_2+1} c_5^{\alpha-1} + 6\alpha\xi_0^2 c_1 c_2^{n_0-2} c_3^{n_1+2} c_4^{n_2} c_5^{\alpha-1} + 6n_2\xi_0^2 c_1 c_2^{n_0} c_3^{n_1} c_4^{n_2-1} c_5^{\alpha}$$
$$+(-4\alpha - n_0 + n_1 - 2n_2 - 3) c_1 c_2^{n_0} c_3^{n_1} c_4^{n_2} c_5^{\alpha}]|0\rangle$$
$$L_{-1}\left| \begin{array}{c} (\lambda,\mu)_B \\ \alpha{+}s\ L{+}1\ L{+}1 \end{array} \right\rangle = [(n_0+n_1+2)\xi_0 c_2^{n_0} c_3^{n_1+1} c_4^{n_2} c_5^{\alpha} + (n_1+1) c_1 c_2^{n_0} c_3^{n_1} c_4^{n_2} c_5^{\alpha}]|0\rangle$$
$$(L_{-1})^2\left| \begin{array}{c} (\lambda,\mu)_B \\ \alpha{+}s\ L{+}2\ L{+}2 \end{array} \right\rangle = [(-2n_0 n_1 - 2n_1^2 - 5n_1)\xi_0 c_2^{n_0+2} c_3^{n_1-1} c_4^{n_2-1} c_5^{\alpha+1}$$
$$+(2n_0 n_1 + 2n_0 + 2n_1^2 + 7n_1 + 5)\xi_0 c_2^{n_0} c_3^{n_1+1} c_4^{n_2} c_5^{\alpha} + (-n_1^2 + n_1) c_1 c_2^{n_0+2} c_3^{n_1-2} c_4^{n_2-1} c_5^{\alpha+1}$$
$$+(2n_0^2 + 4n_0 n_1 + 11n_0 + 2n_1^2 + 11n_1 + 15)/2\xi_0^2 c_1 c_2^{n_0} c_3^{n_1} c_4^{n_2-1} c_5^{\alpha}$$
$$+(-n_0 + 2n_1^2 + 3n_1 - 1)/2 c_1 c_2^{n_0} c_3^{n_1} c_4^{n_2} c_5^{\alpha}]|0\rangle.$$

Using the above actions of the operators Q_0, L_{-1} and L_{-1}^2 on eigenvectors (36) and extracting the coefficients at $c_1, ..., c_5$, we arrive to a set of equations with respect to unknown coefficients:

$\tilde{a}_1^{(0)}$, $\tilde{a}_0^{(0)}$, $\tilde{a}_{-1}^{(0)}$, $\tilde{a}_0^{(1)}$, $\tilde{a}_1^{(1)}$, $\tilde{a}_{-1}^{(1)}$, $\tilde{a}_0^{(2)}$, $\tilde{a}_1^{(2)}$, $\tilde{a}_1^{(2)}$. From formula (34) and from action of the operators Q_0, L_{-1} and L_{-1}^2 on functions (36) we obtain:

$$Q_0 \left| \begin{array}{c} (\lambda,\mu)_B \\ \alpha\ L\ L \end{array} \right\rangle - \sum_{s=0,,\pm 1} \left\{ \tilde{a}_s^{(0)} \left| \begin{array}{c} (\lambda,\mu)_B \\ \alpha{+}s\ L\ L \end{array} \right\rangle + \tilde{a}_s^{(1)} L_{-1} \left| \begin{array}{c} (\lambda,\mu)_B \\ \alpha{+}s\ L{+}1\ L{+}1 \end{array} \right\rangle \right.$$
$$\left. + \tilde{a}_s^{(2)} (L_{-1})^2 \left| \begin{array}{c} (\lambda,\mu)_B \\ \alpha{+}s\ L{+}2\ L{+}2 \end{array} \right\rangle \right\} = 0. \qquad (37)$$

The solution of the set of equations obtained by extraction of coefficients at the same powers of the operators c_1,...,c_5 gives values of unknown coefficients $\tilde{a}_1^{(0)}$, $\tilde{a}_0^{(0)}$, $\tilde{a}_{-1}^{(0)}$, $\tilde{a}_0^{(1)}$, $\tilde{a}_1^{(1)}$, $\tilde{a}_{-1}^{(1)}$, $\tilde{a}_0^{(2)}$, $\tilde{a}_1^{(2)}$, $\tilde{a}_1^{(2)}$. Finally, from (35) we arrive to needed values of $a_1^{(0)}$, $a_0^{(0)}$, $a_{-1}^{(0)}$, $a_0^{(1)}$, $a_1^{(1)}$, $a_{-1}^{(1)}$, $a_0^{(2)}$, $a_1^{(2)}$, $a_1^{(2)}$. In result, the action of zero component Q_0 of the quadrupole operator onto the nonorthogonal BM basis (12), i.e. the coefficients $a_s^{(k)}$ of expansion (28), reads as:

$$\begin{aligned}
& a_0^{(2)} = \frac{6(\lambda+\mu-L-2\alpha-\beta)}{((L+2)(2L+3))^{1/2}}, \quad a_{-1}^{(2)} = \frac{12\alpha}{((L+2)(2L+3))^{1/2}}, \quad a_{-1}^{(2)} = 0, \qquad (38)\\
& a_0^{(1)} = -6\frac{2\alpha\beta(L+2\alpha-\mu+1)+(\lambda+\mu-L-2\alpha)[\mu-2\alpha]}{(L+2)(L+1)^{1/2}} - \frac{6\beta}{(L+1)^{1/2}},\\
& a_{-1}^{(1)} = \frac{12\alpha([L]-\mu+2\alpha)}{(L+2)(L+1)^{1/2}}, \quad a_1^{(1)} = \frac{6\beta(\lambda+\mu-L-2\alpha-\beta)[\mu-2\alpha-\beta]}{(L+2)(L+1)^{1/2}},\\
& a_0^{(0)} = 4\alpha\frac{L(L+1)-3(L+2\alpha-\mu+\beta)^2}{(L+1)(2L+3)} - 2(\lambda+\mu-L-\beta-2\alpha)\frac{L(L+1)-3(\mu-2\alpha)^2}{(L+1)(2L+3)}\\
& -(L-[2\mu]+4\alpha+\beta)\left(1+\frac{3\beta}{L+1}\right),\\
& a_{-1}^{(0)} = \frac{[12\alpha](L-\mu+2\alpha)(L-\mu+2\alpha-1)}{(L+1)(2L+3)},\\
& a_1^{(0)} = -\frac{6(\lambda+\mu-L-2\alpha-\beta)(\mu-2\alpha-\beta)(\mu-2\alpha-\beta-1)}{(L+1)(2L+3)},\\
& \beta = \begin{cases} 0, & \lambda+\mu-L \text{ even},\\ 1, & \lambda+\mu-L \text{ odd}. \end{cases}
\end{aligned}$$

Note, there are five misprints in formulas (2.4) of Ref. [14], that are corrected in the above expressions (38). They are marked by the square brackets.

Output of Step 6. The set of matrix elements $q_{i,j,k}^{(\lambda,\mu)}(L)$ has been calculated with algorithm implemented in Fortran. The obtained results for $\lambda,\mu = 0,...,10$, where $\lambda \geq \mu$ (the corresponding sets of values α and L (for example see tables 1 of ref. [12])) coincide up to 10 digits with results of calculations obtained with help of symbolic algorithm [12] implemented in Wolfram Mathematica. Note that the coefficients $q_{i,j,k}^{(\lambda,\mu)}(L)$ for up to $\mu = 3$ were calculated as well and their values are equal to those presented in Table 1 of Ref. [14] except values for the following sets of indices: $k = 0$,$\mu = 3$: $q_{1,1,k}^{(\lambda,\mu)}(L)$ for $\lambda - L$ even, $q_{1,0,k}^{(\lambda,\mu)}(L)$ and $q_{0,1,k}^{(\lambda,\mu)}(L)$ for $\lambda - L$ odd; $k = 1$, $\mu = 3$: $q_{1,1,k}^{(\lambda,\mu)}(L)$ for $\lambda - L$ odd, $q_{0,0,k}^{(\lambda,\mu)}(L)$ and $q_{1,0,k}^{(\lambda,\mu)}(L)$ for $L = \lambda + 1$, $\lambda - L$ odd, $q_{0,0,k}^{(\lambda,\mu)}(L)$ for $L = \lambda + 2$, $\lambda - L$ even. The corrected expressions are shown in Appendix.

4.2. Calculations of action of the quadrupole operator onto the orthonormalized BM basis
The matrix elements of the quadrupole operators, generators of the group SU(3), can be expressed as the reduced matrix elements by means of the Wigner–Eckart theorem

$$\left\langle \begin{array}{c}(\lambda,\mu)\\ j,L+k,M\end{array} \middle| Q_m \middle| \begin{array}{c}(\lambda,\mu)\\ i,L,M'\end{array} \right\rangle = \frac{(LM'\,2m|L+k,M)}{\sqrt{2(L+k)+1}} \left\langle \begin{array}{c}(\lambda,\mu)\\ j,L+k\end{array} \middle\| Q \middle\| \begin{array}{c}(\lambda,\mu)\\ i,L\end{array} \right\rangle . \quad (39)$$

The corresponding reduced matrix elements are determined by the formula

$$\left\langle \begin{array}{c}(\lambda,\mu)\\ j,L+k\end{array} \middle\| Q \middle\| \begin{array}{c}(\lambda,\mu)\\ i,L\end{array} \right\rangle = (-1)^k \frac{\sqrt{2L+1}}{(L+k,L,20|LL)} q^{(\lambda,\mu)}_{i,j,k}(L), \quad (40)$$

where the coefficients $q^{(\lambda,\mu)}_{i,j,k}(L)$ are defined by (32). In this definition, $k \geq 0$. Dimension of subspace of the ket vectors $|(\lambda,\mu)iLM\rangle$ at fixed λ and μ are defined by formula (7). The dimension of this subspace determines the complexity of the above algorithms, i.e., requirements on the computer memory and execution time.

5. Conclusions

We present the practical algorithm implemented in Fortran for constructing the non-canonical Bargmann–Moshinsky (BM) basis with the highest weight vectors of SO(3) irreps., which can be used for calculating spectra and electromagnetic transitions in molecular and nuclear physics. The orthonormalisation algorithm [15] applied in Section 3, as well as recursion algorithm [12], allows one to calculate the orthonormalized BM basis in Fortran and Wolfram Mathematica, respectively. The distinct advantage of such orthonormalisation is that it does not involve any square root operation on the expressions coming from the previous recursion steps of the conventional Gram–Schmidt algorithm. This makes the proposed method very suitable for large-scale calculations of spectral characteristics (especially close to resonances) of quantum systems under consideration and to study their analytical properties for understanding the dominant symmetries. The formalism of partner groups $G = \mathrm{SU}(3) \times \overline{\mathrm{SU}(3)}$ allows for simulation of the intrinsic properties of quantum systems (also nuclei), including their intrinsic symmetries. The presented nuclear SU(3) model is extended and allows for additional intrinsic structure, especially it allows to construct terms having required point symmetries. Calculations of spectral characteristics of the above nuclei models and study of their dominant symmetries will be done in our next publications.

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Appendix

There are misprints in expressions of the coefficients $q^{(\lambda,3)}_{i,j,k}$ in Table 1 of Ref. [14], that are corrected in the below expressions. For $\lambda - L$ even:

$$q^{(\lambda,3)}_{1,1,0} = \left(\frac{12(-2+L)(-1+L)(2-L-\lambda)(6+L+\lambda)}{Y_3(\lambda,L)} + 6(2+\lambda) - L(3+2\lambda+L(15+2\lambda)) \right) \frac{1}{(1+L)(3+2L)}.$$

For $\lambda - L$ odd:

$$q^{(\lambda,3)}_{1,0,0} = q^{(\lambda,3)}_{0,1,0} = -\frac{12\,(3(2+\lambda)(3+\lambda)(4+L+\lambda)(3-L+\lambda)(-2+L)(-1+L)(3+L)(2+L))^{1/2}}{\tilde{Y}_3(\lambda,L)(1+L)(3+2L)},$$

$$q_{1,1,1}^{(\lambda,3)}=\frac{6(2(-1+L)(7+L+\lambda)-Y_3(\lambda,L+1))}{(1+L)}\left(\frac{L(2+\lambda)(1-L+\lambda)}{\tilde{Y}_3(\lambda,L)Y_3(\lambda,L+1)(2+L)(3+2L)}\right)^{1/2}.$$

For $L=\lambda+1$ and $\lambda-L$ odd:

$$q_{0,0,1}^{(\lambda,3)}=\frac{30(4+\lambda)}{(2+\lambda)}\left(\frac{6(-1+\lambda)}{(3+\lambda)(20+\lambda)(5+2\lambda)}\right)^{1/2},$$

$$q_{1,0,1}^{(\lambda,3)}=12\left(\frac{\lambda(4+\lambda)}{\tilde{Y}_3(\lambda,\lambda+1)(2+\lambda)}\right)^{1/2}.$$

For $L=\lambda+2$ and $\lambda-L$ even:

$$q_{0,0,1}^{(\lambda,3)}=-\frac{6(3\lambda)^{1/2}}{(3+\lambda)},$$

where

$$Y_3(\lambda,L)=4(\lambda+L+6)(\lambda-L+2)+3(L+2)(L+3),$$
$$\tilde{Y}_3(\lambda,L)=4(\lambda+L+5)(\lambda-L+3)+(L+2)(L+3).$$

Thus, table 1 of Ref. [14] together with the above expressions have been used to test the *Step 6* of the proposed procedure implemented in Fortran.

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