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On calculation of quadrupole operator in orthogonal Bargmann-Moshinsky basis of SU(3) group

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Abstract. Construction of orthonormal states of the noncanonical Bargmann-Moshinsky basis in a nonmultiplicity-free case is presented. It is implemented by means of the both Gram-Schmidt procedure and solving eigenvalue problem of the Hermitian labeling operator of an envelope algebra of the SU(3) group. Calculations of the quadrupole and Bargmann-Moshinsky operators and its matrix elements needed for construction of the nuclear models are tested. Comparison of results in the integer and floating point calculations with help of the proposed procedures implemented in Wolfram Mathematica is given.

1. Introduction

The quadrupole momentum operator is one of the most important quantities applied in nuclear physics modeling and large-scaled calculations and treated as generator of SU(3) group [1, 2, 3, 4]. It should be noted that the quadrupole momentum is an essential part in construction of the Hamiltonians for nuclear models with a tetrahedral and octahedral symmetries [5, 6], which are studied by modern experiments [7, 8]. However, in spite of a long history [9], there are still no sufficient efficient and cost effective algorithms and programs for constructing the required orthogonal SU(3) bases of the non-canonical group reduction chain of subgroups SU(3)$\supset$ SO(3) $\supset$ SO(2) and computing tensor operators in these bases similar as a conventional program implemented in the canonical Gel'fand-Tseitlin basis [10]. Another problem is that the above non-canonical group reduction chain is known of one label missing to characterize the states completely [11, 12, 13, 14]. Solving these problem using adapted versions of Gram-Schmidt procedure for construction of an orthogonal Bargmann-Moshinsky(BM) basis [15] has been subject of our study given in the recent papers [16, 17, 18]. Below they are labeled as I, II and III and their main results are summarized briefly.

The degeneracy problem for SO(3) states in the SU(3) representation can be also solved by introducing of an additional Hermitian operator $X^{(3)}$ proposed by Bargmann and Moshinsky [15] of an enveloping algebra of the SU(3) group [19]. The eigenvalues of the operator $X^{(3)}$ provide the missing label for the state vectors.

In this paper we developed effective procedures for computing matrices of the quadrupole operators as well as the matrices of the operator $X^{(3)}$ in the orthogonal BM basis. The developed procedure for calculation of quadrupole operators was applied to calculate the spectrum of the Hamiltonian with the quadrupole-quadrupole interaction exhibited a tetrahedral/octahedral symmetry. It should be noted that the developed procedures allow both numerical and exact symbolic implementation. All developed procedures were implemented in Wolfram Mathematica, which allows for a comprehensive study of their effectiveness.

The paper is organized as follows. In section 2 the procedure of calculations of the orthogonal BM basis is described. In section 3 the scheme of evaluation of matrix elements of tensor operator components is given. In section 4 the spectrum of the tetrahedral/octahedral quadrupole-quadrupole Hamiltonian is calculated. In Conclusions further applications of the elaborated procedures are outlined.

2. The orthogonal Bargmann-Moshinsky basis

2.1. Classification of Bargmann-Moshinsky states

The non-canonical BM basis corresponding to the subgroup chain SU(3)$\supset$ SO(3) $\supset$ SO(2) is indexed by the quantum numbers λ and μ, L and M of the respective group SU(3), SO(3) and SO(2). In the case of the BM basis, α is an additional index that is used to unambiguously distinguish the equivalent SO(3) irreps L in a given SU(3) irrep λ and μ. In the case of the Elliott basis, the additional index K is used instead of α for the same purpose. Note the set of quantum numbers λ, μ, L, α (or K) must be consistent according to the subgroup chain

$$|u_\alpha\rangle \equiv \left| \begin{array}{c} (\lambda\mu)_B \\ \alpha L M \end{array} \right\rangle \quad \begin{array}{ccccc} \mathrm{SU(3)} & \supset & \mathrm{SO(3)} & \supset & \mathrm{SO(2)} \\ (\lambda\mu) & \alpha & L & & M \end{array} \tag{1}$$

The ranges of quantum numbers are determined by the following relations:

$$\lambda, \mu = 0, 1, 2, \ldots \quad \text{and} \quad \lambda \geq \mu; \tag{2}$$

$$K = \mu, \mu - 2, \mu - 4, ..., 1 \text{ or } 0; \tag{3}$$

$$\alpha = \frac{1}{2}(\mu - K); \quad \alpha = 0, 1, 2, \ldots \alpha_{\max}; \quad \alpha_{\max} = \begin{cases} \frac{\mu}{2}, & \mu \text{ even}, \\ \frac{\mu-1}{2}, & \mu \text{ odd}; \end{cases} \tag{4}$$

$$K = 0: \quad L = \lambda, \lambda-2, \lambda-4, ..., 1 \text{ or } 0; \tag{5}$$

$$K \neq 0: \quad L_{\min} = K; \quad L_{\max} = \mu - 2\alpha + \lambda - \beta; \quad \beta = \begin{cases} 0, & \lambda+\mu-L \text{ even}, \\ 1, & \lambda+\mu-L \text{ odd}; \end{cases} \tag{6}$$

$$M = -L, \ldots, +L. \tag{7}$$

2.2. Overlap Integrals of non-orthogonal BM Basis

The construction of a basis is mainly based on an efficient procedure for calculating the overlap integrals. A very effective procedure for the overlap integrals of the non-orthogonal basis of BM was proposed by [20]. We developed the procedure for calculating these overlap integrals and checked its results with the results provided by the authors [20] in I and II:

$$\begin{aligned}
&\langle u_{\alpha'}|u_\alpha\rangle \equiv \langle u_\alpha|u_{\alpha'}\rangle = \left\langle \begin{array}{c|c} (\lambda,\mu)_B & (\lambda,\mu)_B \\ \alpha, L, L & \alpha', L, L \end{array} \right\rangle = C_1(\lambda, L, \Delta)(\lambda+2)^\beta (L-\mu+2\alpha)! \\
&\times(\lambda - L + \mu - 2\alpha' - \beta)!!(\mu - 2\alpha' - \beta + \Delta - 1)!! \\
&\times \sum_{l,z} \begin{pmatrix} \alpha' \\ \frac{1}{2}(l-\beta-\Delta) \end{pmatrix} (-1)^{(\mu+2\alpha-\Delta-\beta)/2+z} \begin{pmatrix} \frac{1}{2}(\mu-2\alpha-\Delta-\beta) \\ z \end{pmatrix} \\
&\times \frac{(\mu-l)!!}{(\mu-l-2z)!!} \frac{(\mu+\beta+\Delta)!!}{(\mu-2\alpha'+l)!!} (l-\Delta+\beta-1)!!(\mu-\Delta-\beta-2z)!! \\
&\times \frac{(\lambda-L+\mu-2\alpha-\beta)!!}{(\lambda-L+\Delta+2z)!!} \frac{(\lambda+L-\Delta+2)!!}{(\lambda+L-\mu+2\alpha+\beta+2z+2)!!} \frac{(L+l)!}{L!} \\
&\times \frac{(\lambda+\mu+L+\beta+2)!!}{(\lambda+L+l+\beta+2z+2)!!} \frac{(\lambda+\beta+2z+1)!}{(\lambda+\beta+1)!} \frac{(\lambda+\mu-l-L+\Delta)!!}{(\lambda-L+\mu-2\alpha'-\beta)!!} \\
&\times C_2(\lambda, L, \Delta, z).
\end{aligned} \tag{8}$$

Here $\alpha \geq \alpha'$ and we use the following notations

$$\beta = \begin{cases} 0, & \lambda+\mu-L \text{ even}, \\ 1, & \lambda+\mu-L \text{ odd}, \end{cases} \qquad \Delta = \begin{cases} 0, & \lambda-L \text{ even}, \\ 1, & \lambda-L \text{ odd}, \end{cases} \qquad \begin{pmatrix} m \\ n \end{pmatrix} = \frac{m!}{n!(m-n)!}, \tag{9}$$

$$C_1(\lambda, L, \Delta) = \begin{cases} 1, & L > \lambda+\Delta, \\ \frac{(\lambda+L+\Delta+1)!!}{(2L+1)!!}, & L \leq \lambda+\Delta, \end{cases} \qquad C_2(\lambda, L, \Delta, z) = \begin{cases} \frac{(\lambda+L+\Delta+1+2z)!!}{(2L+1)!!}, & L > \lambda+\Delta, \\ \frac{(\lambda+L+\Delta+1+2z)!!}{(\lambda+L+\Delta+1)!!}, & L \leq \lambda+\Delta. \end{cases}$$

Note, the upper alternative in definition of the coefficients C_1 and C_2 corresponds to the overlap integrals which contain only λ in their final expression. The summation parameter z runs from 0 to $\frac{1}{2}(-2\alpha-\beta-\Delta+\mu)$ except when $z < \frac{1}{2}(-\Delta-\lambda+L)$. The summation parameter l runs from $\beta+\Delta$ to $2\alpha'+\beta+\Delta$ except when $\mu-l$ or $l-\Delta-\beta$ is odd. We check also applicability of the above expressions of the overlap $\langle u_\alpha|u_{\alpha'}\rangle$ in the case of values $\lambda < \mu$ in benchmark calculations of matrices of the BM operator $X^{(3)}$ and its eigenvalues given in section 3.

2.3. Adaptation of the Gram-Schmidt orthonormalization procedure

The developed universal algorithm for orthonormalizing the noncanonical basis SU(3) with vectors of highest weights of irreducible representations (irreps) of SO(3) is based on the Gram-Schmidt orthonormalization procedure adopted in accordance with I and II

$$|\phi_i\rangle \equiv \left| \begin{array}{c} (\lambda,\mu) \\ i, L, L \end{array} \right\rangle = \sum_{\alpha=0}^{\alpha_{\max}} A_{i,\alpha}^{(\lambda,\mu)}(L) \left| \begin{array}{c} (\lambda,\mu)_B \\ \alpha, L, L \end{array} \right\rangle, \quad A_{i,\alpha}^{(\lambda,\mu)}(L) = 0, \quad \text{if } i > \alpha. \tag{10}$$

Here, a multiplicity index i is introduced to differentiate the orthonormalized BM states and takes the same range of values as α. $A^{(\lambda,\mu)}_{i,\alpha}(L)$ denotes matrix elements of the upper triangular matrix $\mathcal{A}$ of the BM basis orthonormalization coefficients.

It should be noted that the developed symbolic orthonormalization algorithm can be called non-standard recursive, or actually iterative, since it traverses the computation graph not from top to bottom, but from bottom to top

$$|\psi_\alpha\rangle = -|u_\alpha\rangle + \sum_{\alpha'=\alpha+1}^{\alpha_{\max}} c_{\alpha\alpha'}|\phi_{\alpha'}\rangle, \text{ when } 0 \le \alpha < \alpha_{\max}. \tag{11}$$

Here $\alpha_{\max}$ is the number of linearly independent BM states $|u_\alpha\rangle$, $|\psi_\alpha\rangle$ is the orthogonalized BM states, $|\phi_\alpha\rangle$ is the orthonormalized BM states and $c_{\alpha\alpha'}$ are linear coefficients. The orthonormalization process (11) starts (somewhat deliberately) by taking $|\psi_{\alpha_{\max}}\rangle = |u_{\alpha_{\max}}\rangle$.

2.4. Calculation of $f^{(n)}_{\alpha,\alpha'}$, $n = 0, 1, \ldots, \alpha_{\max K} - 1$, and $\langle\psi_\alpha|\psi_\alpha\rangle$

In this algorithm, it is necessary to introduce and iteratively calculate the convenient intermediate values $f^{(n)}_{\alpha,\alpha'}$, where n denotes the iteration number. $\alpha_{\max K}$ is the maximal α value for which there is a BM state for this particular L. The iteration starts at $n = 0$ by calculation of all $f^{(n)}_{\alpha,\alpha'}$ which are determined by the overlap integrals $\langle u_{\alpha'}|u_\alpha\rangle$ of BM states

$$f^{(0)}_{\alpha,\alpha'} = \langle u_\alpha|u_{\alpha'}\rangle, \tag{12}$$
$$\alpha = \alpha_{\min K}, \alpha_{\min K}+1, \ldots, \alpha_{\max K}-1 \text{ and } \alpha < \alpha' \le \alpha_{\max K};$$
$$f^{(1)}_{\alpha,\alpha'} = -f^{(0)}_{\alpha,\alpha'} + \frac{f^{(0)}_{\alpha,\alpha_{\max K}} f^{(0)}_{\alpha',\alpha_{\max K}}}{\langle u_{\alpha_{\max K}}|u_{\alpha_{\max K}}\rangle}, \tag{13}$$
$$\alpha = \alpha_{\min K}, \alpha_{\min K}+1, \ldots, \alpha_{\max K}-2 \text{ and } \alpha < \alpha' \le \alpha_{\max K}-1;$$
$$f^{(n)}_{\alpha,\alpha'} = f^{(n-1)}_{\alpha,\alpha'} + \frac{f^{(n-1)}_{\alpha,\alpha_{\max K-n+1}} f^{(n-1)}_{\alpha',\alpha_{\max K-n+1}}}{\langle\psi_{\alpha_{\max K-n+1}}|\psi_{\alpha_{\max K-n+1}}\rangle}, \tag{14}$$
$$\alpha = \alpha_{\min K}, \alpha_{\min K}+1, \ldots, \alpha_{\max K}-n-1 \text{ and } \alpha < \alpha' \le \alpha_{\max K}-n;$$
$$\langle\psi_\alpha|\psi_\alpha\rangle = \langle u_\alpha|u_\alpha\rangle - \sum_{\alpha'=\alpha+1}^{\alpha_{\max K}} \frac{\left(f^{(\alpha_{\max K}-\alpha')}_{\alpha,\alpha'}\right)^2}{\langle\psi_{\alpha'}|\psi_{\alpha'}\rangle}. \tag{15}$$

Here the indices are in the indicated ranges. In the next step of the iteration $n = 1$, the calculation of $f^{(1)}_{\alpha,\alpha'}$ is determined by the formula (13). For all subsequent steps of the iteration $n > 1$, $f^{(n)}_{\alpha,\alpha'}$ is determined by the formula (14). Here, the normalizing integral is determined by the formula (15). One can see that to calculate in symbolic analytical form $f^{(n)}_{\alpha,\alpha'}$ the square root operation cannot be applied, see I and II. It should be noted that all the $f^{(n)}_{\alpha,\alpha'}$ values at step n of the iteration can be calculated solely from the values of $f^{(n-1)}_{\alpha,\alpha'}$and normalization integrals obtained at the previous step $n-1$ of the iteration.

2.5. Orthonormalization of the basis of Bargmann-Moshinsky

Having calculated the normalization integrals by means of (8)–(9) and Eqs. (12)–(15), one may directly calculate the required coefficients of matrix $\mathcal{A}$. The formulas for calculating them are very simple

(i) $\alpha = \alpha' = \alpha_{\max K}$:

$$A_{\alpha_{\max K},\alpha_{\max K}} = \langle u_{\alpha_{\max K}}|u_{\alpha_{\max K}}\rangle^{-1/2}. \tag{16}$$

(ii) $\alpha = \alpha'$ and $\alpha = \alpha_{\min K}, \alpha_{\min K}+1, \ldots, \alpha_{\max K}-1$:

$$A_{\alpha,\alpha} = -\langle\psi_\alpha|\psi_\alpha\rangle^{-1/2}, \tag{17}$$

(iii) $\alpha < \alpha' < \alpha_{\max K}$:

$$A_{\alpha,\alpha'} = \frac{1}{\langle\psi_{\alpha'}|\psi_{\alpha'}\rangle}\sum_{\alpha''=\alpha}^{\alpha'-1} A_{\alpha,\alpha''} f_{\alpha'',\alpha'}^{(\alpha_{\max K}-\alpha')}, \tag{18}$$

(iv) $\alpha = \alpha_{\min K}, \alpha_{\min K}+1, \ldots, \alpha_{\max K}-1$ and $\alpha' = \alpha_{\max K}$:

$$A_{\alpha,\alpha_{\max K}} = -\frac{1}{\langle\psi_{\alpha_{\max K}}|\psi_{\alpha_{\max K}}\rangle}\sum_{\alpha''=\alpha}^{\alpha_{\max K}-1} A_{\alpha,\alpha''} f_{\alpha'',\alpha_{\max K}}^{(0)}. \tag{19}$$

It should be noted that the square root operation is applied only at the last stage of calculating coefficient of matrix $\mathcal{A}$.

2.6. Test condition

The orthonormalization property of the matrix of orthonormalization coefficients of the matrix $\mathcal{A}$ has the following form. Product of the nonzero blocks of the indicated matrices is the unity matrix. The matrix elements of the matrix $\mathcal{U}$ are the overlap integrals of the BM states. The equality of the product of these matrices to the identity matrix is actually the final test for the correctness of orthonormalization. Because the BM vectors $|u_\alpha\rangle$ are linearly independent, one can require the orthonormalization properties for the vectors $|\phi_i\rangle$

$$\langle\phi_i|\phi_j\rangle = \delta_{ij}. \tag{20}$$

From Eq. (20) there may be derived the orthonormalization property of the orthonormalization coefficients $A_{\alpha,\alpha'}$ of matrix $\mathcal{A}$

$$\mathcal{A}\,\mathcal{U}\tilde{\mathcal{A}} = \mathcal{I}. \tag{21}$$

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

$$\mathcal{A} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \mathbf{A} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathcal{U} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \mathbf{U} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathcal{I} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \mathbf{I} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{U} = \mathbf{A}^{-1}\tilde{\mathbf{A}}^{-1}. \tag{22}$$

Here the matrices $\mathbf{A}$, $\tilde{\mathbf{A}} = \mathbf{A}^T$ is transposed matrix $\mathbf{A}$, $\mathbf{U}$ and $\mathbf{I}$ 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 $\mathbf{I}$ is the unit matrix, and the entries of the matrix $\mathbf{U}$ are the overlap integrals $\langle u_\alpha|u_{\alpha'}\rangle$. The Eq. (21) may be used for control of consistency and accuracy of calculations.

3. The matrix elements of tensor operator components

3.1. The action of the zero component of the quadrupole operator onto the BM basis

The procedure for calculating the matrices of a quadrupole operator can be developed according to the method proposed in [21, 22] and recalculated in II and III. The action of the zero component of Q_0 onto nonorthogonal BM vectors reads as

$$Q_0 \left| \begin{array}{c} (\lambda,\mu)_B \\ \alpha, L, L \end{array} \right\rangle = \sum_{\substack{k=0,1,2 \\ s=0,\pm1}} a_s^{(k)} \left| \begin{array}{c} (\lambda,\mu)_B \\ \alpha+s, L+k, L \end{array} \right\rangle, \tag{23}$$

Using the inverse transformation of the orthonormalization matrix $(A^{-1})^{(\lambda\mu)}_{\alpha,i}(L)$ connected nonorthogonal and orthogonal BM bases

$$\left| \begin{array}{c} (\lambda,\mu)_B \\ \alpha, L, L \end{array} \right\rangle = \sum_{i=0}^{\alpha} (A^{-1})^{(\lambda\mu)}_{\alpha,i}(L) \left| \begin{array}{c} (\lambda,\mu) \\ i, L, L \end{array} \right\rangle, \tag{24}$$

we have action of zero component of Q_0 on orthogonal BM basis vector

$$Q_0 \left| \begin{array}{c} (\lambda,\mu) \\ i, L, L \end{array} \right\rangle = \sum_{\substack{j=0,\ldots,\alpha_{\max} \\ k=0,1,2}} q^{(\lambda\mu)}_{ijk}(L) \left| \begin{array}{c} (\lambda,\mu) \\ j, L+k, L \end{array} \right\rangle. \tag{25}$$

Here matrix elements $q^{(\lambda\mu)}_{ijk}(L)$ are calculated

$$q^{(\lambda\mu)}_{ijk}(L) = \sum_{\substack{\alpha=0,\ldots,\alpha_{\max} \\ s=0,\pm1}} A^{(\lambda\mu)}_{i,\alpha}(L) a^{(k)}_s (A^{-1})^{(\lambda\mu)}_{(\alpha+s),j}(L+k) \tag{26}$$

via the coefficients $a^{(k)}_s$ determined by formulas

$$a^{(2)}_0 = \frac{6(\lambda+\mu-L-2\alpha-\beta)}{[(L+2)(2L+3)]^{1/2}}, \quad a^{(2)}_{-1} = \frac{12\alpha}{[(L+2)(2L+3)]^{1/2}}, \quad a^{(2)}_{-1} = 0,$$

$$a^{(1)}_0 = -6\frac{2\alpha\beta(L+2\alpha-\mu+1)+(\lambda+\mu-L-2\alpha-\beta)(\mu-2\alpha-\beta)}{(L+2)(L+1)^{1/2}} - \frac{6\beta}{(L+1)^{1/2}},$$

$$a^{(1)}_{-1} = \frac{12\alpha(\lambda-\mu+2\alpha)}{(L+2)(L+1)^{1/2}}, \quad a^{(1)}_1 = \frac{6\beta(\lambda+\mu-L-2\alpha-\beta)}{(L+2)(L+1)^{1/2}},$$

$$a^{(0)}_0 = 4\alpha\frac{L(L+1)-3(L+2\alpha-\mu+\beta)^2}{(L+1)(2L+3)} - 2(\lambda+\mu-L-\beta-2\alpha)\frac{L(L+1)-3(\mu-2\alpha)^2}{(L+1)(2L+3)}$$

$$-(L-\mu+4\alpha+\beta)\left(1+\frac{3\beta}{L+1}\right),$$

$$a^{(0)}_{-1} = \frac{6(\lambda+\mu-L-2\alpha-\beta)(L-\mu+2\alpha)(L-\mu+2\alpha-1)}{(L+1)(2L+3)},$$

$$a^{(0)}_1 = -\frac{6(\lambda+\mu-L-2\alpha-\beta)(\mu-2\alpha-\beta)(\mu-2\alpha-\beta-1)}{(L+1)(2L+3)},$$

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

The analytical expressions for the $q^{(\lambda\mu)}_{ijk}(L)$ coefficients for values up to $\mu = 3$ were presented in [22] and were used to verify the procedures developed by us for $q^{(\lambda\mu)}_{ijk}(L)$ coefficients calculations in III.

3.2. The matrix elements of the quadrupole operator components

The reduced matrix elements of the quadrupole operator are related to the previously determined coefficients $q^{(\lambda\mu)}_{ijk}(L)$ by the following formula

$$\left\langle \begin{array}{c} (\lambda\mu) \\ j, L+k \end{array} \right\| Q^{(2)} \left\| \begin{array}{c} (\lambda\mu) \\ i, L \end{array} \right\rangle = (-1)^k \frac{\sqrt{2L+1}}{(L+k, L, 20|LL)} q^{(\lambda,\mu)}_{i,j,k}(L). \tag{27}$$

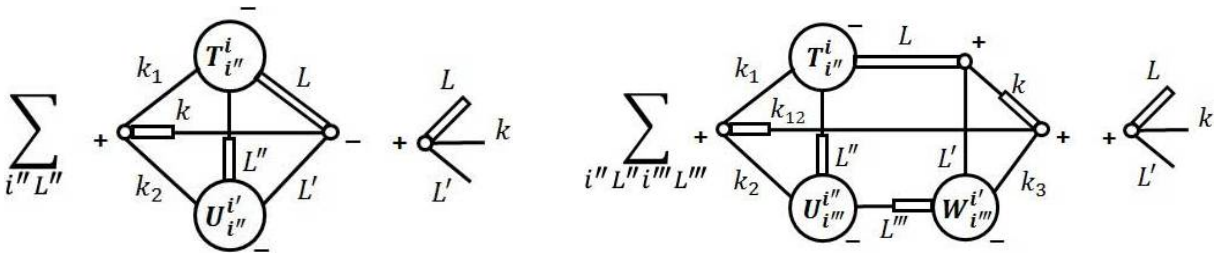

Figure 1. Calculations of tensor product of two and three tensor operators in graphical form.

The matrix elements of the quadrupole operator components can be obtained from the reduced matrix elements using the Wigner-Eckart theorem

$$\left\langle \begin{array}{c}(\lambda\mu)\\ jL'M'\end{array}\middle|\, Q^{(2)}_p \,\middle|\begin{array}{c}(\lambda\mu)\\ iLM\end{array}\right\rangle = \frac{(LM\,2p|L',M')}{\sqrt{2L'+1}} \left\langle \begin{array}{c}(\lambda\mu)\\ j,L'\end{array}\middle\|\, Q^{(2)} \,\middle\|\begin{array}{c}(\lambda\mu)\\ i,L\end{array}\right\rangle. \tag{28}$$

Here the conventional notation of $O(3)$ Clebsch-Gordan coefficients [23] is used. The dimension of the matrix of the quadrupole operator for given values of μ and λ can be calculated by the following formula

$$D_{\lambda\mu} = \frac{1}{2}(\lambda+1)(\mu+1)(\lambda+\mu+2). \tag{29}$$

3.3. $Q \cdot Q$ matrix

The quadratic Casimir operator of SU(3) group and its eigenvalues of a subspace for given λ, μ read as

$$C_2(SU(3)) = Q\cdot Q + 3L\cdot L = 4(\lambda^2+\mu^2+\lambda\mu+3\lambda+3\mu), \tag{30}$$

where the scalar product of the quadrupole operators is given by the formula

$$Q\cdot Q = \sum_{\eta=-2}^{2} (-1)^{\eta} Q_{\eta} Q_{-\eta}, \tag{31}$$

which was verified in integer arithmetic calculations.

3.4. Illustration of $\left(L^{(1)}\cdot L^{(1)}\right)$ calculation by graphical method

The effective expression for the matrix elements of the operator $X^{(3)}$ was derived by the graphical method [24](see fig. 1). The great advantage of the graphical method is that usually it can significantly simplify the momentum recoupling coefficients that are presented in formulas

$$\begin{aligned}\langle iLM|\,[T^{(k_1)}\otimes U^{(k_2)}]^{(k)}_q\,|i'L'M'\rangle &= \sum_{i''L''M''q_1,q_2} (k_1q_1\,k_2q_2|kq)\,\langle iLM|\,T^{(k_1)}_{q_1}\,|i''L''M''\rangle\\ &\times \langle i''L''M''|\,U^{(k_2)}_{q_2}\,|i'L'M'\rangle = (L'M'\,kq|LM)\sum_{i''L''}[(2L+1)(2L''+1)]^{-1/2}\\ &\times \langle iL\|\,T^{(k_1)}\,\|i''L''\rangle\,\langle i''L''\|\,U^{(k_2)}\,\|i'L'\rangle\,\langle (L',(k_1,k_2)k)L|((L',k_2)L'',k_1)L\rangle,\end{aligned} \tag{32}$$

where coefficients $\langle (L',(k_1,k_2)k)L|((L',k_2)L'',k_1)L\rangle$ read as

$$\begin{aligned}\langle (L',(k_1,k_2)k)L|((L',k_2)L'',k_1)L\rangle &= \frac{1}{2L+1}\sum_{q_1q_2qM'M''M}(k_1q_1\,k_2q_2|kq)(L'M'\,kq|LM)\\ &\times(L'M'\,k_2q_2|L''M'')(L''M''\,k_1q_1|LM) = (-1)^{k_1}(2k_1+1)^{-1/2}\,\delta_{k_1,k_2}\,\delta_{L,L'}\,\Delta(k_1L''L).\end{aligned} \tag{33}$$

3.5. Illustration of $\left(L^{(1)} \cdot L^{(1)}\right)$ *calculation*

Using this relation between the scalar product and the tensor product of zero rank and the expression for the reduced matrix element of the angular momentum, we obtain the correct formula for the scalar product of the angular momentum operators

$$[T^{(k)} \otimes U^{(k)}]_0^{(0)} = (-1)^k (2k+1)^{-1/2} \, (T^{(k)} \cdot U^{(k)}), \tag{34}$$

$$\langle iL \| \, L^{(1)} \, \| i''L'' \rangle = [L(L+1)(2L+1)]^{1/2} \, \delta_{iL,i''L''}, \tag{35}$$

$$\langle iLM | \, (L^{(1)} \cdot L^{(1)}) \, | i'L'M' \rangle = L(L+1) \, \delta_{iLM,i'L'M'}, \tag{36}$$

$$\left\langle \begin{array}{c} (\lambda\mu) \\ i, L, L \end{array} \right| \left(L^{(1)} \cdot L^{(1)}\right) \left| \begin{array}{c} (\lambda\mu) \\ i, L', L' \end{array} \right\rangle = -\sqrt{3}\delta_{LL'} \tag{37}$$

$$\times \sum_{m_1=-1}^{1} (1m_1 1 - m_1|00) \left\langle \begin{array}{c} (\lambda\mu) \\ i, L, L \end{array} \right| L^{(1)}_{m_1} \left| \begin{array}{c} (\lambda\mu) \\ i, L, L-m_1 \end{array} \right\rangle \left\langle \begin{array}{c} (\lambda\mu) \\ i, L, L-m_1 \end{array} \right| L^{(1)}_{-m_1} \left| \begin{array}{c} (\lambda\mu) \\ i, L, L \end{array} \right\rangle .$$

It should be noted that the same numerical values gives and direct summation of angular momentum matrix elements. This type of procedure can be used for testing purposes.

3.6. Illustration of $X^{(3)} = \left([L^{(1)} \otimes L^{(1)}]^{(2)} \cdot Q^{(2)}\right)$ *calculation by graphical method*

In the case of three operators, their general tensor product can be expressed in graphical form as follows (see fig. 1). The appeared angular momentum recoupling coefficient can be significantly simplified by the graphical method

$$\begin{aligned}
&\langle iLM | \left[[T^{(k_1)} \otimes U^{(k_2)}]^{(k_{12})} \otimes W^{(k_3)} \right]^{(k)}_q | i'L'M' \rangle \\
&= \sum_{i''L''M''q_1,q_2} \; \sum_{i'''L'''M'''q_{12},q_3} (k_1 q_1 \, k_2 q_2 | k_{12} q_{12}) (k_{12} q_{12} \, k_3 q_3 | kq) \\
&\times \langle iLM | \, T^{(k_1)}_{q_1} \, | i''L''M'' \rangle \, \langle i''L''M'' | \, U^{(k_2)}_{q_2} \, | i'''L'''M''' \rangle \, \langle i'''L'''M''' | \, W^{(k_3)}_{q_3} \, | i'L'M' \rangle \\
&= (L'M' \, kq | LM) \sum_{i''L''i'''L'''} [(2L+1)(2L''+1)(2L'''+1)]^{-1/2} \\
&\times \langle iL \| \, T^{(k_1)} \, \| i''L'' \rangle \, \langle i''L'' \| \, U^{(k_2)} \, \| i'''L''' \rangle \, \langle i'''L''' \| \, W^{(k_3)} \, \| i'L' \rangle \\
&\times \langle (L', ((k_1, k_2)k_{12}, k_3)k)L | (((L', k_3)L''', k_2)L'', k_1)L \rangle,
\end{aligned} \tag{38}$$

where coefficients $\langle (L', ((k_1, k_2)k_{12}, k_3)k)L | (((L', k_3)L''', k_2)L'', k_1)L \rangle$ are determined similar to (33) and calculated following the graphical method [24].

3.7. Matrix elements of $X^{(3)} = \left([L^{(1)} \otimes L^{(1)}]^{(2)} \cdot Q^{(2)}\right)$ *operator*

We present the result of our calculation for the operator $X^{(3)}$ that coincides with the expression of the operator $X^{(3)}$ given in the article [22] with the exception of the numerical factor $1/\sqrt{6}$

$$\left\langle \begin{array}{c} (\lambda\mu) \\ j, L', M' \end{array} \right| X^{(3)} \left| \begin{array}{c} (\lambda\mu) \\ i, L, M \end{array} \right\rangle = \frac{1}{\sqrt{6}} (L+1)(2L+3) \; q^{(\lambda\mu)}_{ij0}(L) \; \delta_{LL'} \; \delta_{MM'}. \tag{39}$$

It should be noted that some numerical factor is quite deliberately used by different authors. The obtained formula of the matrix elements of the operator $X^{(3)}$ was verified with results that

give a direct summation of the matrix elements of these operators

$$\left\langle \begin{array}{c}(\lambda\mu)\\ j,L',L'\end{array}\right| X^{(3)} \left|\begin{array}{c}(\lambda\mu)\\ i,L,L\end{array}\right\rangle = \sqrt{5}\delta_{LL'}\sum_{m_1=-2}^{2}\sum_{m_4=-1}^{1}(2m_1 2-m_1|00)$$
$$\times(1m_1-m_4 1m_4|2m_1)\left\langle \begin{array}{c}(\lambda\mu)\\ j,L,L\end{array}\right| L^{(1)}_{m_1-m_4} \left|\begin{array}{c}(\lambda\mu)\\ j,L,L-m_1+m_4\end{array}\right\rangle \qquad (40)$$
$$\times\left\langle \begin{array}{c}(\lambda\mu)\\ j,L,L-m_1+m_4\end{array}\right| L^{(1)}_{m_4} \left|\begin{array}{c}(\lambda\mu)\\ j,L,L-m_1\end{array}\right\rangle \left\langle \begin{array}{c}(\lambda\mu)\\ j,\,L,L-m_1\end{array}\right| Q^{(2)}_{-m_1} \left|\begin{array}{c}(\lambda\mu)\\ i,\,L,L\end{array}\right\rangle .$$

3.8. Matrix elements of $\tilde{X}^{(3)}=\left([L^{(1)}\otimes Q^{(2)}]^{(1)}\cdot L^{(1)}\right)$ *operator*

Another form of the operator $X^{(3)}$ was proposed in [19]. In this case, the expressions obtained by the graphical method (38) and with direct summation have the following form

$$\left\langle \begin{array}{c}(\lambda\mu)\\ j,L',M'\end{array}\right| \tilde{X}^{(3)} \left|\begin{array}{c}(\lambda\mu)\\ i,L,M\end{array}\right\rangle = \sqrt{\frac{5}{2}}\left(-\frac{1}{\sqrt{10}}\right)(L+1)(2L+3)\; q^{(\lambda\mu)}_{ij0}(L)\;\delta_{LL'}\;\delta_{MM'}, \qquad (41)$$

$$\left\langle \begin{array}{c}(\lambda\mu)\\ j,L',L'\end{array}\right| \tilde{X}^{(3)} \left|\begin{array}{c}(\lambda\mu)\\ i,L,L\end{array}\right\rangle = \sqrt{\frac{5}{2}}(-\sqrt{3})\;\delta_{LL'}\sum_{m_1=-2}^{2}\sum_{m_4=-1}^{1}(2m_1 2-m_1|00)$$
$$\times(1m_1-m_4 1m_4|2m_1)\left\langle \begin{array}{c}(\lambda\mu)\\ j,L,L\end{array}\right| L^{(1)}_{m_1-m_4} \left|\begin{array}{c}(\lambda\mu)\\ j,L,L-m_1+m_4\end{array}\right\rangle \qquad (42)$$
$$\times\left\langle \begin{array}{c}(\lambda\mu)\\ j,L,L-m_1+m_4\end{array}\right| L^{(1)}_{m_4} \left|\begin{array}{c}(\lambda\mu)\\ j,L,L-m_1\end{array}\right\rangle \left\langle \begin{array}{c}(\lambda\mu)\\ j,\,L,L-m_1\end{array}\right| Q^{(2)}_{-m_1} \left|\begin{array}{c}(\lambda\mu)\\ i,\,L,L\end{array}\right\rangle .$$

3.9. Calculation of the matrix $\tilde{X}^{(3)}=\left([L^{(1)}\otimes Q^{(2)}]^{(1)}\cdot L^{(1)}\right)$ *and its eigenvalues*

The resulting expression for the matrix elements of the operator $\tilde{X}^{(3)}$ gives the same numerical results as in [19]. We present example of calculation of the matrix $\tilde{X}^{(3)}$ with $\mu=6$, $\lambda=6$ and $L=6$ for comparison with result of [19] at $\lambda=k_1-k_2$ and $\mu=k_2$, i.e. $k_1=12$ and $k_2=6$. For example, here is the matrix $\tilde{X}^{(3)}$, calculated exactly and numerically, as well as the eigenvalues of the matrix:

$$\tilde{\mathbf{X}}^{(3)}=\begin{pmatrix} -\frac{2407509}{3455} & -\frac{18\sqrt{44049486}}{3455} & 0 & 0\\ -\frac{18\sqrt{44049486}}{3455} & -\frac{9677048733}{102692965} & -\frac{720\sqrt{20733455}}{29723} & 0\\ 0 & -\frac{720\sqrt{20733455}}{29723} & \frac{1976289111}{10492219} & \frac{36\sqrt{4577342}}{353}\\ 0 & 0 & \frac{36\sqrt{4577342}}{353} & \frac{212751}{353}\end{pmatrix} \qquad (43)$$

$$\tilde{\mathbf{X}}^{(3)}=\begin{pmatrix} -696.818813314038 & -34.5776023854303 & 0 & 0\\ -34.5776023854303 & -94.2328301943565 & -110.300046158617 & 0\\ 0 & -110.300046158617 & 188.357592516893 & 218.189816246354\\ 0 & 0 & 218.189816246354 & 602.694050991501\end{pmatrix}$$

Numerical eigenvalues E_n of eigenvalue problem $\tilde{\mathbf{X}}^{(3)}\mathbf{C}=E_n\mathbf{C}$ read as

$$E_n=\{698.844211758832,\ -698.844211758832,\ -138.429648887718,\ 138.429648887718\}\,.$$

Table 1. The example of spectrum $E_n \equiv E_{\lambda,\mu,\nu}$ 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 $\nu_{\max}$ denote degeneration of eigenvalues due to the intrinsic tetrahedral/octahedral symmetry.

(λ,μ)	$D_{\lambda\mu}$	$\gamma C_2(SU(3))$	Exact eigenvalues	Numerical eigenvalues	$\nu_{\max}$
$(1,0)$	15	96	$\frac{12}{5}\left(1+\sqrt{89}\right)$	25.0415547	3
			$\frac{12}{5}\left(-1-\sqrt{65}\right)$	−21.7494186	3
			$\frac{12}{5}\left(1-\sqrt{89}\right)$	−20.2415547	3
			$\frac{12}{5}\left(-1+\sqrt{65}\right)$	16.9494186	3
			$\frac{48}{5}$	9.6000000	1
			$-\frac{24}{5}$	−4.8000000	2

We have also agreement of our calculations of eigenvalues of the operator $\tilde{X}^{(3)}$ with benchmark results presented in [10] up to a constant factor appearing in a definition of the operator $\tilde{X}^{(3)}$. Moreover, at the case of values $\mu > \lambda$ eigenvalues of the operator $X^{(3)}$ differ only sign if the values of $\lambda > \mu$ are only interchanged, as pointed out in [25, 26]. So, we are sure that we correctly calculated the matrix $\tilde{X}^{(3)}$ and its eigenvalues.

4. Spectrum of the tetrahedral/octahedral quadrupole-quadrupole Hamiltonian

We present a benchmark example that is related to the problem of existence of higher symmetries in nuclei. An influence of point symmetries within the nuclear SU(3) approximation has been proposed in [6] and investigated in II floating points arithmetic for example the low lying energy levels $E_n \equiv E_{\lambda,\mu,\nu}$ of the Hamiltonian:

$$H \equiv H/h_{4Q} = \gamma C_2(SU(3)) + H''_{4Q}/h_{4Q},\ H|\lambda,\mu,\nu>= E_n|\lambda,\mu,\nu> . \tag{44}$$

Here we perform calculation of matrix of one of the quadrupole-quadrupole terms that can simulate both tetrahedral and octahedral nuclear symmetry with Hamiltonian H''_{4Q}

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

To illustrate the effect of this term on the energy spectrum, the eigenvalues of H''_{4Q} for irr. $\mu = 0$, $\lambda = 1$ were calculated. The computational results for the example of spectrum of Hamiltonian (44) are presented in Table 1. 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.(29) that is determined a complexity of the above algorithm; $C_2(SU(3))$ marks the eigenvalues of the second order Casimir operator (30); E_n presents the energy levels that results after diagonalization of the Hamiltonian (44); $\nu = 1, ..., \nu_{\max}$ is the degeneration $\nu_{\max}$ of the corresponding energy levels E_n. The computations were done with integer arithmetic and numerically to 10-digit precision.

The obtained results of exact and numerical calculations are presented in Table 1 here in two columns respectively. These results indicate correct degeneracy of the eigenvalues expected be for interactions with tetrahedral symmetry.

5. Conclusion

We present the new, extremely fast and universal symbolic algorithm for construction of the orthonormalized non-canonical SU(3) basis with the highest weight vectors of SO(3) irreps. The proposed orthonormalization algorithm allows one to implement analytic, exact and numerical

calculations. The high efficiency of the program implemented in the Wolfram Mathematica was illustrated by exact as well as numerical orthonormalisation of the BM basis up to extremely high quantum numbers λ and μ which is not given by other symbolic algorithms known in the literature [9]. The efficient exact as well as numerical procedures for calculation of the quadrupole operator as well as the BM operator $X^{(3)}$ matrices up to high λ and μ values were developed and implemented. The presented benchmark calculations of spectrum of the quadrupole-quadrupole interaction with Tetrahedral/Octahedral symmetry demonstrate efficiency of the proposed method for calculation of spectral characteristics (especially close to resonances) of quantum systems under consideration and to study their analytical properties for understanding the dominant symmetries.

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