Construction of the Orthogonal Bargmann-Moshinsky Basis of SU(3) Group

S.I. Vinitsky
(Joint Institute for Nuclear Research, Dubna, Russia)

A. Deveikis
Vytautas Magnus University, Kaunas, Lithuania
A. Pędrak
National Centre for Nuclear Research, Warsaw, Poland
A. Góźdź
(Institute of Physics, University of M. Curie-Skłodowska, Lublin, Poland),
A.A. Gusev, V.P. Gerdt
(JINR)

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ЯДЕРНАЯ ФИЗИКА
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О РЕАЛИЗАЦИЯХ ФИЗИЧЕСКОГО БАЗИСА $SU(3)$ И ВЕРОЯТНОСТИ $E2$-ПЕРЕХОДОВ В СХЕМЕ $SU(3)$

Г. Н. АФАНАСЬЕВ, С. А. АВРАМОВ, П. П. РАЙЧЕВ

ОБЪЕДИНЕННЫЙ ИНСТИТУТ ЯДЕРНЫХ ИССЛЕДОВАНИЙ

(Поступила в редакцию 23 ноября 1971 г.)

В рамках $SU(3)$-схемы проанализированы вероятности переходов. Показано, что можно выбрать операторы Ω_1 и Ω_2, достаточно четко разделяющие вращательные полосы.

1. Мы начинаем с базиса Баргмана — Мошинского (Б.— М.) [1]. Кратко опишем его. Генераторы $SU(3)$ выбираем в виде

$$L_{\mu\nu} = L_{\mu\nu}(x) + L_{\mu\nu}(y), \quad Q_{\mu\nu} = Q_{\mu\nu}(x) + Q_{\mu\nu}(y),$$
$$L_{\mu\nu}(x) = x_\mu p_\nu - x_\nu p_\mu, \quad L_{\mu\nu}(y) = y_\mu q_\nu - y_\nu q_\mu,$$
$$Q_{\mu\nu}(x) = x_\mu p_\nu + x_\nu p_\mu - {}^2/_3\delta_{\mu\nu}xp, \quad Q_{\mu\nu}(y) = y_\mu q_\nu + y_\nu q_\mu - {}^2/_3\delta_{\mu\nu}yq.$$

Мы предполагаем фоковскую реализацию операторов рождения x, y и уничтожения p, q:

$$p_\mu = \frac{\partial}{\partial x_\mu} = (x_\mu)^+, \quad q_\mu = \frac{\partial}{\partial y_\mu} = (y_\mu)^+, \quad \mu = 1, 2, 3,$$
$$[p_\mu, x_\nu] = [q_\mu, y_\nu] = \delta_{\mu\nu}.$$

Остальные коммутаторы равны нулю.

Введем операторы

$$C = xp + yq, \quad T_1 = \frac{1}{\sqrt{2}}xq, \quad T_{-1} = \frac{1}{\sqrt{2}}yp, \quad T_0 = \frac{1}{2}(xp - yq).$$

C есть оператор Казимира $U(3)$ и равен сумме чисел частиц сортов x и y. Удобно считать, что x, y несут соответственно проекции $(\pm{}^1/_2)$ изоспина. Тогда T_μ можно интерпретировать как операторы группы изоспина. Операторы (xx), (yy), (xy) рождают пары частиц с нулевым угловым мо-

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A new procedure for constructing basis vectors of $SU(3) \supset SO(3)$

Feng Pan [a,b,*], Shuli Yuan [a], Kristina D. Launey [b], Jerry P. Draayer [b]

[a] Department of Physics, Liaoning Normal University, Dalian 116029, China
[b] Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803-4001, USA

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Abstract

A simple and effective algebraic angular momentum projection procedure for constructing basis vectors of $SU(3) \supset SO(3) \supset SO(2)$ from the canonical $U(3) \supset U(2) \supset U(1)$ basis vectors is outlined. The expansion coefficients are components of the null-space vectors of a projection matrix with, in general, four nonzero elements in each row, where the projection matrix is derived from known matrix elements of the $U(3)$ generators in the canonical basis. The advantage of the new procedure lies in the fact that the Hill–Wheeler integral involved in the Elliott's projection operator method used previously is avoided, thereby achieving faster numerical calculations with improved accuracy. Selected analytical expressions of the expansion coefficients for the $SU(3)$ irreps $[n_{13}, n_{23}]$, or equally, $(\lambda, \mu) = (n_{13} - n_{23}, n_{23})$ with λ and μ the $SU(3)$ labels familiar from the Elliott model, are presented as examples for $n_{23} \leq 4$. Explicit formulae for evaluating $SO(3)$-reduced matrix elements of $SU(3)$ generators are derived. A general formula for evaluating the $SU(3) \supset SO(3)$ Wigner coefficients is given, which is expressed in terms of the expansion coefficients and known $U(3) \supset U(2)$ and $U(2) \supset U(1)$ Wigner coefficients. Formulae for evaluating the elementary Wigner coefficients of $SU(3) \supset SO(3)$, i.e., for the $SU(3)$ coupling $[n_{13}, n_{23}] \otimes [1, 0]$, are explicitly given with some analytical examples shown to check the validity of the results. However, the Gram–Schmidt orthonormalization is still needed in order to provide orthonormalized basis vectors.

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Analytical form of the orthonormal basis of the decomposition $SU(3) \supset O(3) \supset O(2)$ for some (λ, μ) multiplets

S Ališauskas†, P Raychev‡ and R Roussev‡

† Academy of Sciences of the Lithuanian SSR, Institute of Physics and Mathematics, Vilnuis, Lithuanian SSR

‡ Bulgarian Academy of Sciences, Institute of Nuclear Researches and Nuclear Energy, Sofia, Bulgaria

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Abstract. An analytical formula for the overlap integrals in the case of the non-canonical basis of Bargmann and Moshinsky has been obtained. These integrals are tabulated for $\mu = 0$, 1, 2, 3, 4 and $\lambda > \mu$. The overlap integrals are used for the construction (by means of the Hilbert–Schmidt procedure) of an orthonormal basis. The transformation coefficients are tabulated for $\mu = 0$, 1, 2, 3 and $\lambda > \mu$.

1. Introduction

The angular momentum associated with the group O(3), which is embedded in the group SU(3), plays a major role in the application of SU(3) in nuclear physics. The corresponding chain of subgroups is

$$SU(3) \supset O(3) \supset O(2). \tag{1.1}$$

The basic functions corresponding to decomposition (1.1) are common eigenfunctions of the second- and third-order Casimir operators C_2 and C_3 of SU(3) and of the angular momentum operators L^2 and L_0 associated with O(3) and O(2) respectively. Chain (1.1), however, is not canonical, i.e. in a given (λ, μ) irreducible representation (IR) of SU(3) there can be more than one state characterised by the quantum numbers (L, M) of the decomposition $O(3) \supset O(2)$. There is one label missing to characterise the states completely and in that sense the construction of the basis is somewhat arbitrary. The 'missing label' problem can be solved in the following way.

(i) The basic functions are constructed as polynomials in some chosen variables. The missing label is introduced by means of a special prescription which leads to a simple labelling of the states by integers. For instance, in the case of the basis of Bargmann and Moshinsky (1961; hereafter referred to as BM) an additional quantum number q (or α) is

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Elliott's $SU(3)$ model and its developments in nuclear physics

A Arima
RIKEN, Wako, Saitama 351-0198, Japan

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Abstract. The $SU(3)$ group, its role in bridging the shell model and the collective model, $SU(3)$-based truncated shell model calculations and puzzles associated with quadrupole quadrupole interaction together with solutions are briefly described. An overview of various important developments resulting from the application of $SU(3)$ symmetry, and its potential in exploring new frontiers of nuclear structure physics is presented.

1. Introduction

Symmetries have played a very important role in understanding the complex nuclear spectra. The striking resemblance of the spectra obtained for ^{19}F in the shell model calculations of Elliott and Flowers [1] and collective model calculations of Paul [2] and the degeneracies in the harmonic oscillator spectrum led to the discovery of Elliott's $SU(3)$ model [3] exactly 40 years ago. I thank the organizers for bestowing on me the honour of reviewing the role of $SU(3)$ symmetry in nuclear structure physics. I take this opportunity to congratulate Phil Elliott upon the profound success of the $SU(3)$ model which has extended even into the present era marked by the ever-widening frontiers of nuclear structure physics.

2. Elliott's $SU(3)$ model

The salient features of $SU(3)$ symmetry are briefly reviewed before embarking upon its applications over the last 40 years. This symmetry is generated by the harmonic oscillator quanta-conserving, momentum-dependent quadrupole (Q) and angular momentum (L) operators, with the quadratic Casimir operator given by

$$C(SU(3)) = \tfrac{2}{3}[2Q \cdot Q + \tfrac{3}{4}L \cdot L]. \tag{1}$$

The eigenvalues of the Casimir operator are

$$\langle\lambda\mu|C(SU(3))|\lambda\mu\rangle = \tfrac{2}{3}(\lambda^2 + \lambda\mu + \mu^2 + 3\lambda + 3\mu) \tag{2}$$

where λ, μ are the difference in quanta in the z and x, x and y directions, respectively.

Shell model calculations with the quadrupole–quadrupole ($Q \cdot Q$) interaction,

$$\begin{aligned} H &= -\kappa\hat{Q}\cdot\hat{Q} \\ &= -\tfrac{3}{4}\kappa C(SU(3)) + \tfrac{3}{8}\kappa\hat{L}\cdot\hat{L} \end{aligned} \tag{3}$$

gives the rotational spectrum,

$$E = -\tfrac{1}{2}\kappa(\lambda^2 + \lambda\mu + \mu^2 - 3\lambda + 3\mu) + \tfrac{3}{8}\kappa L(L+1). \tag{4}$$

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POINT SYMMETRIES IN THE NUCLEAR SU(3) PARTNER GROUPS MODEL*

A. Góźdź[a], A. Pędrak[b], A.A. Gusev[c], S.I. Vinitsky[c,d]

[a]Institute of Physics, Maria Curie-Skłodowska University
pl. Marii Curie-Skłodowskiej 1, 20-031 Lublin, Poland
[b]National Centre for Nuclear Research, Warszawa, Poland
[c]Joint Institute for Nuclear Research, Dubna, Russia
[d]RUDN University, 6 Miklukho-Maklaya, 117198 Moscow, Russia

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The algebraic approach which allows for simulation of symmetries of a nucleus with respect to the laboratory and intrinsic frames is presented. The formalism is based on the partner groups (a group and the corresponding intrinsic group) idea. An illustrative example is related to the successful SU(3) Elliot nuclear model. An example of schematic Hamiltonian is chosen to have tetrahedral or octahedral symmetry.

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1. Introduction

The classical rotation is a well-understood phenomenon in which the orientation of a body is changing with time. On the other hand, the quantum rotation allows to determine only the probability of a given orientation of the "rotating" body and, in fact, the time dependence is not needed. In both cases, the rotational motion can be described as a motion on the rotation group manifold (the space of SO(3) group parameters). Usually, in the case of rotations, this manifold is parametrized by the set of Euler angles $\Omega = (\Omega_1, \Omega_2, \Omega_3)$. The quantum state space for this motion is not the group manifold itself but the space of square integrable complex functions of Euler angles denoted by $L^2(SO(3), d\mu(\Omega))$.

The simplest SU(3) model Hamiltonian consists of the quadrupole-quadrupole interaction, the rotational term and the other terms constructed from generators of the partner groups $G = \mathrm{SU}(3) \times \overline{\mathrm{SU}(3)}$, see [Góźdź, A., 2018] 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 [Varshalovitch, D.A., 1975]. These interaction terms can simulate either the tetrahedral or octahedral nuclear symmetry [Dudek, J., 2002].

The low part of spectrum at $L = 0$ of hamiltonian $H/h_{4Q} = \gamma' C_2(\mathrm{SU}(3)) + H''_{4Q}/h_{4Q}$:

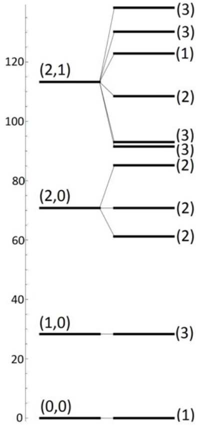

Fig. 1. Example of spectrum of Hamiltonian (24) for $\gamma' = 1.5$. The pair (λ, μ) labels the irreducible representations of the group SU(3) and the label (n), where $n = 1, 2, 3$ denote degeneration of eigenvalues due to the intrinsic tetrahedral/octahedral symmetry.

The SU(3) collective nuclear models in the orthogonal non-canonical Bargmann–Moshinsky (BM) Basis [Bargmann, V., Moshinsky, M. 1961]

$$H\left|\begin{array}{c}(\lambda,\mu)_B\\ E,L,M\end{array}\right\rangle = E\left|\begin{array}{c}(\lambda,\mu)_B\\ E,L,M\end{array}\right\rangle,\ \left|\begin{array}{c}(\lambda,\mu)\\ E,L,M\end{array}\right\rangle = \sum_{\alpha} C_E^{\alpha}\left|\begin{array}{c}(\lambda,\mu)_B\\ \alpha,L,M\end{array}\right\rangle,\ \to \left\langle\begin{array}{c}(\lambda,\mu)\\ E,L,M\end{array}\right| Q_m \left|\begin{array}{c}(\lambda,\mu)\\ E',L',M'\end{array}\right\rangle. \quad (5)$$

A possible Hamiltonian H used in this schematic nuclear model [Arima, A., 1989]

$$H = \gamma C_2(\mathrm{SU}(3)) - \kappa Q\cdot Q + \beta L\cdot L = (\gamma-\kappa)C_2(\mathrm{SU}(3)) + (3\kappa+\beta)L\cdot L, \quad (6)$$

To solve this problem we need to construct the orthonormal basis in the space spanned by the non-canonical Bargmann–Moshinsky (BM) vectors [a]

$$\left|\begin{array}{c}(\lambda,\mu)\\ f_i,L,L\end{array}\right\rangle = \sum_{\alpha=0}^{\alpha_{\max}} A_{i,\alpha}^{(\lambda,\mu)}(L)\left|\begin{array}{c}(\lambda,\mu)_B\\ \alpha,L,L\end{array}\right\rangle. \quad (7)$$

[a] It should be noted that the used states $\left|\begin{array}{c}(\lambda,\mu)_B\\ \alpha,L,L\end{array}\right\rangle$ differ from the states (3.8) given by [Moshinsky, M., 1975] in the definition of the number a and coincide up to a phase factor $(-1)^{\alpha}$.

Here multiplicity index i is introduced to differentiate the orthonormalized states and $A_{i,\alpha}^{(\lambda,\mu)}(L)$ are the BM basis orthonormalization coefficients. These coefficients fulfill the following condition

$$A_{i,\alpha}^{(\lambda,\mu)}(L) = 0, \qquad \text{if } i > \alpha. \quad (8)$$

Because the BM vectors (5) are linearly independent, one can require the orthonormalization properties for the vectors (17)

$$\left\langle\begin{array}{c}(\lambda,\mu)\\ f_i,L,L\end{array}\middle|\begin{array}{c}(\lambda,\mu)\\ f_k,L,L\end{array}\right\rangle = \delta_{ik}. \quad (9)$$

Overlap Integrals of BM Basis [Bargmann, V., Moshinsky, M. 1961]

Commutation relations of the spherical tensors $L_\nu(\nu = \pm 1, 0)$, $Q_\nu(\nu = \pm 2, \pm 1, 0)$

$$[L_\nu, L_{\nu'}] = -\sqrt{2}(1\nu 1\nu'|1\nu+\nu')L_{\nu+\nu'}, \qquad [Q_\nu, L_{\nu'}] = -\sqrt{6}(2\nu 1\nu|2\nu+\nu)Q_{\nu+\nu'},$$
$$[Q_\nu, Q_{\nu'}] = 3\sqrt{10}(2\nu 2\nu'|1\nu+\nu')L_{\nu+\nu'}.$$

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 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 [Alisauskas, S., 1981] [a]. Let us introduce the notation for the vectors of this basis:

$$\left\langle \alpha \middle| \alpha' \right\rangle = \left\langle \begin{array}{c} (\lambda,\mu)_B \\ \alpha, L, M \end{array} \middle| \begin{array}{c} (\lambda,\mu)_B \\ \alpha', L, M \end{array} \right\rangle \tag{10}$$

Here the quantum numbers λ, μ label irreducible representations (irreps), $\lambda, \mu = 0, 1, 2, \ldots$ and $\lambda > \mu$; L, M are the quantum numbers of angular momentum $\mathbf{L}\cdot\mathbf{L}$ 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 subspace irrep for given λ, μ can be calculated by using the following formula:

$$D_{\lambda\mu} = \frac{1}{2}(\lambda+1)(\mu+1)(\lambda+\mu+2). \tag{11}$$

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[a] Alisauskas, S., Raychev, P., Roussev, R.: Analytical form of the orthonormal basis of the decomposition $SU(3) \supset O(3) \supset O(2)$ for some (λ, μ) multiplets. J. Phys. G: Nucl. Phys. 7, 1213–1226 (1981)

Overlap Integrals of BM Basis

In order to perform classification of the BM states (5) one should determine the 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 former quantities is rather cumbersome. The easiest way to get the allowed values of α and L is by using the symbolic algorithm 1 that consists of the following steps:

Step 1.

Firstly we should start with choosing some particular value of the quantum number μ. For the following consideration, it is convenient to introduce auxiliary label K [Elliott, J.P., 1958] which varies in the ranges

$$K = \mu, \mu - 2, \mu - 4, ..., 1 \text{ or } 0, \qquad \text{since } \lambda > \mu. \tag{12}$$

The label K is related to α by

$$\alpha = \frac{1}{2}(\mu - K). \tag{13}$$

So, for every fixed μ, the set of possible values of K can be obtained directly from the definition of K from (12). Now, the set of allowed values of α may be determined from these K values using relation (13).

Overlap Integrals of BM Basis

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:

$$L = \lambda, \lambda - 2, \lambda - 4, ..., 1 \text{ or } 0. \tag{14}$$

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 (12) there exists a number of the corresponding α numbers. It means that for every particular μ, there will be a number of pairs $(\alpha, L_{\min})$. The maximum value of L is defined by the expression $L_{\max} = \mu - 2\alpha + \lambda - \beta$, where

$$\beta = \begin{cases} 0, & \lambda + \mu - L \text{ even}, \\ 1, & \lambda + \mu - L \text{ odd}. \end{cases} \tag{15}$$

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 μ value, and the number $L_{\max}$ is also determined. An illustrative example for calculation of allowed values of α and L is presented in Tables 1a and 1b at $K \neq 0$ and $K = 0$, respectively. It should be noted that the set of allowed values of L for overlap integrals is given by the intersection of these sets for the corresponding $< bra|$ and $|ket >$ vectors.

Overlap Integrals of BM Basis

The overlap integral of the non-canonical BM states presented in [Alisauskas, S., 1981]

$$\left\langle \alpha' \middle| \alpha \right\rangle = \left\langle \begin{array}{c} (\lambda,\mu)_B \\ \alpha, L, L \end{array} \middle| \begin{array}{c} (\lambda,\mu)_B \\ \alpha', L, L \end{array} \right\rangle = C_1(\lambda, L, \Delta)(\lambda+2)^{\beta}(L-\mu+2\alpha)!$$
$$\times(\lambda - L + \mu - 2\alpha' - \beta)!!(\mu - 2\alpha' - \beta + \Delta - 1)!!$$
$$\times \sum_{l,z} \begin{pmatrix} \alpha' \\ \frac{1}{2}(l-\beta-\Delta) \end{pmatrix} (-1)^{(\mu+2\alpha-\Delta-\beta)/2+z} \begin{pmatrix} \frac{1}{2}(\mu-2\alpha-\Delta-\beta) \\ z \end{pmatrix}$$
$$\times \frac{(\mu-l)!!}{(\mu-l-2z)!!} \frac{(\mu+\beta+\Delta)!!}{(\mu-2\alpha'+l)!!}(l-\Delta+\beta-1)!!(\mu-\Delta-\beta-2z)!!$$
$$\times \frac{(\lambda-L+\mu-2\alpha-\beta)!!}{(\lambda-L+\Delta+2z)!!} \frac{(\lambda+L-\Delta+2)!!}{(\lambda+L-\mu+2\alpha+\beta+2z+2)!!} \frac{(L+l)!}{L!}$$
$$\times \frac{(\lambda+\mu+L+\beta+2)!!}{(\lambda+L+l+\beta+2z+2)!!} \frac{(\lambda+\beta+2z+1)!}{(\lambda+\beta+1)!} \frac{(\lambda+\mu-l-L+\Delta)!!}{(\lambda-L+\mu-2\alpha'-\beta)!!}$$
$$\times C_2(\lambda, L, \Delta, z). \qquad (16)$$

Here $\alpha \geq \alpha'$ and β from (15) and we use the following notations

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

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

Overlap Integrals of BM Basis

Table 1a. The allowed values of α, $L_{\min}$, and $L_{\max}$ for up to $\mu = 5$ when $K \neq 0$.

μ	α	$L_{\min}$	$L_{\max}(\lambda - L$ even$)$	$L_{\max}(\lambda - L$ odd$)$
1	0	1	λ	$\lambda + 1$
2	0	2	$\lambda + 2$	$\lambda + 1$
3	0	3	$\lambda + 2$	$\lambda + 3$
	1	1	λ	$\lambda + 1$
4	0	4	$\lambda + 4$	$\lambda + 3$
	1	2	$\lambda + 2$	$\lambda + 1$
5	0	5	$\lambda + 4$	$\lambda + 5$
	1	3	$\lambda + 2$	$\lambda + 3$
	2	1	λ	$\lambda + 1$

Table 1b. The allowed values of α and L for up to $\mu = 5$ when $K = 0$.

μ	α	L, $(\lambda - L$ even$)$
0	0	$\lambda, \lambda - 2, \lambda - 4, ..., 1$ or 0
2	1	$\lambda, \lambda - 2, \lambda - 4, ..., 1$ or 0
4	2	$\lambda, \lambda - 2, \lambda - 4, ..., 1$ or 0

The above algorithm was realized in the form of the program implemented in the computer algebra system Wolfram Mathematica 10.1. The typical running time of calculating the irreducible representations $\mu = 4$ and $\mu = 8$ is 3 and 57 seconds and memory is 35 and 47 Mb, respectively using the PC Intel Pentium CPU 1.50 GHz 4GB 64bit Windows 8.

Table 2. Overlap integrals of non-canonical BM basis for $\mu = 4$.

$(\alpha\|\alpha')$	L	$\lambda - L$ even	L	$\lambda - L$ odd
$(2\|2)$	$0, \ldots, \lambda$	$\langle u_2\|u_2\rangle$		
$(2\|1)$	$2, \ldots, \lambda$	$\langle u_2\|u_1\rangle$		
$(2\|0)$	$4, \ldots, \lambda$	$\langle u_2\|u_0\rangle$		
$(1\|1)$	$2, \ldots, \lambda$	$\langle u_1\|u_1\rangle$	$2, \ldots, \lambda+1$	$\langle \tilde{u}_1\|\tilde{u}_1\rangle$
$(1\|1)$	$\lambda+2$	$\langle u'_1\|u'_1\rangle$		
$(1\|0)$	$4, \ldots, \lambda$	$\langle u_1\|u_0\rangle$	$4, \ldots, \lambda+1$	$\langle \tilde{u}_1\|\tilde{u}_0\rangle$
$(1\|0)$	$\lambda+2$	$\langle u'_1\|u'_0\rangle$		
$(0\|0)$	$4, \ldots, \lambda$	$\langle u_0\|u_0\rangle$	$4, \ldots, \lambda+1$	$\langle \tilde{u}_0\|\tilde{u}_0\rangle$
$(0\|0)$	$\lambda+2$	$\langle u'_0\|u'_0\rangle$	$\lambda+3$	$\langle \tilde{u}'_0\|\tilde{u}'_0\rangle$
$(0\|0)$	$\lambda+4$	$\langle u''_0\|u''_0\rangle$		

Table 3. Overlap integrals of the non-canonical BM basis. for $\mu = 4$ and $\lambda - L$ even.

	$\mu = 4$ and $\lambda - L$ even
	$\langle u_2\|u_2\rangle = 8L!(\lambda-L)!!(\lambda+L+1)!!(3L^4+6L^3$ $-(8\lambda(\lambda+8)+135)L^2-2(4\lambda(\lambda+8)+69)L+8(\lambda+3)^2(\lambda+5)^2)/(2L+1)!!$
	$\langle u_2\|u_1\rangle = 8L!(-\lambda+L-2)(\lambda+L+6)(\lambda-L)!!(\lambda+L+1)!!$ $\times(3(L-1)L-2(2\lambda(\lambda+8)+33))/(2L+1)!!$
	$\langle u_2\|u_0\rangle = 24L!(\lambda-L+2)(\lambda-L+4)(\lambda+L+4)$ $\times(\lambda+L+6)(\lambda-L)!!(\lambda+L+1)!!/(2L+1)!!,$
$(*)$	$\langle u_1\|u_1\rangle = -4(L-2)!(\lambda-L+2)!!(\lambda+L+1)!!\Big(6L^5+6(\lambda+5)L^4$ $-(\lambda(7\lambda+59)+150)L^3-(\lambda+6)(\lambda(7\lambda+55)+118)L^2$ $-(\lambda+2)(\lambda(5\lambda+48)+129)L-6(\lambda+2)(\lambda(\lambda+10)+27))/(2L+1)!!$
$(*)$	$\langle u'_1\|u'_1\rangle = 4(\lambda+2)(\lambda+3)(\lambda+4)(\lambda+35)\lambda!.$
	$\langle u_1\|u_0\rangle = 24(L-2)!(\lambda-L+4)(\lambda+L+6)(\lambda-L+2)!!$ $\times(\lambda+L(\lambda+L(\lambda+L+4)+2)+2)(\lambda+L+1)!!/(2L+1)!!$
	$\langle u'_1\|u'_0\rangle = 96(\lambda+2)(\lambda+3)(\lambda+4)\lambda!$
$(*)$	$\langle u_0\|u_0\rangle = 24(L-4)!(\lambda-L+4)!!(\lambda+L+1)!!(9(\lambda+2)(\lambda+4)$ $+L^6+2(\lambda+3)L^5+8(\lambda+2)(\lambda+3)L+(\lambda(\lambda+4)-8)L^4$ $-2(\lambda+3)(\lambda+6)L^3+(\lambda(5\lambda+38)+88)L^2)/(2L+1)!!,$
	$\langle u'_0\|u'_0\rangle = 48(\lambda+2)(\lambda+3)(\lambda+4)(2\lambda^2+\lambda+3)(\lambda-2)!$

Table 4. Overlap integrals of non-canonical BM basis for $\mu = 5$.

$(\alpha\vert\alpha')$	L	$\lambda - L$ even	L	$\lambda - L$ odd
$(2\vert 2)$	$1, \ldots, \lambda$	$\langle u_2\vert u_2\rangle$	$1, \ldots, \lambda+1$	$\langle \tilde{u}_2\vert \tilde{u}_2\rangle$
$(2\vert 1)$	$3, \ldots, \lambda$	$\langle u_2\vert u_1\rangle$	$3, \ldots, \lambda+1$	$\langle \tilde{u}_2\vert \tilde{u}_1\rangle$
$(2\vert 0)$	$5, \ldots, \lambda$	$\langle u_2\vert u_0\rangle$	$5, \ldots, \lambda+1$	$\langle \tilde{u}_2\vert \tilde{u}_0\rangle$
$(1\vert 1)$	$3, \ldots, \lambda$	$\langle u_1\vert u_1\rangle$	$3, \ldots, \lambda+1$	$\langle \tilde{u}_1\vert \tilde{u}_1\rangle$
$(1\vert 1)$	$\lambda+2$	$\langle u_1'\vert u_1'\rangle$	$\lambda+3$	$\langle \tilde{u}_1'\vert \tilde{u}_1'\rangle$
$(1\vert 0)$	$5, \ldots, \lambda$	$\langle u_1\vert u_0\rangle$	$5, \ldots, \lambda+1$	$\langle \tilde{u}_1\vert \tilde{u}_0\rangle$
$(1\vert 0)$	$\lambda+2$	$\langle u_1'\vert u_0'\rangle$	$\lambda+3$	$\langle \tilde{u}_1'\vert \tilde{u}_0'\rangle$
$(0\vert 0)$	$5, \ldots, \lambda$	$\langle u_0\vert u_0\rangle$	$5, \ldots, \lambda+1$	$\langle \tilde{u}_0\vert \tilde{u}_0\rangle$
$(0\vert 0)$	$\lambda+2$	$\langle u_0'\vert u_0'\rangle$	$\lambda+3$	$\langle \tilde{u}_0'\vert \tilde{u}_0'\rangle$
$(0\vert 0)$	$\lambda+4$	$\langle u_0''\vert u_0''\rangle$	$\lambda+5$	$\langle \tilde{u}_0''\vert \tilde{u}_0''\rangle$

Table 5. Overlap integrals of the non-canonical BM basis. for $\mu = 5$ and $\lambda - L$ even.

$\mu = 5$ and $\lambda - L$ even
$\langle u_2\vert u_2\rangle = 24(\lambda+2)(L+1)(L-1)!(\lambda-L)!!(\lambda+L+1)!!$ $\times(-(4\lambda(\lambda+10)+109)L^2 - 2(2\lambda(\lambda+10)+55)L$ $+8(\lambda(\lambda+10)(\lambda(\lambda+10)+49)+603) + L^4 + 2L^3)/(2L+1)!!$
$\langle u_2\vert u_1\rangle = 24(\lambda+2)(L+1)(-\lambda+L-2)(\lambda+L+8)(L-1)!$ $\times((L-1)L - 2(\lambda(\lambda+10)+27))(\lambda-L)!!(\lambda+L+1)!!/(2L+1)!!$
$\langle u_2\vert u_0\rangle = 24(\lambda+2)(L+1)(-\lambda+L-4)(-\lambda+L-2)(\lambda+L+6)$ $\times(L-1)!(\lambda+L+8)(\lambda-L)!!(\lambda+L+1)!!/(2L+1)!!$
$\langle u_1\vert u_1\rangle = 12(\lambda+2)(L+1)(L-3)!(\lambda-L+2)!!(\lambda+L+1)!!$ $\times((\lambda(3\lambda+29)+96)L^3 + (\lambda(\lambda(3\lambda+53)+316)+680)L^2$ $+(\lambda(\lambda(7\lambda+100)+487)+716)L - 2L^5 - 2(\lambda+7)L^4$ $+2(\lambda(\lambda(7\lambda+102)+491)+684))/(2L+1)!!$
$\langle u_1'\vert u_1'\rangle = 12(\lambda+2)(\lambda+3)^2(\lambda+4)(\lambda+5)(\lambda+20)(\lambda-1)!$
$\langle u_1\vert u_0\rangle = 24(\lambda+2)(L+1)(\lambda-L+4)(\lambda+L+8)(L-3)!(\lambda-L+2)!!$ $\times(5\lambda + L(3\lambda + L(\lambda+L+6)+8)+12)(\lambda+L+1)!!/(2L+1)!!$
$\langle u_1'\vert u_0'\rangle = 96(\lambda+2)(\lambda+3)^2(\lambda+4)(\lambda+5)(\lambda-1)$
$\langle u_0\vert u_0\rangle = 24(\lambda+2)(L+1)(L-5)!(\lambda-L+4)!!(\lambda+L+1)!!$

Orthonormalisation of BM Basis

Let us construct the orthonormal basis in the space spanned by the non-canonical BM vectors (5), $(M = L)$. For this purpose, we propose a bit more efficient form of the Gram–Schmidt orthonormalisation procedure

$$\left| \begin{array}{c} (\lambda,\mu) \\ f_i, L, L \end{array} \right\rangle = \sum_{\alpha=0}^{\alpha_{\max}} A_{i,\alpha}^{(\lambda,\mu)}(L) \left| \begin{array}{c} (\lambda,\mu)_B \\ \alpha, L, L \end{array} \right\rangle . \tag{17}$$

Here multiplicity index i is introduced to differentiate the orthonormalized states and $A_{i,\alpha}^{(\lambda,\mu)}(L)$ are the BM basis orthonormalization coefficients. These coefficients fulfill the following condition

$$A_{i,\alpha}^{(\lambda,\mu)}(L) = 0, \quad \text{if } i > \alpha. \tag{18}$$

Because the BM vectors (5) are linearly independent, one can require the orthonormalization properties for the vectors (17)

$$\left\langle \begin{array}{c} (\lambda,\mu) \\ f_i, L, L \end{array} \middle| \begin{array}{c} (\lambda,\mu) \\ f_k, L, L \end{array} \right\rangle = \delta_{ik}. \tag{19}$$

Orthonormalisation of BM Basis

In the case of the subset of three independent BM vectors (5) indicated by the displayed values of labels, expansion (17) takes the form ($\mu = 4$, $\lambda - L$ even))

$$\left| \begin{array}{l} (\lambda,\mu) \\ f_2, L, L \end{array} \right\rangle = A_{2,2}^{(\lambda,\mu)}(L) \left| \begin{array}{l} (\lambda,\mu)_B \\ 2, L, L \end{array} \right\rangle,$$

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

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

$$A_{2,2}^{(\lambda,4)}(L) = \left(\langle u_2|u_2\rangle\right)^{-1/2}, \qquad A_{1,1}^{(\lambda,4)}(L) = -\langle \psi_1|\psi_1\rangle^{-1/2}, \qquad A_{1,2}^{(\lambda,4)}(L) = \langle \psi_1|\psi_1\rangle^{-1/2} \frac{\langle u_2|u_1\rangle}{\langle u_2|u_2\rangle},$$

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

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

$$\langle \psi_0|\psi_0\rangle = \langle u_0|u_0\rangle - \frac{\langle u_2|u_0\rangle^2}{\langle u_2|u_2\rangle} - \frac{1}{\langle \psi_1|\psi_1\rangle} \left(-\langle u_1|u_0\rangle + \frac{\langle u_2|u_1\rangle\langle u_2|u_0\rangle}{\langle u_2|u_2\rangle} \right)^2,$$

$$\langle \psi_1|\psi_1\rangle = \langle u_1|u_1\rangle - \frac{\langle u_2|u_1\rangle^2}{\langle u_2|u_2\rangle}.$$

Orthonormalisation of BM Basis

The Gram–Schmidt orthonormalization symbolic algorithm 2. Step 1.

Step 1. First one needs to organize the loop running over all indices $\alpha = \alpha_{\max}, \alpha_{\max} - 1, ..., 0$ of a given set of the BM states. Then the first orthonormalization coefficients of the orthogonal BM states (i.e., some linear combination of initial states (5)) for a given value of α are calculated by the formula

$$b_{\alpha,\alpha_{\max}} = \frac{\langle u_\alpha | u_{\alpha_{\max}} \rangle}{\langle u_{\alpha_{\max}} | u_{\alpha_{\max}} \rangle^{1/2}}, \qquad (20)$$

where the $\langle u_\alpha | u_{\alpha'} \rangle$ denotes the overlap integrals (16).

Orthonormalisation of BM Basis

Step 2.

Step 2. Secondly one needs to organize the inner loop inside the loop defined in Step 1. of this algorithm. This inner loop should run over all indices $\alpha' = \alpha_{\max} - 1, \alpha_{\max} - 2, ..., \alpha + 1$ of a given set of BM states. For the following calculations, it is convenient to introduce the intermediate quantity

$$f_{\alpha,\alpha'} = -\langle u_\alpha | u_{\alpha'} \rangle + \frac{\langle u_\alpha | u_{\alpha_{\max}} \rangle \langle u_{\alpha_{\max}} | u_{\alpha'} \rangle}{\langle u_{\alpha_{\max}} | u_{\alpha_{\max}} \rangle}. \quad (21)$$

Now the orthonormalization coefficients for the BM states for any given values of α and α' are calculated by the formula

$$b_{\alpha,\alpha'} = \frac{f_{\alpha,\alpha'}}{\langle \psi_{\alpha'} | \psi_{\alpha'} \rangle^{1/2}}. \quad (22)$$

Here the normalization integral is defined as

$$\langle \psi_\alpha | \psi_\alpha \rangle = \langle u_\alpha | u_\alpha \rangle - \sum_{i=\alpha+1}^{\alpha_{\max}} b_{\alpha,i}^2. \quad (23)$$

Orthonormalisation of BM Basis

Step 3.

Step 3. Now we make the recursive step and calculate the next quantity $f_{\alpha,\alpha'}$ from the results of the previous step

$$f_{\alpha,\alpha'-1} = f_{\alpha,\alpha'\to\alpha'-1} + \frac{1}{\langle\psi_{\alpha'}|\psi_{\alpha'}\rangle} f_{\alpha\to\alpha'-1,\alpha'} f_{\alpha,\alpha'}. \tag{24}$$

Here the arrows in the right hand side of the (24) indicate that the quantity $f_{\alpha,\alpha'}$ obtained at the previous step is used with the appropriate substitution of indices. Having calculated the quantity $f_{\alpha,\alpha'}$, the expression of the next orthonormalization coefficient $b_{\alpha,\alpha'}$ can be obtained by Eq. (22). The steps of the orthonormalization algorithm defined above are recursively repeated doing the loop over all allowed values of indices α and α'.

Step 4.

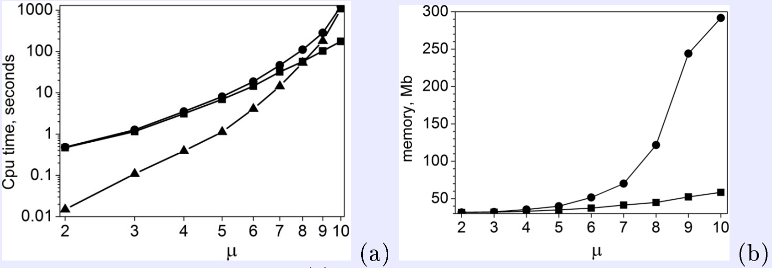
Step 4. Finally, we should to collect all the coefficients in the recursively obtained analytical expansion representing the orthonormalized state for every independent BM state (5). In this way, we get the required orthonormalization coefficients of expansion (17).

Orthonormalisation of BM Basis

Table 6. Transformation coefficients $A_{i,\alpha}^{(\lambda,\mu)}(L)$ for $\mu = 4$.

α	i	L	$\lambda - L$ even	$\lambda - L$ odd
2	2	$0, 1, \ldots, \lambda$	$A_{2,2}^{(\lambda,4)}(L)$	—
	1	$2, 3, \ldots, \lambda$	$A_{1,2}^{(\lambda,4)}(L)$	—
	0	$4, 5, \ldots, \lambda$	$A_{0,2}^{(\lambda,4)}(L)$	—
1	1	$2, 3, \ldots, \lambda+1$	$A_{1,1}^{(\lambda,4)}(L)$	$\tilde{A}_{1,1}^{(\lambda,4)}(L)$
		$\lambda+2$	$A_{1,1}^{(\lambda,4)}(\lambda+2)$	—
	0	$4, 5, \ldots, \lambda+1$	$A_{0,1}^{(\lambda,4)}(L)$	$\tilde{A}_{0,1}^{(\lambda,4)}(L)$
		$\lambda+2$	$A_{0,1}^{(\lambda,4)}(\lambda+2)$	—
0	0	$4, 5, \ldots, \lambda+1$	$A_{0,0}^{(\lambda,4)}(L)$	$\tilde{A}_{0,0}^{(\lambda,4)}(L)$
		$\lambda+2$	$A_{0,0}^{(\lambda,4)}(\lambda+2)$	—
		$\lambda+3$	—	$\tilde{A}_{0,0}^{(\lambda,4)}(\lambda+3)$
		$\lambda+4$	$A_{0,0}^{(\lambda,4)}(\lambda+4)$	—

The above algorithm was realized in the form of the program implemented in the computer algebra system Wolfram Mathematica 10.1. The typical running time of calculating the irreducible representations $\mu = 4$ is 30 seconds and memory is 60Mb using the PC Intel Pentium CPU 1.50 GHz 4GB 64bit Windows 8.
Recursive calculation of the quantities $f_{\alpha,\alpha'}$ (24) and the normalization integrals (23) do not involve any square root operation. This distinct feature of the proposed orthonormalization algorithm may make the large scale symbolic calculations feasible.



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 by means of Algorithm 1 code(squares) and execution of the othonormalization Gram–Schmidt procedure by means of Algorithm 2 code (triangles).

The orthonormalization numerical algorithm

$$\sum_{\alpha'=0}^{\alpha_{\max}} \left(\left\langle \alpha \middle| \alpha' \right\rangle - \Lambda_i(L)\delta_{\alpha\alpha'} \right) C_{\alpha' i}(L) = 0$$

For $\Lambda_i \neq 0$ one gets the following basis of orthonormal states

$$\left| \begin{array}{c} (\lambda,\mu) \\ f_i, L, L \end{array} \right\rangle = \sum_{\alpha=0}^{\alpha_{\max}} C_{\alpha i}^{(\lambda,\mu)}(L) \left| \begin{array}{c} (\lambda,\mu)_B \\ \alpha, L, L \end{array} \right\rangle, \quad \sum_{\alpha=0}^{\alpha_{\max}} C_{\alpha i}^{(\lambda,\mu)}(L) C_{\alpha i'}^{(\lambda,\mu)}(L) = \delta_{ii'}. \tag{25}$$

The Action of the Zero Component of the Quadrupole Operator onto the Orthogonal Basis

Following the paper [Raychev, P., 1981], we determine the action of the zero component of the second order generator of SU(3) group onto the BM basis vectors[a]

$$Q_0 \left| \begin{array}{l} (\lambda,\mu)_B \\ \alpha, L, L \end{array} \right\rangle = \sum_{\substack{k=0,1,2 \\ s=0,\pm 1}} a_s^{(k)} \left| \begin{array}{l} (\lambda,\mu)_B \\ \alpha+s, L+k, L \end{array} \right\rangle, \tag{26}$$

where the coefficients $a_s^{(k)} \equiv a_s^{(k)}(\alpha)$ can be calculated as in [Afanasjev, G.N., 1973] and they have the form given in [Raychev, P., 1981], and the inverse transformation $\tilde{A}_{i,\alpha}^{(\lambda\mu)}(L)$ from formula (17)

$$\left| \begin{array}{l} (\lambda,\mu)_B \\ \alpha, L, L \end{array} \right\rangle = \sum_{i=0}^{\alpha} \tilde{A}_{i,\alpha}^{(\lambda\mu)}(L) \left| \begin{array}{l} (\lambda,\mu) \\ f_i, L, L \end{array} \right\rangle, \tag{27}$$

where conventional relations take place

$$\sum_i \tilde{A}_{i,\alpha'}^{(\lambda\mu)}(L) A_{i,\alpha}^{(\lambda\mu)}(L) = \delta_{\alpha',\alpha} \quad \text{and} \quad \sum_\alpha \tilde{A}_{i',\alpha}^{(\lambda\mu)}(L) A_{i,\alpha}^{(\lambda\mu)}(L) = \delta_{i',i}. \tag{28}$$

---

[a] It should be noted that the used states differ from the states (3.8) given by [Moshinsky, M., 1975] in the definition of the number a and coincide up to a phase factor $(-1)^\alpha$ in l.h.s. and $(-1)^{\alpha+s}$ in r.h.s..

The Action of the Zero Component of the Quadrupole Operator onto the Orthogonal Basis

Using (26), (27), and (28), one obtains the action of the zero component of the quadrupole operator onto the orthogonal BM basis vectors

$$Q_0 \left| \begin{array}{l} (\lambda,\mu) \\ f_i, L, L \end{array} \right\rangle = \sum_{\substack{j=0,\ldots,\alpha_{\max} \\ k=0,1,2}} q_{ijk}^{(\lambda\mu)}(L) \left| \begin{array}{l} (\lambda,\mu) \\ f_j, L+k, L \end{array} \right\rangle, \tag{29}$$

where the coefficients $q_{ijk}^{(\lambda\mu)}(L)$ are calculated by the formula

$$q_{ijk}^{(\lambda\mu)}(L) = \sum_{\substack{\alpha=0,\ldots,\alpha_{\max} \\ s=0,\pm 1}} A_{i,\alpha}^{(\lambda\mu)}(L) a_s^{(k)} \tilde{A}_{j,(\alpha+s)}^{(\lambda\mu)}(L+k), \tag{30}$$

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

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

The Action of the Zero Component of the Quadrupole Operator onto the Orthogonal Basis

The matrix elements of the quadrupole operators, generators of the group SU(3) can be reduced to the calculation of the reduced matrix elements by means of the Wigner–Eckart theorem

$$\left\langle \begin{matrix} (\lambda\mu) \\ jL+kM \end{matrix} \middle| Q_m \middle| \begin{matrix} (\lambda\mu) \\ iLM' \end{matrix} \right\rangle = \frac{(LM'\,2m|L+k,M)}{\sqrt{2(L+k)+1}} \left\langle \begin{matrix} (\lambda\mu) \\ j,L+k \end{matrix} \middle\| Q \middle\| \begin{matrix} (\lambda\mu) \\ i,L \end{matrix} \right\rangle . \quad (32)$$

The corresponding reduced matrix element is determined by formula

$$\left\langle \begin{matrix} (\lambda\mu) \\ j,L+k \end{matrix} \middle\| Q \middle\| \begin{matrix} (\lambda\mu) \\ i,L \end{matrix} \right\rangle = (-1)^k \frac{\sqrt{2L+1}}{(L+k,L,20|LL)} q_{i,j,k}^{(\lambda,\mu)}(L), \quad (33)$$

where the coefficients $q_{i,j,k}^{(\lambda,\mu)}(L)$ are defined by (30). 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 (11). The dimension of this subspace determines the complexity of the above algorithms, i.e., required computer memory and execution time.

In this paper, the new results for the coefficients $q_{ijk}^{(\lambda\mu)}(L)$ in the orthonormal BM basis with the highest weight vectors of SO(3) irreps for $\mu = 4$ were calculated. Note that the coefficients $q_{ijk}^{(\lambda\mu)}(L)$ for up to $\mu = 3$ were calculated as well and their values are equal to those presented in Table 1 of Ref. [Raychev, P., 1981].

The zero component of the quadrupole operator into the nonorthogonal BM basis

The zero component of the quadrupole operator Q_0 into the nonorthogonal BM basis, i.e. the coefficients $a_s^{(k)} \equiv a_s^{(k)}(\alpha) = (-1)^s q_s^{(k)}(\alpha)$ of expansion (26) reads as

$$q_0^{(2)} = \frac{12\sigma}{[(l+2)(2l+3)]^{1/2}}, \quad q_{-1}^{(2)} = \frac{12\alpha}{[(l+2)(2l+3)]^{1/2}}, \quad q_{-1}^{(2)} = 0,$$

$$q_0^{(1)} = 12\frac{\alpha\beta(l_1+1)+\sigma(l_2+\beta)}{(l+2)(l+1)^{1/2}} - \frac{6\beta}{(l+1)^{1/2}},$$

$$q_{-1}^{(1)} = -\frac{12\alpha l_1}{(l+2)(l+1)^{1/2}}, \quad q_1^{(1)} = -\frac{12\sigma\beta l_2}{(l+2)(l+1)^{1/2}},$$

$$q_0^{(0)} = 4\alpha\frac{l(l+1)-3(l_1+\beta)^2}{(l+1)(2l+3)} - 4\sigma\frac{l(l+1)-3(l_2+\beta)^2}{(l+1)(2l+3)} - (l_1-l_2)\left(1+\frac{3\beta}{l+1}\right),$$

$$q_{-1}^{(0)} = \frac{12\alpha l_1(l_1-1)}{(l+1)(2l+3)},$$

$$q_1^{(0)} = -\frac{12\sigma l_2(l_2-1)}{(l+1)(2l+3)},$$

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

where $T = \lambda/2$, $n = 2\mu+\lambda$, $l_1 = L+2\alpha-n/2+T$, $l_2 = n/2-T-2\alpha-\beta$.

Resume

- We present the practical symbolic algorithm implemented in Mathematica 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 proposed recursive orthonormalisation algorithm allows one to find the analytical expressions of the orthonormalized basis. The distinct advantage of adapted Gram–Schmidt orthonormalisation is that it does not involve any square root operation on the expressions coming from the previous recursion steps.
- This makes the proposed method very suitable for 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 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.

THANK YOU FOR YOUR ATTENTION