Supplemental material to the paper: Orthonormal basis and the matrix elements for algebraic models of partner groups $\mathrm{SU}(3) \times \overline{\mathrm{SU}(3)}$

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Abstract. A new class of algebraic models based on partner groups idea allowing to describe both the external laboratory and the intrinsic degrees of freedom of a given physical system is used. Such models are, to some extend, successors of the generalized rotor model in which the Hamiltonian was constructed from the angular momentum operators. The algebraic-group method and procedures described in this paper are dedicated for searching higher order point symmetries in nuclei. The main part of the elaborated procedures are realized as an open access code `SU3BMB` implemented in the Wolfram Mathematica computes the orthonormal $\mathrm{SU}(3) \supset \mathrm{SO}(3)$ non-canonical Bargmann-Moshinsky (BM) basis labelled by Elliot's (λ, μ) and the angular momentum (L, M) quantum numbers. It also calculate all basic ingredients required to calculate required matrix elements of the group generators, e.g. required for calculating of spectra of the Hamiltonians constructed from the generators of the partner groups $\mathrm{SU}(3) \times \overline{\mathrm{SU}(3)}$. The proposed method uses a new symbolic-numerical non-standard recursive and fast orthonormalization procedure based on the Gram-Schmidt orthonormalization algorithm. Efficiency of the elaborated procedures and the code for large scale calculation is shown by benchmark calculations of orthogonalization matrix, reduced quadrupole matrix elements and degeneracy spectrum of the tetrahedral algebraic model.

Keywords: Bargmann-Moshinsky SU(3) basis, Gram-Schmidt orthonormalization, quadrupole operator , partner groups $\mathrm{SU}(3) \times \overline{\mathrm{SU}(3)}$ algebraic nuclear models

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1. The set of equations cited in the paper and in Refs. [1, 2, 3, 4, 5, 6]

$$\left\langle \begin{array}{c} \lambda\mu \\ i'L'M' \end{array} \middle| T_{lm} \middle| \begin{array}{c} \lambda\mu \\ iLM \end{array} \right\rangle = \frac{(LMlm|L'M')}{\sqrt{2L'+1}} \left\langle \begin{array}{c} \lambda\mu \\ i'L' \end{array} \middle\| T_l \middle\| \begin{array}{c} \lambda\mu \\ iL \end{array} \right\rangle . \quad (5)$$

$$H_{SU(3)} = -\kappa Q \cdot Q + \beta L \cdot L = -\kappa C_2(\mathrm{SU(3)}) + (3\kappa+\beta)L^2 \, . \quad (9)$$

$$C_2(SU(3)) = Q \cdot Q + 3L \cdot L \quad (11)$$

$$\langle C_2(SU(3))\rangle_{(\lambda,\mu)} = 4(\lambda^2+\mu^2+\lambda\mu+3\lambda+3\mu). \quad (12)$$

$$D_{\lambda\mu} = \frac{1}{2}(\lambda+1)(\mu+1)(\lambda+\mu+2). \quad (13)$$

$$H_{3QL} = i\left[(\bar{Q}\otimes\bar{L})_{32} - (\bar{Q}\otimes\bar{L})_{3,-2}\right], \quad (14)$$

$$H_{4QQ} = \left[\sqrt{\frac{14}{5}}(\bar{Q}\otimes\bar{Q})_{40} + (\bar{Q}\otimes\bar{Q})_{4,-4} + (\bar{Q}\otimes\bar{Q})_{44}\right], \quad (16)$$

$$\langle u_\alpha|u_{\alpha'}\rangle = \langle \hat{u}_\alpha|N^{-1}_{\alpha\alpha}N^{-1}_{\alpha'\alpha'}|\hat{u}_{\alpha'}\rangle,\ \langle u_\alpha|u_\alpha\rangle = 1. \quad (24)$$

$$|\phi_i\rangle = \sum_{\alpha=0}^{\alpha_{\max}} A_{i,\alpha}|u_\alpha\rangle = \sum_{\alpha=0}^{\alpha_{\max}} \hat{A}_{i,\alpha}|\hat{u}_\alpha\rangle, \qquad \mathbf{A} = \hat{\mathbf{A}}\mathbf{N}. \quad (25)$$

$$\begin{aligned}
\langle \hat{u}_\alpha|\hat{u}_{\alpha'}\rangle &= \left\langle \begin{array}{c} (\lambda,\mu)_B \\ \alpha, L, L \end{array} \middle| \begin{array}{c} (\lambda,\mu)_B \\ \alpha', L, L \end{array} \right\rangle = C_1(\lambda,L,\Delta)(\lambda+2)^\beta(L-\mu+2\alpha)! \\
&\times (\lambda-L+\mu-2\alpha'-\beta)!!(\mu-2\alpha'-\beta+\Delta-1)!! \\
&\times \sum_{l,z} \begin{pmatrix} \alpha' \\ \frac{1}{2}(l-\beta-\Delta) \end{pmatrix} (-1)^{(\mu+2\alpha-\Delta-\beta)/2+z} \begin{pmatrix} \frac{1}{2}(\mu-2\alpha-\Delta-\beta) \\ z \end{pmatrix} \\
&\times \frac{(\mu-l)!!}{(\mu-l-2z)!!}\frac{(\mu+\beta+\Delta)!!}{(\mu-2\alpha'+l)!!}(l-\Delta+\beta-1)!!(\mu-\Delta-\beta-2z)!! \\
&\times \frac{(\lambda-L+\mu-2\alpha-\beta)!!}{(\lambda-L+\Delta+2z)!!}\frac{(\lambda+L-\Delta+2)!!}{(\lambda+L-\mu+2\alpha+\beta+2z+2)!!}\frac{(L+l)!}{L!} \\
&\times \frac{(\lambda+\mu+L+\beta+2)!!}{(\lambda+L+l+\beta+2z+2)!!}\frac{(\lambda+\beta+2z+1)!}{(\lambda+\beta+1)!}\frac{(\lambda+\mu-l-L+\Delta)!!}{(\lambda-L+\mu-2\alpha'-\beta)!!} \\
&\times C_2(\lambda,L,\Delta,z). \quad (34)
\end{aligned}$$

$$\mathcal{A}\,\mathcal{U}\mathcal{A}^T = \mathcal{I}. \quad (45)$$

$$\mathcal{A} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \mathbf{A} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \mathcal{U} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \mathbf{U} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \mathcal{I} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \mathbf{I} & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (46)$$

$$\mathbf{A} = \begin{pmatrix} A_{\alpha_{\min K},\alpha_{\min K}} & \cdots & A_{\alpha_{\min K},\alpha_{\max K}} \\ \vdots & \ddots & \vdots \\ A_{\alpha_{\max K},\alpha_{\min K}} & \cdots & A_{\alpha_{\max K},\alpha_{\max K}} \end{pmatrix}. \quad (47)$$

$$\mathbf{U}=\begin{pmatrix} \langle u_{\alpha_{\min K}}|u_{\alpha_{\min K}}\rangle & \dots & \langle u_{\alpha_{\min K}}|u_{\alpha_{\max K}}\rangle \\ \vdots & \ddots & \vdots \\ \langle u_{\alpha_{\max K}}|u_{\alpha_{\min K}}\rangle & \dots & \langle u_{\alpha_{\max K}}|u_{\alpha_{\max K}}\rangle \end{pmatrix}. \tag{48}$$

$$q^{(\lambda\mu)}_{ijk}(L)=\sum_{\substack{\alpha=0,\dots,\alpha_{\max}\\ s=0,\pm1}} A^{(\lambda\mu)}_{i,\alpha}(L)N^{-1}_{\alpha,\alpha}a^{(k)}_s N_{\alpha+s,\alpha+s}(A^{-1})^{(\lambda\mu)}_{j,(\alpha+s)}(L+k), \tag{54}$$

$$\begin{aligned}
&a^{(2)}_0=\frac{6(\lambda+\mu-L-2\alpha-\beta)}{((L+2)(2L+3))^{1/2}},\;\; a^{(2)}_{-1}=\frac{12\alpha}{((L+2)(2L+3))^{1/2}},\;\; a^{(2)}_{-1}=0,\\
&a^{(1)}_0=-6\frac{2\alpha\beta(L+2\alpha-\mu+1)+(\lambda+\mu-L-2\alpha)[\mu-2\alpha]}{(L+2)(L+1)^{1/2}}-\frac{6\beta}{(L+1)^{1/2}},\\
&a^{(1)}_{-1}=\frac{12\alpha([L]-\mu+2\alpha)}{(L+2)(L+1)^{1/2}},\;\; a^{(1)}_1=\frac{6\beta(\lambda+\mu-L-2\alpha-\beta)[\mu-2\alpha-\beta]}{(L+2)(L+1)^{1/2}},\\
&a^{(0)}_0=4\alpha\frac{L(L+1)-3(L+2\alpha-\mu+\beta)^2}{(L+1)(2L+3)}-2(\lambda+\mu-L-\beta-2\alpha)\frac{L(L+1)-3(\mu-2\alpha)^2}{(L+1)(2L+3)}\\
&-(L-[2\mu]+4\alpha+\beta)\left(1+\frac{3\beta}{L+1}\right),\\
&a^{(0)}_{-1}=\frac{[12\alpha](L-\mu+2\alpha)(L-\mu+2\alpha-1)}{(L+1)(2L+3)},\\
&a^{(0)}_1=-\frac{6(\lambda+\mu-L-2\alpha-\beta)(\mu-2\alpha-\beta)(\mu-2\alpha-\beta-1)}{(L+1)(2L+3)},\\
&\beta=\begin{cases}0, & \lambda+\mu-L \text{ even},\\ 1, & \lambda+\mu-L \text{ odd}.\end{cases}
\end{aligned} \tag{55}$$

2. Description of the program SU3BMB [2]

The program `SU3BMB` computes the orthonormal SU(3) $\supset$ SO(3) non-canonical Bargmann-Moshinsky basis. Using this basis it calculates matrices of the quadrupole and the angular momentum operators Q and L and by the anti-isomorphism of partners groups $\bar{Q}$ and $\bar{L}$. Using these matrices it calculates, as the test, the matrix of the tetrahedral Hamiltonian $H_{SU(3)}+\gamma_{3QL}H_{3QL}+\gamma_{4QQ}H_{4QQ}$ operator and it finds its eigenvalues.

Remark 3. Using as the pattern the above Hamiltonian $H_{SU(3)}+\gamma_{3QL}H_{3QL}+\gamma_{4QQ}H_{4QQ}$ one can write any other SU(3) $\times$ $\overline{\mathrm{SU}(3)}$ Hamiltonian. It is not useful to construct a universal procedure for calculating any arbitrary Hamiltonian because of its complexity [7]. It can be specify by user for a case that interests him (see, for example [3]). Other examples we will consider in a separated paper.

The program allows for choosing:

- the values of the quantum numbers labeling SU(3) irreducible representation λ and μ, the value of the angular momentum L, the value of the index denoting different components of the quadrupole operator and angular momentum operator η, and the values of the variational coefficients: κ, β, γ_{3QL} and γ_{4QQ} as appropriate in the corresponding computation case;

- the desired computation for the chosen values of the quantum numbers and variational coefficients:
  - calculation of the overlap integrals of SU(3) BM basis given by expression (34) for the specified values of (λ, μ, L);
  - calculation of the SU(3) BM basis orthonormalization coefficients defined by expression (25) for the specified values of (λ, μ, L);
  - the orthonormality test of the BM basis using the condition (45) for the specified values of (λ, μ, L);
  - calculation of the quadrupole operator Q matrix in the BM basis by formula (5) for the specified values of (λ, μ, η);
  - a test of the matrices Q comparing the calculated matrix of the scalar product of the Q operators for the specified values of (λ, μ) against the well-known results given by equalities (11) and (12) ;
  - calculation of the matrix of the operator H_{3QL} defined by equation (14) and its eigenvalues for the specified values of (λ, μ);
  - calculation of the matrix of the operator H_{4QQ} defined by equation (16) and its eigenvalues for the specified values of (λ, μ);
  - calculation of the matrix of the operator $H_{SU(3)} + \gamma_{3QL} H_{3QL}$ and its eigenvalues for the specified values of $(\lambda, \mu, \kappa, \beta, \gamma_{3QL})$, where the operator $H_{SU(3)}$ is defined by expression (9);
  - calculation of the matrix of the operator $H_{SU(3)} + \gamma_{4QQ} H_{4QQ}$ and its eigenvalues for the specified values of $(\lambda, \mu, \kappa, \beta, \gamma_{4QQ})$;
  - calculation of the matrix of the operator $H_{SU(3)} + \gamma_{3QL} H_{3QL} + \gamma_{4QQ} H_{4QQ}$ and its eigenvalues for the specified values of $(\lambda, \mu, \kappa, \beta, \gamma_{3QL}, \gamma_{4QQ})$;
  - calculation of the possible values of the L of the BM basis for the specified values of (λ, μ);
  - calculation of the possible values of the α of the BM basis for the specified values of (λ, μ);
  - calculation of the angular momentum operator L matrix in the BM basis for the specified values of (λ, μ, η);
  - call of the pattern of a procedure to be implemented by user;
  - timing of all chosen computation procedures for the specified values of input parameters;
  - calculation of the operator q matrix in the BM basis for the specified values of (λ, μ, L, k);
- the desired computation and output precision:
  - a number of significant digits in the numerical calculations;
  - a number of output digits of calculation results transferred to the notebook

and the working file;

- the desired output:
  - only to the notebook;
  - only to the file;
  - to the notebook and file at the same time.

The program `SU3BMB` performs the following tasks:

- reads input data from the provided file `input.txt`;
- performs computation of one or more quantities chosen in the input file;
- if required, evaluation of the accuracy of the calculated BM basis or/and quadrupole operator matrices may be output only as message/verdict or as complete results;
- prints the results to the notebook or/and output file `output.txt`.

On user demand the output of the program `SU3BMB` may contains the following information:

- in the case of the overlap integrals of SU(3) BM basis calculation: input data, dimension of the overlap integrals matrix, values of ($\alpha_{\min}$, $\alpha_{\min K}$, $\alpha_{\max K}$, $\alpha_{\max}$), and the calculated matrix $\mathcal{U}^{\mu\lambda}(L)$;
- in the case of the SU(3) BM basis orthonormalization coefficients calculation: input data, dimension of the matrix of the products of BM basis vectors, values of ($\alpha_{\min}$, $\alpha_{\min K}$, $\alpha_{\max K}$, $\alpha_{\max}$), and the calculated matrix $\mathcal{A}^{\mu\lambda}(L)$;
- in the case of the orthonormality test of the BM basis: input data, only message/verdict if the BM basis is orthonormalized or not;
- in the case of Q_η calculation: input data, dimension of the matrix, specification of SU(3) BM states (i, L, M), and the calculated matrix of this operator;
- in the case of the Q matrices test: input data, only verdict if the calculated matrix of the scalar product of the Q operators is equal to the corresponding matrix which values are given by known Casimir operators eigenvalues or the matrix itself as well as the verdict;
- in the case of H_{3QL}, H_{4QQ}, $H_{SU(3)} + \gamma_{3QL}H_{3QL}$, $H_{SU(3)} + \gamma_{4QQ}H_{4QQ}$, and $H_{SU(3)} + \gamma_{3QL}H_{3QL} + \gamma_{4QQ}H_{4QQ}$ calculations: input data, dimension of the matrix, specification of SU(3) BM states (i, L, M), the calculated matrix of this operator, and the eigenvalues of this matrix.
- in the case of L boundaries calculation: input data, $L^{\text{one}}_{\min}$, $L^{\text{all}}_{\min}$, $L^{\text{all}}_{\max}$, and $L^{\text{one}}_{\max}$;
- in the case of α boundaries calculation: input data, and interval of allowed values;
- in the case of L_η calculation: input data, dimension of the matrix, specification of SU(3) BM states (i, L, M), and the calculated matrix of this operator;
- in the case of timing of the chosen procedures: input data, time of calculation of the every procedure and the total time of calculation;
- in the case of q calculation: input data, dimension of the matrix, and the calculated matrix of this operator;

Table 1. Input to computer code SU3BMB

line 1	# outputMode prec outPrec
line 2	2 200 5
line 3	# outputUn outputAn testON outputQ testQQ0 outputH3QL outputH4QQ outputHSU3H3QL outputHSU3H4QQ outputHSU3H3QLH4QQ outputLboundaries outputAboundaries outputL outputTimeTest userFunction qsmall
line 4	0 0 0 0 0 0 0 1 1 1 0 0 0 0 0 0
line 5	# outputUn: lambda mu L
line 6	11 10 6
line 7	# outputAn: lambda mu L
line 8	11 10 6
line 9	# testON: lambda mu L
line 10	11 10 6
line 11	# outputQ: lambda mu eta
line 12	2 1 1
line 13	# testQQ0: lambda mu
line 14	2 1
line 15	# outputH3QL: lambda mu
line 16	2 1
line 17	# outputH4QQ: lambda mu
line 18	2 0

3. Input file

Below we present the input file for the program SU3BMB used to obtain entries in Table 3.

A description of the format for the input parameters is given in Tables 1 and 2. All parameters are entered in fixed order separated by a single space.

Input data to the program `SU3BMB` can be provided using a file of the following form:

(i) Names the parameters which values we introduce in the next row.

(ii) Contains: the first number specifies output mode (0 to the notebook, 1 to the file, 2 to the notebook and the file), the second number specifies precision of numerical calculations (the number of significant digits in the numerical calculations), and the third number specifies output precision (the number of output digits of calculation results);

(iii) Names the parameters which one needs to introduce in the next row;

(iv) Contains a list of switches: the first is 1 - calculation of the normalized BM overlap

Table 2. Input to computer code SU3BMB (continuation)

`line 19`	`# outputHSU3H3QL: lambda mu kappa beta gamma3QL`
`line 20`	`2 1 1.5 1.5 0.1`
`line 21`	`# outputHSU3H4QQ: lambda mu kappa beta gamma4QQ`
`line 22`	`2 0 1.5 1.5 0.1`
`line 23`	`# outputHSU3H3QLH4QQ: lambda mu kappa beta gamma3QL gamma4QQ`
`line 24`	`2 0 1.5 1.5 0.1 0.1`
`line 25`	`# outputLboundaries: lambda mu`
`line 26`	`17 7`
`line 27`	`# outputAboundaries: lambda mu L`
`line 28`	`120 60 31`
`line 29`	`# outputL: lambda mu eta =(-1,0,1)`
`line 30`	`2 1 1`
`line 31`	`# outputTimeTest: lambda mu L`
`line 32`	`11 10 6`
`line 33`	`# userFunction: lambda mu`
`line 34`	`1 1`
`line 35`	`# qsmall: lambda mu L k`
`line 36`	`11 10 6 2`

integrals, the second is 1 - calculation of the $SU(3)$ BM basis orthonormalization coefficients, the third is 1 - message/verdict about the BM basis orthonormalization test, the third is 2 - output of the matrix of the product of BM basis vectors as well as the verdict, the fourth is 1 - calculation of the Q_η matrix, the fifth is 1 - verdict if the calculated matrix of the scalar product of the Q operators is equal to the corresponding matrix which values are given by the known Casimir operators eigenvalues or the matrix itself as well as the verdict, the sixth is 1 - calculation and diagonalization of the H_{3QL} matrix, the seventh is 1 - calculation and diagonalization of the H_{4QQ} matrix, the eighth is 1 - calculation and diagonalization of the $H_{SU(3)} + \gamma_{3QL} H_{3QL}$ matrix, the ninth is 1 - calculation and diagonalization of the $H_{SU(3)} + \gamma_{4QQ} H_{4QQ}$ matrix, the tenth is 1 - calculation and diagonalization of the $H_{SU(3)} + \gamma_{3QL} H_{3QL} + \gamma_{4QQ} H_{4QQ}$ matrix (the 0 turns off and greater than 0 turns on the specified case of calculations).

(v) Names the variables which values we introduce in the next row.

(vi) Contains the values of (λ, μ, L) for which one calculates the normalized BM overlap integrals.

(vii) Names the variables which values we introduce in the next row;

(viii) Contains the values of (λ, μ, L) for which one calculates the $SU(3)$ BM basis orthonormalization coefficients.

(ix) Names the variables which values we introduce in the next row.
(x) Contains the values of (λ, μ, L) for BM basis orthonormalization test.
(xi) Names the variables which values we introduce in the next row.
(xii) Contains the values of $(\lambda, \mu, \eta = -2, -1, 0, +1, +2)$ for calculation of the Q_η matrix.
(xiii) Names the variables which values we introduce in the next row.
(xiv) Contains the values of (λ, μ) for the Q matrices test.
(xv) Names the variables which values we introduce in the next row.
(xvi) Contains the values of (λ, μ) for calculation and diagonalization of the H_{3QL} matrix.
(xvii) Names the variables which values we introduce in the next row.
(xviii) Contains the values of (λ, μ) for calculation and diagonalization of the H_{4QQ} matrix.
(xix) Names the variables which values we introduce in the next row.
(xx) Contains the values of $(\lambda, \mu, \kappa, \beta, \gamma_{3QL})$ for calculation and diagonalization of the $H_{SU(3)} + \gamma_{3QL} H_{3QL}$ matrix.
(xxi) Names the variables which values we introduce in the next row.
(xxii) Contains the values of $(\lambda, \mu, \kappa, \beta, \gamma_{4QQ})$ for calculation and diagonalization of the $H_{SU(3)} + \gamma_{4QQ} H_{4QQ}$ matrix.
(xxiii) Names the variables which values we introduce in the next row.
(xxiv) Contains the values of $(\lambda, \mu, \kappa, \beta, \gamma_{3QL}, \gamma_{4QQ})$ for calculation and diagonalization of the $H_{SU(3)} + \gamma_{3QL} H_{3QL} + \gamma_{4QQ} H_{4QQ}$ matrix.
(xxv) Names the variables which values we introduce in the next row.
(xxvi) Contains the values (λ, μ) for which the function `Lboundaries` calculates an interval of the allowed values of the angular momentum L.
(xxvii) Contains names the variables which values we introduce in the next row.
(xxviii) Contains the values (λ, μ) and L for which the function `Aboundaries` outputs an interval of possible values of the index α.
(xxix) Names the variables which values we introduce in the next row.
(xxx) Contains the values (λ, μ) and $\eta = -1, 0, 1$ for which the function `Lmatrix` calculates the matrix of the angular momentum operator L_η.
(xxxi) Names the variables which values we introduce in the next row.
(xxxii) Contains the default values (λ, μ) and L for which the CPU time test is calculated if these values are not specified for every chosen individual case.
(xxxiii) Names the variables which values we introduce in the next row.
(xxxiv) Contains the values (λ, μ) for which the `userFunction` is used.
(xxxv) Names the variables which values we introduce in the next row.
(xxxvi) Contains the values (λ, μ, L, k) for calculation of corresponding q–coefficients matrix.

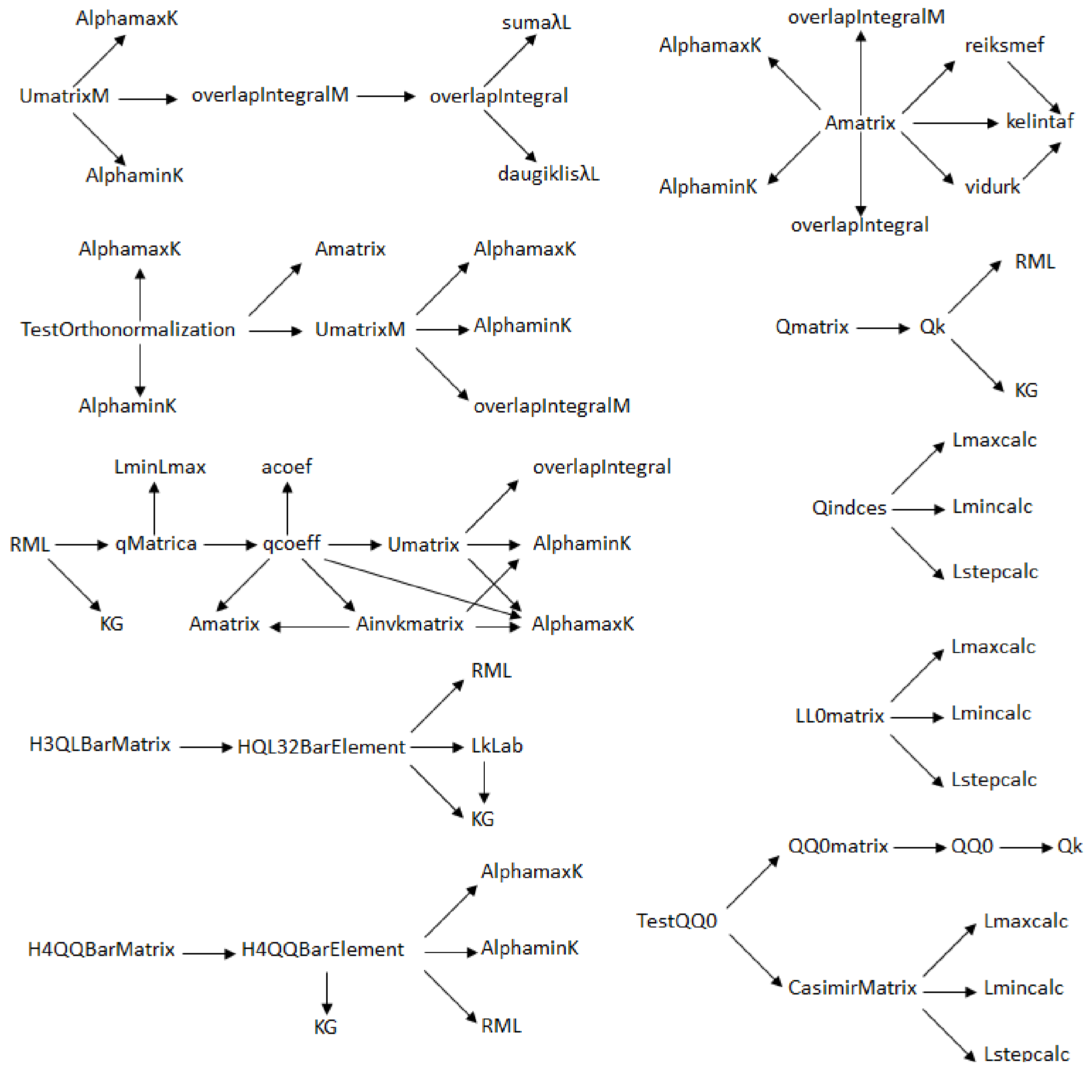

Figure 1. The block scheme of the program `SU3BMB`.

The corresponding input and output files are specified in readme.txt file and presented in the forthcoming archive file.

The program `SU3BMB` contains the following functions:

- `H4QQBarMatrix` calculates the matrix of the H_{4QQ} operator for the given values of λ and μ;
- `H4QQBarElement` calculates the matrix elements of the H_{4QQ} operator;
- `H3QLBarMatrix` calculates the matrix of the H_{3QL} operator for the given values of λ and μ;
- `HQL32BarElement` calculates the matrix element of the H_{3QL} operator;
- `TestQQ0` tests if the calculated matrix of the scalar product of the Q operators is equal to the corresponding matrix which values are given by known eigenvalues of the Casimir operators;

Table 3. The examples of spectrum of Hamiltonians: $E_{C_2(SU(3))}$ of $H_{SU(3)}$ (9), E_{3QL} of $H_{SU(3)} + \gamma_{3QL} H_{3QL}$ (14), E_{4QQ} of $H_{SU(3)} + \gamma_{4QQ} H_{4QQ}$ (16), and E of $H_{SU(3)} + \gamma_{3QL} H_{3QL} + \gamma_{4QQ} H_{4QQ}$ for $(\kappa = 1.5, \beta = 1.5, \gamma_{3QL} = 0.1, \gamma_{4QQ} = 0.1)$. The pair (λ, μ) labels the irreps of the group SU(3) of the dimension $D_{\lambda\mu}$ from Eq. (13) and the label ν denote degeneration of eigenvalues due to the intrinsic tetrahedral/octahedral symmetry.

(λ, μ)	$D_{\lambda\mu}$	$E_{C_2(SU(3))}(\nu)$	$E_{3QL}(\nu)$	$E_{4QQ}(\nu)$	$E(\nu)$	CPU time (s)
$(0,0)$	1	0.0000 (1)	0.0000 (1)	0.0000 (1)	0.0000 (1)	0.05
$(1,0)$	3	-12.000 (3)	-12.000 (3)	-12.000 (3)	-12.000 (3)	0.8
$(2,0)$	6	-60.000 (1)	-60.000 (1)	-60.000 (1)	-60.000 (1)	5.
		-24.000 (5)	-24.490 (1)	-24.960 (3)	-24.960 (3)	
			-24.000 (3)	-22.560 (2)	-23.050 (1)	
			-23.510 (1)		-22.070 (1)	
$(2,1)$	15	-84.000 (3)	-84.003 (3)	-84.062 (3)	-84.065 (3)	90.
		-60.000 (5)	-60.490 (1)	-60.480 (2)	-60.970 (1)	
		-24.000 (7)	-60.009 (3)	-59.822 (3)	-59.990 (1)	
			-59.510 (1)	-24.418 (3)	-59.831 (3)	
			-24.213 (3)	-23.698 (3)	-24.486 (3)	
			-24.000 (1)	-23.040 (1)	-23.618 (3)	
			-23.775 (3)		-23.040 (1)	

- `QQ0matrix` calculates the matrix of the scalar product of the quadrupole operators for the given values of λ and μ;
- `QQ0` calculates the matrix element of the scalar product of the quadrupole operators;
- `Qmatrix` calculates the matrix of the quadrupole operator for the given values of λ, μ, and η;
- `Qk` calculates the matrix element of the quadrupole operator;
- `RML` calculates the reduced matrix element of the quadrupole operator;
- `qMatrica` is the auxiliary function that precalculates all coefficients $q_{ijk}^{(\lambda\mu)}(L)$ defined in Eq. (54) for the given values of λ and μ;
- `qcoeff` is the auxiliary function that calculates the coefficients $q_{ijk}^{(\lambda\mu)}(L)$ defined in Eq. (54) for given values of indices;
- `acoef` is the auxiliary function of the function qcoeff that calculates the coefficient $a_s^{(k)}$ defined in Eq. (55);
- `Qindces` outputs the indices of the matrix of the quadrupole operator for the given values of λ and μ;
- `CasimirMatrix` calculates the matrix of the scalar product of the quadrupole operators for the given values of λ and μ using eigenvalues of the $SU(3)$ Casimir operator;
- `LL0matrix` calculates the matrix of the scalar product of angular momentum operators for the given values of λ and μ;

- `LkLab` calculates the matrix element of the angular momentum operator in the laboratory system;
- `KG` calculates the value of the Clebsch–Gordan coefficients and returns zero if any one of the non-vanishing-conditions is not satisfied;
- `TestOrthonormalization` tests if the BM basis is orthonormalized for the given values of λ, μ and L;
- `Amatrix` returns the matrix of the BM basis orthonormalization coefficients $\mathcal{A}^{\mu\lambda}(L)$ for the given values of λ, μ and L (see (46) and (47));
- `Ainvkmatrix` returns the inverse matrix of the matrix $\mathcal{A}^{\mu\lambda}(L)$ for the given values of λ, μ and L;
- `vidurk` adds the next normalization integral, calculated for the given value of index α of not orthonormal BM state, to the list of normalization integrals of the orthogonalized BM states;
- `reiksmef` returns the value of the quantity $f^{(n)}_{\alpha,\alpha'}$ for given values of indices of not orthonormal BM states;
- `kelintaf` returns the sequence number in the linear storage of the quantity $f^{(n)}_{\alpha,\alpha'}$ for given values of indices of not orthonormal BM states;
- `UmatrixM` returns the matrix $\mathcal{U}^{\mu\lambda}(L)$ which entries are the normalized overlap integrals calculated for given values of λ, μ and L, see (24), (46) and (48);
- `Umatrix` returns the matrix $\hat{\mathcal{U}}^{\mu\lambda}(L)$ which entries are the not normalized overlap integrals calculated for given values of λ, μ and L, see (34), (46) and (48);
- `overlapIntegralM` returns the value of the normalized overlap integral $\langle u_\alpha | u_{\alpha'} \rangle$ of the BM states, it is the appropriate matrix element of the matrix, see (24);
- `overlapIntegral` returns the value of the not normalized overlap integral $\langle \hat{u}_\alpha | \hat{u}_{\alpha'} \rangle$ of the BM states which is calculated for given values of indices of not orthonormal BM states, see (34);
- `suma`λ`L` is an internal function of the function `overlapIntegral`, see (34);
- `daugiklis`λ`L` is an internal function of the function `overlapIntegral`, see (34);
- `LminLmax` returns the minimal and maximal values of the angular momentum quantum number of the existing BM state for the given values of λ and μ;
- `Lmaxcalc` returns the maximal value of the angular momentum quantum number of the existing BM state for the given values of λ, μ and α;
- `Lmincalc` returns the minimal value of the angular momentum quantum number of the existing BM state for the given values of λ, μ and α;
- `Lstepcalc` returns the step value of the angular momentum quantum numbers of the existing BM state for the given values of λ, μ and α;
- `AlphamaxK` returns the maximal sequence number of the existing BM state for the given values of λ, μ and L in the list of the maximal possible number of BM states for the given value of μ;

- `AlphaminK` returns the minimal sequence number of the existing BM state for the given values of λ, μ and L in the list of the maximal possible number of BM states for the given value of μ;
- `Lboundaries` is the auxiliary function which outputs the intervals of the possible values of the angular momentum L for a given irreducible representation labelled by λ and μ of the group SU(3).
- `Aboundaries` is the auxiliary function which outputs intervals of possible values of the index α for the given values of λ, μ and L.
- `Lmatrix` calculates the matrix of the orbital angular for given values of λ, μ and η.
- `userCalculations` calculates the user defined operator for given values of λ and μ.

The dependency of the functions of the program `SU3BMB`, i.e. its block scheme is presented in Figure (1).

Supporting Information Available

The following files available free of charge.

• supp.pdf Supplemental material contains description of the code `SU3BMB`.

• su3bmb.zip Supplemental material contains the code `SU3BMB`.nb, readme.txt and test examples.

This material is available free of charge via the Internet at
http://theor.jinr.ru/∼vinitsky/su3bmb.html

4. References

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