Symmetrized Vibrational-Rotational Basis for Collective Nuclear Models

A.A. Gusev, S.I. Vinitsky
Joint Institute for Nuclear Research, Dubna, Russia

A. Gózdź, A. Dobrowolski, A. Szulerecka
Institute of Physics, Department of Mathematical Physics, University of Maria Curie-Skłodowska, Lublin, Poland

A. Pędrak
National Centre for Nuclear Research, Warsaw, Poland
E-mail: vinitsky@theor.jinr.ru

Abstract. The generalized projection operators for the intrinsic group acting in the space \( L_2(SO(3)) \) and in the space spanned by the eigenfunctions of a multidimensional harmonic oscillator are constructed. New symbolic-numerical algorithm implemented in computer algebra system for generating irreducible representations of the point symmetry groups in the rotor + shape vibrational space of a nuclear collective model in the intrinsic frame is presented. The efficiency of the algorithm is investigated by calculating the bases of irreducible representations subgroup \( D_{4y} \) of octahedral group in the intrinsic frame of a quadrupole-octupole collective nuclear model. The discrete variable representation algorithm proposed for solving eigenvalue problem, describing vibrational-rotational motion of collective nuclear model in intrinsic frame.

1. Introduction
The most efficient way of construction of collective models in nuclear and molecular physics is using of the so called intrinsic frame [1] The most useful is the rotating intrinsic frame. However, to construct vibrational-rotational basis of the collective models in an intrinsic frame one needs to notice some important features of this notion [2] and the technique of generalized projection operators [3].

In this paper we propose a simple and effective algorithm for numerical construction of such basis for the vibrational + rotational collective motion based on algorithms elaborated in refs. [4, 5]. We consider application of the algorithm on the example of construction of the rotation-vibrational quadrupole-octupole basis of the irreducible representation (irr.) \( A1 = \Gamma_1 \) of the point group \( D_4 \) group (in classification of Ref. [6]) in the intrinsic frame considered in the zero and one-phonon approximation, as in ref.[7]. Structure of the paper is following. In Section 2, a setting of intrinsic frame and symmetrization groups are presented In Section 3, a setting of quadrupole-octupole harmonic oscillator in rotating frame is formulated. In Section 4, parametric vibration basis functions of irr. \( A1 = \Gamma_1 \) of intrinsic dihedral \( D_4 \) point group are derived. In Section 5, an
algorithm for construction of orthonormal vibrational-rotational basis is presented. In Section 6, solving an eigenvalue problem in the intrinsic frame using discrete variable representation (DVR) is described.

2. Intrinsic frame and symmetrization group

The classical rotation is well understood phenomenon in which the orientation of a body is changing with time. Contrary, the quantum rotation allows to determine only the probability of a given orientation and there is no time variable in the wave function.

The notion of the quantum rotational motion allows to define the rotating intrinsic frame, for the collective variables \( \{ \alpha^{(\text{lab})} \} \) defined by the equation of surface [1]:

\[
R(\alpha^{(\text{lab})}; \theta, \phi) = R_0 \left( 1 + \sum_{\lambda \mu} \alpha^{(\text{lab})}_{\lambda \mu} \star Y_{\lambda \mu}(\theta, \phi) \right). \tag{1}
\]

The corresponding collective variables in the intrinsic frame we denote by \( \{ \alpha_{\lambda} \} \). They can be obtained by the quantum rotation of the laboratory collective variables \( \{ \alpha^{(\text{lab})} \} \) with the rotation operator \( \hat{R}(\Omega) \)

\[
\alpha^{(\text{lab})}_{\lambda} = \hat{R}(\Omega^{-1}) \alpha_{\lambda} \tag{2}
\]

assuming, in addition, that the rotation group \( \text{SO}(3) \equiv \hat{R}(\Omega) \) parameters, represented by the Euler angles \( \Omega = (\Omega_1, \Omega_2, \Omega_3) \), are considered as a part of intrinsic variables. The intrinsic variables \( \alpha_{\lambda} \) are invariant in respect to the laboratory rotations \( \hat{R}(\Omega) \). It is important to notice that inclusion of the Euler angles into the set of intrinsic variables makes this set of variables redundant, 3 variable more than needed. It implies that, the definition of the intrinsic frame requires three additional conditions which leads the same number of variables in both frames

\[
F_k(\alpha, \Omega) = 0, \quad \text{where } k = 1, 2, 3. \tag{3}
\]

In this way one can obtain a new description of a physical system, e.g. a nucleus, in which the rotational motion can be directly described by the Euler angles, i.e. we start to work in the rotating frame.

An interesting question is how to investigate symmetries of a nucleus in the intrinsic frame. It is clear, that the transformations furnishing an intrinsic symmetry group have to be defined in the intrinsic frame.

A convenient definition of intrinsic groups was formulated in [2] in the following form: for each element \( g \) of the group \( G \), one can define a corresponding operator \( \hat{g} \) in the group linear space \( L_G \) as:

\[
\hat{g}|S\rangle = |Sg\rangle, \quad \text{for all } |S\rangle \in L_G, \tag{4}
\]

where all elements inside the ket vectors \( S = \sum_{g \in G} c_g g \), here \( c_g \) are the complex numbers, form a group algebra of the group \( G \). In this definition the notion of the group linear space \( L_G \) is used. This space is defined as the linear space spanned by all possible formal linear combinations of the elements of the group \( G \)

\[
L_G = \left\{ |S\rangle : |S\rangle = \sum_{g \in G} c_g g, \text{ where } c_g \in \mathbb{C} \right\}. \tag{5}
\]

It looks like the group algebra mentioned above, but, it is important that the elements of \( L_G \) have to be considered only as vectors, not as the elements of the group algebra. The group formed by the collection of the operators \( \hat{g} \) is called the intrinsic group \( \mathcal{G} \) related to the group \( G \).
One of the most important property of the intrinsic group $\mathcal{G}$ is that this group commutes with its partner group $G$ (this can be called a laboratory group, because it acts in the laboratory frame):

$$[G, \mathcal{G}] = 0. \quad (6)$$

The groups $G$ and $\mathcal{G}$ are anti-isomorphic. The required anti-isomorphism between the partner groups $G$ and $\mathcal{G}$ is given by

$$\phi_G : \mathcal{G} \to G, \text{ where } \phi_G(\bar{g}) = g \text{ and } \phi_G(\bar{g}\bar{g}') = \phi_G(g')\phi_G(\bar{g}). \quad (7)$$

This property suggests that the partner groups $G$ and $\mathcal{G}$ have a lot of common properties as e.g. similar structure of representations, decompositions of the Kronecker products, the Clebsch-Gordan coefficients and many others.

As an example let us consider a relation among representations of both groups. Because the partner groups commute one can find common basis $|\Gamma mk\rangle$ for representations of the group $G$ and the group $\mathcal{G}$. The representations are defined as:

$$g|\Gamma mk\rangle = \sum_{m'} \Delta^{(\Gamma)}_{m'm}(g)|\Gamma m'k\rangle, \quad \bar{g}|\Gamma mk\rangle = \sum_{k'} \bar{\Delta}^{(\Gamma)}_{k'k}(\bar{g})|\Gamma mk'\rangle. \quad (8)$$

To compare both representation one can use as the basis in the form of the generalized projection operators (elements of the group linear space $L_G$) $[3]$

$$|\Gamma mk\rangle = \frac{\dim[\Gamma]}{\text{card}(G)} \sum_{g \in G} \Delta^{(\Gamma)}_{mk}(g)\star g, \quad (9)$$

where $\dim[\Gamma]$ denotes the dimension of the representation $\Gamma$ and $\text{card}(G)$ is the number of elements in the group $G$. This allows to calculate (8)

$$\bar{g}|\Gamma mk\rangle = \frac{\dim[\Gamma]}{\text{card}(G)} \sum_{g' \in G} \Delta^{(\Gamma)}_{mk}(g')\star g' = \frac{\dim[\Gamma]}{\text{card}(G)} \sum_{g' \in G} \Delta^{(\Gamma)}_{mk}(g'g^{-1})\star g'$$

$$= \frac{\dim[\Gamma]}{\text{card}(G)} \sum_{g' \in G} \sum_{k'} \Delta^{(\Gamma)}_{mk'}(g')\star \Delta^{(\Gamma)}_{k'k}(g')\star g' = \sum_{k'} \Delta^{(\Gamma)}_{kk'}(g)|\Gamma mk'\rangle, \quad (10)$$

where $\Delta^{(\Gamma)}_{mm'}(g)$ are matrix elements of the representation $\Gamma$ of the group $G$. Comparing both expression one can see that the matrices of both representations are related. The representations of the intrinsic group are transposed representations of the partner group

$$\bar{\Delta}^{(\Gamma)}_{mk}(g) = \Delta^{(\Gamma)}_{km}(g). \quad (11)$$

A bit different are definitions of irreducible tensors in respect to the laboratory group $G$ and the intrinsic group $\mathcal{G}$. By definition the irreducible tensors in respect to the laboratory group $G$ transform as

$$\bar{g}T^{(\Gamma)}_m\bar{g}^{-1} = \sum_i \Delta^{(\Gamma)}_{im}(g)\bar{T}^{(\Gamma)}_i. \quad (12)$$

The tensors in respect to the intrinsic group $\mathcal{G}$, due to the anti-isomorphism between both groups, have to be defined in the following way

$$\bar{g}\bar{T}^{(\Gamma)}_{k}\bar{g}^{-1} = \sum_i \Delta^{(\Gamma)}_{ik}(g^{-1})\bar{T}^{(\Gamma)}_i. \quad (13)$$

As an example, let us consider the action of the intrinsic group in the collective space consisted of the square integrable functions of the deformation parameters and the Euler angles. The intrinsic
rotation operators \( \hat{R}(\bar{g}_1, \bar{g}_2) \in \text{SO}(3)_\alpha \times \text{SO}(3)_\Omega \) (the indices \( \alpha \) and \( \Omega \) show the variables which are affected by the corresponding group) are defined as follows

\[
\hat{R}(\bar{g}_1, \bar{g}_2) f(\alpha, \Omega) = f(\{\hat{g}_1\alpha\}, \Omega \phi_G(\bar{g}_2)^{-1}),
\]

where \( \bar{g}_1 \in \text{SO}(3)_\alpha \) and \( \bar{g}_2 \in \text{SO}(3)_\Omega \). The action of the group \( \text{SO}(3)_\alpha \) onto the deformation variables is a bit non-standard and is given by the following equation

\[
\hat{g}_1 \alpha = \sum_{\mu'} D^\lambda_{\mu'\mu}(\phi_G(\bar{g}_1)^{-1}) \alpha \mu',
\]

where \( D^\lambda_{\mu'\mu} \) are Wigner functions [8]. The intrinsic group \( \text{SO}(3) \) corresponding to the laboratory rotation group \( \text{SO}(3) \) defined in the laboratory frame consists of all rotations \( \hat{R}(\bar{g}, \bar{g}) \) for which the deformation parameters and the Euler angles are rotated with the same angles. The required anti-isomorphism between the partner groups \( \text{SO}(3) \) and \( \text{SO}(3) \) is given by (7). It is important to notice that, in general, not all transformations \( (\bar{g}_1, \bar{g}_2) \in \text{SO}(3)_\alpha \times \text{SO}(3)_\Omega \)

\[
(\bar{g}_1, \bar{g}_2): \ (\alpha, \Omega) \rightarrow (\alpha', \Omega')
\]

are allowed in the intrinsic frame. They are allowed if they do not break the conditions which define the intrinsic frame (3)

\[
(\hat{g}_1, \hat{g}_2) F_k(\alpha, \Omega) = F_k(\hat{g}_1 \alpha, \Omega \hat{g}_2^{-1}) = 0, \quad \text{where} \quad k = 1, 2, 3.
\]

For example, in the case of the quadrupole collective variables \( \alpha_2 \) with the standard Bohr condition which define the intrinsic frame: \( \alpha_{2\pm 1} = 0 \) and \( \alpha_{22} = \alpha_{2-2} \), the allowed intrinsic rotations \( \hat{R}(\bar{g}_1, \bar{g}_2) \in \text{SO}(3)_\alpha \times \text{SO}(3)_\Omega \) have to fulfill the following conditions

\[
\hat{R}(\bar{g}_1, e_G) \alpha_{2\pm 1} = 0 \quad \text{and} \quad \hat{R}(\bar{g}_1, e_G) \alpha_{22} = \hat{R}(\bar{g}_1, e_G) \alpha_{2-2},
\]

where the second argument represents the unit element of the group \( \text{SO}(3)_\Omega \). The Bohr conditions allow for the arbitrary rotations \( \bar{g}_2 \in \text{SO}(3)_\Omega \).

Using the conditions (18) the allowed rotations of the deformation parameters \( \alpha \) have to satisfy the following equations

\[
D^2_{0,\pm 1}(\bar{g}_1^{-1}) = 0, \quad D^2_{2\pm 1}(\bar{g}_1^{-1}) + D^2_{2\pm 1}(\bar{g}_1^{-1}) = 0, \quad D^2_{02}(\bar{g}_1^{-1}) = 0, \quad D^2_{0,-2}(\bar{g}_1^{-1}) = 0,
\]

\[
D^2_{2,-2}(\bar{g}_1^{-1}) + D^2_{2,-2}(\bar{g}_1^{-1}) = D^2_{-22}(\bar{g}_1^{-1}) + D^2_{22}(\bar{g}_1^{-1})).
\]

In this case, the octahedral point group \( \Omega_\alpha \subset \text{SO}(3)_\alpha \) acting only on the variables \( \alpha \) provide the solution of the set of equations (19).

In practice, the transformation from the laboratory frame to the intrinsic frame is not a one-to-one function. In principle, there are two possibilities to achieve uniqueness of transformation from the laboratory to the intrinsic frame:

- first, one can define the appropriate region of the intrinsic collective variables in which the transformation from the laboratory to intrinsic frame is a one-to-one function,
- second, one can allow for the whole range of collective variables but then one needs to fulfil some special conditions for physical states.

However, narrowing of the domain of transformations is not a physical solution. For example, narrowing the ranges of Euler angles \( \Omega \) destroys the angular momentum operators – the operators
become ill defined. To keep the appropriate physical properties in space of state one have to accept that the second possibility.

For further purpose it is useful to define the special group of intrinsic transformations \( \tilde{h} \in \mathcal{G}_S \):

\[
(\alpha, \Omega) \rightarrow \tilde{h}(\alpha', \Omega'),
\]

(20)

where \( \alpha = \{\alpha_{\lambda \mu}\} \) and which leave invariant the laboratory variables as function of the intrinsic variables:

\[
\alpha^{(\text{lab})}(\alpha', \Omega') = \alpha^{(\text{lab})}(\alpha, \Omega), \quad F_k(\alpha', \Omega') = F_k(\alpha, \Omega) = 0, \text{ for } k = 1, 2, 3,
\]

(21)

where \( \alpha^{(\text{lab})}(\alpha, \Omega) = R(\Omega^{-1})\alpha \), see (2). The group \( \mathcal{G}_S \) we call the symmetrization group. The symmetrization group decomposes the collective manifold into orbits of physically equivalent points.

Let the function \( \Psi^{(\text{lab})} \) denotes a state vector of a nucleus in the laboratory frame. The corresponding state vector in the intrinsic frame has to fulfil the obvious equation

\[
\Psi(\alpha, \Omega) = \Psi^{(\text{lab})}(\alpha^{(\text{lab})})
\]

(22)

which represents the fact that the wave function of the physical system written in the laboratory frame has to be well and uniquely defined function. However, after transformation of Eq. (22) with the elements of the symmetrization group we potentially change \( \Psi \) and do not change the laboratory state vector:

\[
\Psi(\alpha', \Omega') = \Psi^{(\text{lab})}(\alpha^{(\text{lab})}).
\]

(23)

To omit the obvious contradiction, we have to define the uniqueness condition for the states in the intrinsic frame

\[
\Psi(\alpha', \Omega') = \Psi(\alpha, \Omega).
\]

(24)

This condition we will call the symmetrization condition. It can be expressed as invariance of the intrinsic state vectors in respect to all transformations \( \tilde{h} \in \mathcal{G}_S \),

\[
\tilde{h}\Psi(\alpha, \Omega) = \Psi(\alpha, \Omega),
\]

(25)

where the group \( \mathcal{G}_S \) is the symmetrization group for a given intrinsic frame.

In quantum mechanics the collective states in the laboratory/intrinsic frame belong the spaces of square integrable functions. In the laboratory frame the quantum state space is usually represented by the whole space \( L^2(\alpha^{(\text{lab})}) \), however, the quantum state space in the intrinsic frame has to be restricted to the subspace of functions satisfying the symmetrization condition (25): \( \mathcal{K}_S \subset L^2(\{\alpha_{\lambda \mu}\}) \). This implies that in calculations we cannot use any standard basis, but we have to construct the basis dedicated to the subspace \( \mathcal{K}_S \).

3. Shape vibrational basis in the intrinsic frame

To define the rotations of intrinsic spherical tensors with respect to intrinsic rotation group, we rewrite the expansion (1) in terms of spherical harmonics \( Y_{lm}(\theta', \phi') \) in the intrinsic frame:

\[
R(\theta, \phi) = R(\theta', \phi') = R_0 \left( 1 + \sum_l a_{l0} Y_{l0}(\theta', \phi') + \sum_{lm} \left( a_{lm} Y^{(+)\text{lab}}_{lm}(\theta', \phi') + b_{lm} Y^{(-)\text{lab}}_{lm}(\theta', \phi') \right) \right),
\]

\[
Y^{(\pm)\text{lab}}_{lm}(\theta', \phi') = i^{(l+1)/2} \left( Y_{lm}(\theta', \phi') \pm (-1)^m Y_{-l-m}(\theta', \phi') \right) / \sqrt{2}.
\]

(26)
Note, that these spherical harmonics are tensors in respect to intrinsic rotations. We rewrite the transformation \( \bar{a}_{\lambda \mu} = \bar{\alpha}_{\lambda \mu}, \) \( \bar{g} \in \mathbb{G} \), between two intrinsic coordinate frames

\[
\bar{a}_{\lambda \mu} = \frac{\lambda}{\mu'} = -\lambda \sum_{\mu'=-\lambda}^{\lambda} D_{\mu \mu'}^{\lambda}(g)^{* (\bar{\alpha}_{\lambda \mu} \cdot Y_{\lambda \mu}(\theta', \varphi')).
\] (27)

We use the relations between the complex-valued coefficients \( \bar{a}_{\lambda \mu}, \lambda_{\mu} \) and real-valued ones \( \bar{a}_{\lambda \mu}, \lambda_{\mu} \)

\[
\bar{a}_{\lambda 0} = \bar{a}_{\lambda 0}, \quad \bar{a}_{\lambda \mu} = (\bar{a}_{\lambda \mu} - i\bar{b}_{\lambda \mu})/\sqrt{2}, \quad \bar{a}_{\lambda \mu} = (-1)^{\mu}(\bar{a}_{\lambda \mu} - i\bar{b}_{\lambda \mu})/\sqrt{2}.
\] (28)

The transformation between both intrinsic frames \( \bar{q} = \bar{M}(g)q \) is represented by a block diagonal matrix \( \lambda = 2, 3, ..., \lambda_{\text{max}} \), with block matrices of the dimension \((2\lambda + 1) \times (2\lambda + 1)\):

\[
\bar{q} = \bar{M}(g)q = \begin{pmatrix} q_{1}(g) \\ q_{3}(g) \end{pmatrix}, \quad \bar{q} = \begin{pmatrix} q_{2}(g) \\ q_{3}(g) \end{pmatrix}, \quad \bar{M}(g) = \begin{pmatrix} \bar{M}_{1}(g) & 0 & \cdots \\ 0 & \bar{M}_{3}(g) & \cdots \\ \cdots & \cdots & \cdots \end{pmatrix}
\] (29)

The transformation of pairs of components \( \bar{q}_{\lambda} = (\bar{a}_{\lambda \lambda}, \bar{b}_{\lambda \lambda})^{T} \) and \( \bar{q}_{\lambda} = (\bar{a}_{\lambda \lambda}, \bar{b}_{\lambda \lambda})^{T} \) are connected by the transformations \( \bar{q}_{\lambda} = \bar{M}_{\lambda}(g)\bar{q}_{\lambda} \), with the blocks matrices \( \bar{M}_{\lambda} \equiv \bar{M}_{\lambda}(g) \) of the following form

\[
\bar{M}_{\lambda} = \begin{pmatrix} C_{1}^{\lambda} + C_{2}^{\lambda} & C_{1}^{\lambda} - C_{2}^{\lambda} & \sqrt{2}C_{1}^{\lambda} & S_{22}^{\lambda} + S_{21}^{\lambda} & S_{22}^{\lambda} - S_{21}^{\lambda} & \cdots \\ 0 & 0 & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix}
\] (30)

where \( C_{\mu \mu'}^{\lambda} = \cos(\mu \alpha + \mu' \gamma) d_{\mu \mu'}^{\lambda}(\beta), \) \( S_{\mu \mu'}^{\lambda} = \sin(\mu \alpha + \mu' \gamma) d_{\mu \mu'}^{\lambda}(\beta), \) and \( d_{\mu \mu'}^{\lambda}(\beta) \) are "reduced" Wigner functions [8]. The inverse transformation is implemented using the transposed matrix \( \bar{M}^{-1} = \bar{M}^{T} \) because \( \bar{M} \) is the orthogonal matrix, i.e. \( \bar{M} \bar{M}^{T} = \bar{M}^{T} \bar{M} = \mathbf{I} \).

The quadrupole-octupole vibrational Hamiltonian \( \hat{H}_{v} \), having the form of that of a harmonic oscillator, can be written in the intrinsic frame as:

\[
\hat{H}_{v}(0) = -\frac{\hbar^{2}}{2B_{2}} \left( \frac{\partial^{2}}{\partial(a_{20})^{2}} + \frac{\partial^{2}}{\partial(a_{22})^{2}} \right) + \frac{B_{2}\omega_{2}^{2}}{2} \left( (a_{20})^{2} + (a_{22})^{2} \right)
\]

\[
+ \frac{\hbar^{2}}{2B_{3}} \left( \sum_{\mu=0}^{3} \frac{\partial^{2}}{\partial(a_{3 \mu})^{2}} + \sum_{\mu=1}^{3} \frac{\partial^{2}}{\partial(b_{3 \mu})^{2}} \right) + \frac{B_{3}\omega_{3}^{2}}{2} \left( \sum_{\mu=0}^{3} (a_{3 \mu})^{2} + \sum_{\mu=1}^{3} (b_{3 \mu})^{2} \right).
\] (31)

\( E_{v}^{N_{23}} = \hbar\omega_{2}(n_{2} + n_{2} + 1) + \hbar\omega_{3}(n_{3} + ... + n_{9} + 7/2), \quad N_{23} = N_{2} + N_{3} = n_{1} + ... + n_{9}. \)

The corresponding eigenfunctions characterized by a set of quantum numbers \( \nu = \{n_{1}, ..., n_{9}\} \) of 9D harmonic oscillator:

\[
\psi_{\nu}^{N_{23}}(q) = \psi_{n_{1}n_{2}}(q_{5}) \psi_{n_{3}n_{4}n_{5}n_{6}}(q_{5}) \psi_{n_{7}n_{8}n_{9}}(q_{5}) \delta_{N_{23} = n_{1} + ... + n_{9}}.
\] (32)
where \( \tilde{N} = (N_2, N_3, N_2) \). They have to satisfy the orthonormalization conditions
\[
\int \psi^N_{\nu}(q)\psi^{K'}_{\nu}(q)dq = \delta_{N,K'}\delta_{n_1 n'_1}...\delta_{n_0 n'_0}.
\] (33)

3.1. Generalized Projection Operators

To construct the appropriate bases in the space of vibrational functions (32) for the intrinsic point groups \( G \) we have to use the action of the generalized projection operators \( \hat{P}_ab \) corresponding to the intrinsic group:
\[
\Psi^{\hat{N}}_{\Gamma ab_{a'\nu}}(q) = \hat{P}^{\Gamma}_{ab}\psi^{\hat{N}}_{\nu}(q) = \frac{\dim(\Gamma)}{\text{card}(G)} \sum_{g \in G} \Delta^{\Gamma}(g)_{ab} \psi^{\hat{N}}_{\nu}(g) = \frac{\dim(\Gamma)}{\text{card}(G)} \sum_{g \in G} \Delta^{\Gamma}(g)_{ab} \psi^{\hat{N}}_{\nu}(\bold{M}(g)q) = \frac{\dim(\Gamma)}{\text{card}(G)} \sum_{g \in G} \Delta^{\Gamma}(g)_{ab} \psi^{N_2}_{n_1 n_2}(\bold{M}_2(g)q_2)_{n_3} \psi^{N_3-N_2}_{N_3-N_2}(\bold{M}_3(g)q_3),
\] (34)

where the matrices of the representations \( \Delta^{\Gamma}(g)_{ab} \) obtained from the action of \( g \in G \) in the space of basis functions of the Cartesian variables are used.

In the above expressions the labels \( N_2 = n_1 + ... + n_9 \), or \( N_2 = N_2 + N_3 \), \( N_3 = n_1 + ... + n_9 \), \( n_1, n_2 = N_2 - n_1 \) run over the full range \( n_1, n_2 = 0, ..., N_2 \) and \( n_3, n_4, ..., n_9 \) run over the full range \( n_3, ..., n_9 = 0, ..., N_3 \) that provides the decomposition of the vibration space for a given \( N_2 \) and \( N_3 \) into the irreducible representations \( \Gamma \).

Note, that the matrices \( \bold{M}_2(g) \) act on the vector \( q_2 = (a_{22}, a_{21}, a_{20}, b_{21}, b_{22})^T \) under the condition \( a_{21} = b_{21} = b_{22} = 0 \), that follows from Bohr constrains (18). They transform pairs of components \( a_{22} \) and \( a_{20} \) into combination of \( \bar{a}_{22} \) and \( \bar{a}_{20} \). In this case we have
\[
\left( \begin{array}{c} \bar{a}_{22} \\ \bar{a}_{20} \end{array} \right) = \bold{M}_2(g) \left( \begin{array}{c} a_{22} \\ a_{20} \end{array} \right), \quad \bold{M}_2(C_{4y}) = \left[ \begin{array}{ccc} \frac{1}{\sqrt{2}} & \frac{\sqrt{3}}{2} & 0 \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{array} \right].
\] (35)

In turn, for the group \( D_{4y} \) the matrices \( \bold{M}_3(g) \) act on the vector \( q_3 = (a_{33}, a_{32}, a_{31}, a_{30}, b_{31}, b_{32}, b_{33})^T \) and transform the pairs \( a_{32}, a_{30} \) into a combination of \( \bar{a}_{32} \) and \( \bar{a}_{30} \), \( a_{33}, a_{31} \) into a combination of \( \bar{a}_{33} \) and \( \bar{a}_{31} \) and \( b_{33}, b_{31} \) into a combination of \( b_{33} \) and \( b_{31} \). An exception is the variable \( b_{32} \) which transforms into itself because it is an invariant of the tetrahedral symmetry. In this case we have
\[
\left( \begin{array}{c} \bar{a}_{33} \\ \bar{a}_{32} \\ \bar{a}_{31} \\ \bar{a}_{30} \end{array} \right) = \bold{M}_3(g) \left( \begin{array}{c} a_{33} \\ a_{32} \\ a_{31} \\ a_{30} \end{array} \right), \quad \bold{M}_3(C_{4y}) = \left[ \begin{array}{cccc} 0 & -\frac{\sqrt{5}}{4} & \frac{\sqrt{3}}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{5}}{4} & 0 & \frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & 0 & \frac{\sqrt{5}}{4} & 0 \\ -\frac{\sqrt{3}}{2} & 0 & \frac{\sqrt{5}}{4} & 0 \end{array} \right].
\] (36)

The vibration basis functions with parameters \( a_{20}, ..., a_{33} \) of irr. \( A_1=\Gamma_1 \) of \( D_{4y} \) have the form
\[
\Psi^{N}_{[n]}(a_{20}, ..., a_{33}; a_{20}^p, ..., a_{33}^p) = \sum_{i=1}^{8} \Psi^{n_i}_{[n]} \times \psi_{n_3}(a_{33}+d_3 a_{33}^p) \psi_{n_4}(a_{33}+d_3 a_{33}^p) \psi_{n_1}(a_{31}+d_1 a_{31}^p) \psi_{n_2}(a_{20}+d_0 a_{20}^p),
\]
where
\[
\Psi^{n_i}_{[n]} = \frac{c_i}{8} \psi_{n_1}(a_{22}-a_{22}) \psi_{n_2}(a_{20}-a_{20}^p) \times \psi_{n_3}(a_{33}+d_3 a_{33}^p) \psi_{n_4}(a_{33}+d_3 a_{33}^p) \psi_{n_1}(a_{31}+d_1 a_{31}^p) \psi_{n_2}(a_{20}+d_0 a_{20}^p),
\]
and
\[
\Psi^{n_i}_{[n]} = \frac{c_i}{8} \psi_{n_1}(\frac{\sqrt{3}}{2} a_{20}+\frac{1}{2} a_{22}-a_{22}^p) \psi_{n_2}(\frac{1}{2} a_{20}-\frac{\sqrt{3}}{2} a_{22}+a_{22}^p) \psi_{n_3}(\frac{\sqrt{10}}{4} a_{30}+\frac{\sqrt{6}}{4} a_{32}) \psi_{n_4}(\frac{\sqrt{6}}{4} a_{30}-\frac{\sqrt{10}}{4} a_{32}),
\]
\(c_1=1, c_2=-(1)^{n_4+n_6}, c_3=-(1)^{n_3+n_5}, c_4=-(1)^{n_3+n_4+n_5+n_6}, c_5=-(1)^{n_2+n_5+n_6}, c_6=-(1)^{n_2+n_4+n_5},
\)
c_7=-(1)^{n_2+n_3+n_6}, c_8=-(1)^{n_2+n_3+n_4}, d_{31}=-(1)^{\lfloor i+1/2\rfloor},
d_{21}=d_0=-(1)^i, d_{11}=-(1)^{\lfloor i+5/4\rfloor}, \) where "\([x]\)" means a greatest integer less than or equal to a number \(x\), and \(\psi_n(a)\) are normalized 1D oscillator functions.

4. Algorithm for construction of the orthonormal vibrational-rotational basis

Calculation of the parametric vibrational-rotational basis functions of irr. \(A_1=\Gamma_1\) of \(D_{4h}\).

**Step 1.** To calculate overlaps,

\[
B_{n_1,\ldots,n_6,K;\nu_1,\ldots,\nu_6,K'}^{JN} = \langle \Psi^{JN}_{n_1,\ldots,n_6,K} | \Psi^{JN}_{\nu_1,\ldots,\nu_6,K'} \rangle,
\]

\[
\Psi^{JN}_{n_1,\ldots,n_6,K}(a_{20},\ldots,a_{33},\Omega) = \sum_{K'-J}^{J} \sum_{i=1}^{8} \Psi_{n_1,\ldots,n_6}^{g_i}(a_{20},\ldots,a_{33}) D_{KK'}^{J}(g_i) r_{MK'}^{J}(\Omega),
\]

where \(r_{MK'}^{J}(\Omega) = \sqrt{2J+1}D_{MK'}^{J}(\Omega)\), form the finite \((2J+1)S\times(2J+1)S\) dimensional hermitian matrix called the Gramm matrix, which we denote here by \(B\).

**Step 2.** Solving the eigenvalue problem of the matrix \(B\) allows to find the orthonormal basis in which this matrix is diagonal:

\[
B_{\lambda_\nu}(s,K) = \lambda_{\nu} \chi_{\nu}(s,K).
\]

For \(\lambda_\nu \neq 0\) one gets the following basis of orthonormal states:

\[
|u_{\nu}\rangle = C_{\nu} \sum_{K'=-J}^{J} \left( \sum_{s=-J}^{J} \sum_{K=-J}^{J} \chi_{\nu}(s,K) \left( \sum_{i=1}^{8} \Psi_{s,K}^{g_i}(a_{20},\ldots,a_{33}) D_{KK'}^{J}(g_i) \right) \right) r_{MK'}^{J}(\Omega),
\]

where \(J, M, \Gamma\), and \(b\) fixed, and \(C_{\nu}\) is the normalization coefficient.

**Step 3.** To calculate the scalar products:

\[
\langle u_{\nu'} | u_{\nu} \rangle = C_{\nu'} C_{\nu} \sum_{s',K',s,K} \chi_{\nu'}(s',K')^{*} \chi_{\nu}(s,K) \langle \Psi^{JN}_{n_1,\ldots,n_6,K'} | \Psi^{JN}_{n_1,\ldots,n_6,K} \rangle = \delta_{\nu\nu'} C_{\nu} C_{\nu} \sum_{s,s,K} \chi_{\nu}(s,K)^{2}.
\]

It means that the states \(|u_{\nu}\rangle\) for which the eigenvalue \(\lambda_{\nu} = 0\) are the zero vectors, and for the cases when \(\lambda_{\nu} \neq 0\) the normalization coefficient is equal: \(C_{\nu} = \left( \lambda_{\nu} \sum_{s,s,K} |\chi_{\nu}(s,K)|^2 \right)^{-1/2}\).

Note that because the eigenequation (38) is, in fact, the eigenequation for the matrix representation of the projection operator \(\hat{P}_{bb}^{\Gamma}\) the eigenvalues are equal to \(\lambda_\nu > 0\). In this way we have obtained the required basis in the projected subspace \(K_{bb}^{\Gamma}\), e.g. \(K_3\) from section 2. Taking into account relation \(\langle r_{MK'}^{J} | r_{MK'}^{J} \rangle = \delta_{KK'}\) we have expression for the matrix \((2J+1)S\times(2J+1)S\) at each \(J > 0\):

\[
B_{\nu_1,\ldots,\nu_6,K_1;\nu_1,\ldots,\nu_6,K_2}(a_{20},\ldots,a_{33}) = \eta_2^{-2} \eta_3^{-4} \sum_{i=1}^{7} \sum_{i=6}^{7} \left( \sum_{s=1}^{8} \sum_{K=-J}^{J} D_{K_2K_1}^{J}(g_s) D_{K_2K_1}^{J}(g_t) \right) W_{K_2} W_{K_1}.
\]

During the integration we use Gauss-Hermite quadratures of \(\nu^{th}\) order at \(\nu = 10\):

\[
\int_{-\infty}^{+\infty} e^{-x^2} f(x) dx = \sum_{i=1}^{\nu} w_i f(x_i), \quad \int_{-\infty}^{+\infty} g(x) dx = \sum_{i=1}^{\nu} W_i g(x_i), \quad W_i = w_i e^{x_i^2}.
\]
Table 1. Output for $v_{11p0}^{ij}(\Omega)$: $\Gamma = \Gamma_1 = A_1$, $J = 0, 2, 4, 5$; $t$ distinguishes equiv.i.r. of $D_{4y}$ point group of intrinsic frame. Here $r_{MK}^{\pm}(\Omega) = (r_{MK}^{L}(\Omega) \pm r_{MK}^{L}(\Omega))/\sqrt{2}$.

| $J$ | $\Gamma$ | $p$ | $q_0$ | $t$ | $v_{11p0}^{ij}(\Omega)$ |
|-----|---------|-----|------|-----|-----------------|
| 0   | $\Gamma_1 = A_1$ | 1   | 1    | 1   | $v_{1111}^{ij}(\Omega) = r_{M0}^{ij}(\Omega)$ |
| 2   | $\Gamma_1 = A_1$ | 1   | 1    | 1   | $v_{1111}^{ij}(\Omega) = (\sqrt{3}r_{M0}^{ij}(\Omega) + 3r_{M2}^{ij}(\Omega))/(2\sqrt{3})$ |
| 4   | $\Gamma_1 = A_1$ | 1   | 1    | 1   | $v_{1111}^{ij}(\Omega) = (\sqrt{3}r_{M0}^{ij}(\Omega) + 2\sqrt{7}r_{M2}^{ij}(\Omega) + 9r_{M4}^{ij}(\Omega))/12$ |
| 4   | $\Gamma_1 = A_1$ | 1   | 1    | 2   | $v_{1111}^{ij}(\Omega) = (-2\sqrt{5}r_{M0}^{ij}(\Omega) + 5r_{M2}^{ij}(\Omega))/(3\sqrt{5})$ |
| 5   | $\Gamma_1 = A_1$ | 1   | 1    | 1   | $v_{5555}^{ij}(\Omega) = (\sqrt{5}r_{M2}^{ij}(\Omega) - r_{M4}^{ij}(\Omega))/2$ |

Here $x_i$ are abscessas (zeros of Hermite polynomials) and $w_i$ are weight factors [9].

Example of calculations of pure rotational basis functions of irr. $A_1 = \Gamma_1$ of $D_{4y}$ symmetrization point group in zero phonon approximation at $N = 0$ is given in table 1. At $J = 0$ and $a_0 = 7/10, a_2 = 1/4, a_2 = a_3 = 0, \eta_2 = \eta_3 = 1$, Gram matrix for $N = 0, 1, s = 1, ..., S$, $S = 7$ have the following eigenvalues $\{\lambda_i\}_{i=1}^T = \{0.9897, 0.2521, 0.0293, 0.8204, 0.0151, -3 \cdot 10^{-17}, -7 \cdot 10^{-19}\}$. From $\lambda_6 = -3 \cdot 10^{-17} \equiv 0, \lambda_7 = -7 \cdot 10^{-19} \equiv 0$ follows $\{X_{s,6}\}_{s=1}^T \equiv 0, \{X_{s,7}\}_{s=1}^T \equiv 0$.

5. DVR algorithm for solving eigenvalue problems in intrinsic frame

One can solve eigenvalue problem describing rotational-vibrational motion of collective nuclear model with potential energy $V(a_{20}, ..., a_{33})$ in intrinsic frame, for example at $J = 0$:

$$\hat{H}_e - E_v \psi_v(a_{20}, ..., a_{33}) = 0, \quad \hat{H}_e = \hat{H}(0) + V(a_{20}, ..., a_{33}),$$

using rotational-vibrational basis $u_0(a_{20}, ..., a_{33})$ of irr $A_1 = \Gamma_1$ of $D_{4y}$ group from Eq. (39) for the quadrupole-octupole harmonic oscillator

$$(\hat{H}(0) - E_v) u_0 = 0, \quad u_0 = C_s \sum_{s'=1}^S X_s(s') \psi_{s'}(a_{20}, ..., a_{33}),$$

where scalar product is calculated similarly to Eq. (41) using Gauss-Hermite quadratures

$$\langle u_{s}^{(0)} | u_{s'}^{(0)} \rangle = \sum_{t=[t_1, ..., t_6]} A_{t' t}^{T} A_{s't}, \quad A_{s't} = W_{t_1}^{1/2} \times ... \times W_{t_6}^{1/2} \sum_{s''=1}^S C_{s''} \psi_{s''}(x_1, ..., x_6) X_{s''}(s''). \quad (43)$$

We seek solution in the form of the Galerkin expansion over the orthogonal basis functions $u_0(a_{20}, ..., a_{33})$ with unknown coefficients $X_{sv}$

$$\psi_v(a_{20}, ..., a_{33}) = \sum_{s'=1}^{S_{max}} u_{s'}^{(0)}(a_{20}, ..., a_{33}) X_{s'v}. \quad (44)$$

Averaging over the basis with scalar product (43) leads to the algebraic eigenvalue problem

$$\sum_{s'=1}^{S_{max}} \left[ \langle u_{s}^{(0)} \mid \hat{H}(0) \mid u_{s'}^{(0)} \rangle + \langle u_{s}^{(0)} \mid V \mid u_{s'}^{(0)} \rangle - V \delta_{ss'} \right] X_{s'v} = 0. \quad (45)$$
We will solve this problem using transformation to the discrete variable representation (DVR)

\[ X_{st'} = \sum_{t=1}^{s'_{\text{max}}} A_{st} Y_{tv}, \quad \sum_{t=1}^{s'_{\text{max}}} A_{st}^T A_{st'} = \delta_{ss'}, \quad \sum_{s=1}^{s'_{\text{max}}} A_{st} A_{st'}^T = \delta_{tt'}, \]

that was successfully applied for solving eigenvalue problems describing large amplitude molecular vibrations [10]. In the DVR the problem (45) is reduced to the following one with respect to the new unknown eigenvectors \( Y_{tv} \)

\[ \sum_{t'=1}^{s'_{\text{max}}} \left[ \sum_{s=1}^{s'_{\text{max}}} A_{st}^T E_s^{(0)} A_{st'} \right] + V \left( \begin{array}{c}
  a_{20} = \frac{x_{i_2}}{\eta_2}, \\
  \vdots \\
  a_{33} = \frac{x_{i_3}}{\eta_3}
\end{array} \right) \delta_{tt'} - E_{vv} \delta_{tt'} \right] Y_{tv} = 0. \]

Here matrix of potential energy \( V \left( \begin{array}{c}
  a_{20} = \frac{x_{i_2}}{\eta_2}, \\
  \vdots \\
  a_{33} = \frac{x_{i_3}}{\eta_3}
\end{array} \right) \) is diagonal matrix which elements is calculated in Gauss-Hermitian nodes (42), while dense real-symmetric matrix of kinetic energy is calculated as product of known eigenvalues \( E_s^{(0)} \) and known symmetric matrixes \( A_{st} \) consisting of basis eigenfunctions in Gauss-Hermitian nodes from Eq. (43). Thus, in the DVR there is no problem of cumbersome numerical calculations of the multiple integrals \( \langle u_s^{(0)} | V | u_{s'}^{(0)} \rangle \). However, it is need to solve the interpolation problem of the potential energy \( V \left( \begin{array}{c}
  a_{20} = \frac{x_{i_2}}{\eta_2}, \\
  \vdots \\
  a_{33} = \frac{x_{i_3}}{\eta_3}
\end{array} \right) \) in Gauss-Hermitian nodes if it is given in a tabular form. Generalization of the above algorithm in the case of \( J > 0 \) is given by direct application of the expression Eq. (39) of the rotational-vibrational basis \( u_s^{(0)} \) at \( -J < K < J \) with corresponding modification of the scalar product Eq. (43) similar to Eq. (41).

6. Resume

New symbolic algorithm implemented in computer algebra system for generating irreducible representations of the point symmetry groups in the rotor + shape vibrational space of a nuclear collective model in the intrinsic frame was presented. The efficiency of the algorithm was investigated by calculating the symmetrized bases of irreducible representations \( \bar{G}_S \) subgroup \( \bar{D}_{4g} \) of octahedral group in the intrinsic frame of a quadrupole-octupole nuclear collective model. The DVR algorithm was proposed for solving eigenvalue problems, describing vibrational-rotational motion of the collective nuclear model in intrinsic frame, that may be solved using the fast eigensolver for dense real-symmetric matrices[11] and MPI technology.

7. Acknowledgment

This work has been partially supported by the Polish–French COPIN collaboration under the project 04-113, the Bogoliubov-Infeld JINR program and the grant RFBR 17–01–00298.

References
[1] Eisenberg J M and Greiner W 1970 Nuclear Theory Vol. 1 (Amsterdam: North-Holland)
[2] Chen J Q, Ping J and Wang F 2002 Group representation theory for physicists (Singapmre: World Sci.)
[3] Barut A and Raczka R 1977 Theory of Group Representations and Applications ( Warszawa: PWN)
[4] Gusev A A et al 2015 Lecture Notes Comp. Sci. 9301 166
[5] Gusev A A et al 2016 Lecture Notes Comp. Sci. 9890 228
[6] Cornwell J F 1984 Group theory in physics (New York: Academic Press)
[7] Szulerecha A, Dobrowolski A and Gódzá A 2014 Phys. Scr. 89 054033
[8] Varshalovich D A, Moskalev A N and Khersonskii V K 1989 Quantum theory of angular momentum (Singapore: World Sci.)
[9] Abramowitz M and Stegun I A 1965 Handbook of Mathematical Functions (New York: Dover)
[10] Bacic Z, Whitnell R M, Brown D and Light J C 1988 Comput. Phys. Commun. 51 35
[11] Bunge C F 2001 Comput. Phys. Commun. 138 92