

Symmetrization problem in a quadrupole-octupole collective approaches

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Idea of intrinsic frame

It is expected that the intrinsic frame:

- excludes contributions from global translational motion;
- introduces rotational degrees of freedom explicitly;
- shows intrinsic symmetries of nuclei;
- separates different kinds of intrinsic motions (sometimes), see, e.g. Bohr Hamiltonian in quadrupole a_0 , a_2 variables.

Surface collective variables

The equation of nuclear surface in the laboratory frame is:

$$R(\theta, \phi) = R_0 \left(1 + \sum_{\lambda\mu} (\alpha_{\lambda\mu}^{lab})^* Y_{\lambda\mu}(\theta, \phi) \right)$$

$\alpha_{\lambda\mu}^{lab}$ are spherical tensors in respect to $SO(3)$.

The equation of nuclear surface has the same form after the transformation to the intrinsic frame:

$$\alpha_{\lambda\mu}^{lab} \rightarrow \alpha_{\lambda\mu} = \sum_{\mu'} D_{\mu'\mu}^{\lambda}(\Omega) \alpha_{\lambda\mu'}^{lab}$$

$(\theta, \phi) \rightarrow (\theta_w, \phi_w)$, where new angles are measured in respect to the intrinsic frame

$\alpha_{\lambda\mu}$ are spherical tensors in respect to $\overline{SO(3)}$.

Intrinsic groups \overline{G}

Jin-Quan Chen, Jialun Ping & Fan Wang: Group Representation Theory for Physicists, World Scientific, 2002.

Def. For each element g of the group G , one can define a corresponding operator \overline{g} in the group linear space \mathcal{L}_G as:

$$\overline{g}S = Sg, \quad \text{for all } S \in \mathcal{L}_G.$$

The group formed by the collection of the operators \overline{g} is called the intrinsic group of G .

IMPORTANT PROPERTY:

$$[G, \overline{G}] = 0$$

Intrinsic group \overline{G}

Action of the rotation intrinsic group $\bar{g} \in \overline{SO(3)}$.

Transformations of coordinates:

$$(\alpha_{\lambda\mu}^{lab})' = \bar{g}\alpha_{\lambda\mu}^{lab} = \alpha_{\lambda\mu}^{lab}$$

$$(\alpha_{\lambda\mu})' = \bar{g}\alpha_{\lambda\mu} = \sum_{\mu'} D_{\mu'\mu}^{\lambda}(g^{-1})\alpha_{\lambda\mu'}$$

$$\Omega' = \bar{g}\Omega = \Omega g.$$

Action in the space of functions of intrinsic variables:

$$\bar{g}\psi(\alpha_{\lambda\mu}, \Omega) = \psi(\bar{g}\alpha_{\lambda\mu}, \bar{g}^{-1}\Omega)$$

Intrinsic vs laboratory frames

One may introduce the intrinsic frame which is tightly associated with a nucleus. This frame always follows the nucleus. In order to describe the nuclear dynamics we need the Euler angles which determine mutual orientation of the intrinsic vs laboratory frame.

The transition from the intrinsic to laboratory frame

$$\begin{cases} \alpha_{\lambda\mu}^{lab} = \sum_{\nu=-\lambda}^{\lambda} D_{\mu\nu}^{\lambda*}(\Omega) \alpha_{\lambda\nu} \\ f_k(\alpha_{\lambda\mu}, \Omega) = 0, \quad k = 1, 2, 3 \end{cases}$$

(e.g. in a pure quadrupole case, ($\lambda = 2$), the conditions $f_k(\alpha_{\lambda\mu}, \Omega) = 0$ are given explicitly as $\alpha_{22} = \alpha_{2-2} \in R$, $\alpha_{21} = \alpha_{2-1} = 0$ set the intrinsic frame along the ellipsoid principal axes)

Uniqueness of quantum states

In practice, the transformation to intrinsic frame is not reversible because of insufficient number of required conditions, an important problem is to discover this ambiguity.

One needs to construct the group of transformations which fulfill the condition $h \in G_s$:

$$(\alpha_{\lambda\nu}, \Omega) \xrightarrow{h} ((\alpha_{\lambda\nu})', \Omega')$$

which leave invariant the corresponding laboratory coordinates:

$$\alpha_{\lambda\mu}^{lab}((\alpha_{\lambda\nu})', \Omega') = \alpha_{\lambda\mu}^{lab}(\alpha_{\lambda\nu}, \Omega)$$

If

$$\Psi(\alpha_{\lambda\mu}, \Omega) = \Psi(\alpha_{\lambda\mu}^{lab})$$

then

$$\Psi((\alpha_{\lambda\mu})', \Omega') = \Psi(\alpha_{\lambda\mu}^{lab})$$

Uniqueness of quantum states

If

$$\Psi(\alpha_{\lambda\mu}, \Omega) = \Psi(\alpha_{\lambda\mu}^{lab})$$

then

$$\Psi((\alpha_{\lambda\mu})', \Omega') = \Psi(\alpha_{\lambda\mu}^{lab})$$

CONTRADICTION; generally while working in the intrinsic frame, for most of square integrable functions $\Psi(\alpha_{\lambda\mu}, \Omega) \neq \Psi((\alpha_{\lambda\mu})', \Omega')$.

The group \bar{G}_s is the SYMMETRIZATION GROUP.

The symmetrization condition for states. For all $\bar{h} \in \bar{G}_s$:

$$\bar{h}\Psi(\alpha_{\lambda\mu}, \Omega) = \Psi(\alpha_{\lambda\mu}, \Omega)$$

The symmetrization group

Let us consider the standard quadrupole case of the collective variables $\alpha_{20}, \alpha_{22}, \Omega$. This definition of intrinsic variables requires 3 conditions

$$\alpha_{2\pm 1} = 0 \text{ and } \alpha_{2-2} = \alpha_{22} \in \mathbb{R}.$$

These requirements give the following set of equations:

$$\begin{aligned} D_{0,\pm 1}^2(g^{-1}) &= 0 \\ D_{-2\pm 1}^2(g^{-1}) + D_{2\pm 1}^2(g^{-1}) &= 0 \\ D_{02}^2(g^{-1}) - D_{0,-2}^2(g^{-1}) &= 0 \\ D_{-2,-2}^2(g^{-1}) + D_{2,-2}^2(g^{-1}) &= D_{-22}^2(g^{-1}) + D_{22}^2(g^{-1}). \end{aligned}$$

The symmetrization group

The symmetrization group is:

$$g \in \bar{O}_h$$

Because the quadrupole variables are invariant in respect to the space inversion, the operation C_i belongs to the symmetrization group.

The generators of the group \bar{O}_h :

$$R_1 \equiv \bar{R}(0, \pi, 0) : (\beta, \gamma) \rightarrow (\beta, \gamma)$$

$$R_2 \equiv \bar{R}(0, 0, \pi/2) : (\beta, \gamma) \rightarrow (\beta, -\gamma)$$

$$R_3 \equiv \bar{R}(\pi/2, \pi/2, \pi/2) : (\beta, \gamma) \rightarrow (\beta, \gamma - \pi/3)$$

E.g. Bohr Hamiltonian

$$\hat{\mathcal{H}}_{Bohr} = \hat{\mathcal{H}}_{vib;2}(\beta, \gamma) + \hat{\mathcal{H}}_{rot}(\Omega) + \hat{\mathcal{H}}_{vr}(\beta, \gamma, \Omega)$$

where

$$\hat{\mathcal{H}}_{vib;2} = \frac{1}{2} \left\{ \frac{1}{\beta^4} \frac{\partial}{\partial \beta} \beta^4 \frac{\partial}{\partial \beta} - \frac{1}{\beta^2 \sin(3\gamma)} \frac{\partial}{\partial \gamma} \sin(3\gamma) \frac{\partial}{\partial \gamma} + \beta^2 \right\} + V(\beta, \gamma)$$

$$\hat{\mathcal{H}}_{rot} = \frac{1}{2} \sum_{k=1,2,3} \frac{J_k^2}{\mathcal{I}_k}$$

$$\hat{\mathcal{H}}_{vr} = \frac{1}{8\beta^4} \sum_{k=1,2,3} \frac{J_k^2}{\sin^2(\gamma - (2\pi/3)k)} - \hat{\mathcal{H}}_{rot}$$

E.g. Bohr Hamiltonian

The vibrational hamiltonian has an octahedral symmetry:

$$\text{Sym}(\hat{\mathcal{H}}_{\text{vib};2}) = \bar{\text{O}}_h.$$

The generators of the group $\bar{\text{O}}_h$:

$$R_1 \equiv \bar{R}(0, \pi, 0) : (\beta, \gamma) \rightarrow (\beta, \gamma)$$

$$R_2 \equiv \bar{R}(0, 0, \pi/2) : (\beta, \gamma) \rightarrow (\beta, -\gamma)$$

$$R_3 \equiv \bar{R}(\pi/2, \pi/2, \pi/2) : (\beta, \gamma) \rightarrow (\beta, \gamma - \pi/3)$$

$\hat{\mathcal{H}}_{\text{vib};2} = \hat{\mathcal{H}}_{\text{vib};2}(\partial/\partial\beta, \partial/\partial\gamma, \beta, \cos(3\gamma))$ is a function of $\bar{\text{O}}_h$ -invariants.

The symmetrization group is here identical to the vibrational Hamiltonian symmetry group.

E.g. Bohr Hamiltonian

The rotational hamiltonian has a dihedral symmetry:

$$\text{Sym}(\hat{\mathcal{H}}_{rot}) = \bar{D}_{2h}.$$

The generators of the group \bar{D}_{2h} :

$$\begin{aligned}\bar{C}_{2y} : (\beta, \gamma) &\rightarrow (\beta, \gamma), & J_k^2 &\rightarrow J_k^2 \\ \bar{C}_{2z} : (\beta, \gamma) &\rightarrow (\beta, \gamma), & J_k^2 &\rightarrow J_k^2\end{aligned}$$

$\hat{\mathcal{H}}_{rot} = \hat{\mathcal{H}}_{rot}(J_x, J_y, J_z)$ is a function of \bar{D}_{2h} -invariants.

The coupling term has also a dihedral symmetry:

$$\text{Sym}(\hat{\mathcal{H}}_{vr}) = \bar{D}_{2h}.$$

E.g. Bohr Hamiltonian

The symmetry group for eigensolutions of the Bohr hamiltonian (weak vib.-rot. coupling):

$$\begin{array}{ccccc} \hat{\mathcal{H}}_{Bohr} & = & \hat{\mathcal{H}}_{vib;2} & + & \hat{\mathcal{H}}_{rot} \\ \downarrow & & \downarrow & & \downarrow \\ \overline{G}_H & = & \overline{O}_h & \times & \overline{D}_{2h} \\ & & \downarrow & & \downarrow \\ & & \Gamma_v & & \Gamma_r \end{array}$$

In general, using the spectral theorem one can always decompose the Hamiltonian into a series of the subhamiltonians of given symmetry

$$\hat{\mathcal{H}} = \sum_G \hat{\mathcal{H}}_G = \sum_G E_G |\Psi_G\rangle \langle \Psi_G|$$

Basis of \overline{O}_h group built of rotational functions

$$\begin{aligned}r_{MK}^J(\Omega) &= \sqrt{2J+1} D_{MK}^J(\Omega)^* \\r_{MK}^{(+J)}(\Omega) &= \frac{1}{\sqrt{2(1+\delta_{K0})}} (r_{MK}^J + r_{M-K}^J), K \geq 0 \\r_{MK}^{(-J)}(\Omega) &= \frac{1}{\sqrt{2}} (r_{MK}^J - r_{M-K}^J), K > 0\end{aligned}$$

$R_{AB}^{JM}(\Omega)$, A-irrep. of \overline{O}_h , B-irrep. of \overline{D}_2 .

$$\begin{aligned}J=0, & \quad R_{A_1A_1K=0}^{J=0M=0}(\Omega) = r_{00}^{(+0)}(\Omega) \\J=1, & \quad \begin{cases} R_{T_1A_1K=0}^{J=1M}(\Omega) = r_{M0}^{(+1)}(\Omega) \\ R_{T_1B_1K=1}^{J=1M}(\Omega) = r_{M1}^{(-1)}(\Omega) \\ R_{T_1B_3K=1}^{J=1M}(\Omega) = r_{M1}^{(+1)}(\Omega) \end{cases}\end{aligned}$$

The schematic model

The quadrupole+octupole model Hamiltonian:

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_{vib} + \hat{\mathcal{H}}_{rot}$$

No vib-rot coupling terms \Rightarrow **the eigenfunctions:**

$$\Psi_{\Gamma JM\nu}(\alpha, \Omega) = \phi_{\Gamma J}(\alpha) R_{JM\nu}(\Omega)$$

The reduced (in respect to $J_3 = M$) matrix elements:

$$\langle \Psi_{\Gamma' J' \nu'} || Q_{\lambda}^{lab} || \Psi_{\Gamma J \nu} \rangle = \sum_{\mu} \langle \phi_{\Gamma' J'} | Q_{\lambda \mu} | \phi_{\Gamma J} \rangle \langle R_{J' \nu'} || D_{\mu}^{\lambda*} || R_{J \nu} \rangle$$

The reduced $B(E\lambda)$ probability:

$$B(E\lambda; (\Gamma J \nu) \rightarrow (\Gamma' J' \nu')) = |\langle \Gamma' J' \nu' || Q_{\lambda}^{lab} || \Gamma J \nu \rangle|^2 / (2J + 1)$$

Another group of symmetrization

Another choice of intrinsic variables ($\alpha_{20}, \alpha_{21}, \Omega$):
 $\alpha_{2\pm 2} = 0$ and $\alpha_{21} = -\alpha_{2-1} \in R$, ($\alpha_{\lambda-\mu} = (-1)^\mu \alpha_{\lambda\mu}^*$).

It leads to the set of equations for allowed rotations and the symmetrization group:

$$\begin{aligned} D_{\pm 20}^2(g)^* &= 0 \\ D_{\pm 2,1}^2(g)^* - D_{\pm 2,-1}^2(g)^* &= 0 \\ D_{10}^2(g)^* + D_{-1,0}^2(g)^* &= 0 \\ D_{11}^2(g)^* - D_{1,-1}^2(g)^* &= D_{-1-1}^2(g)^* - D_{-11}^2(g)^*. \end{aligned}$$

The symmetrization group is:

$$g \in \overline{D}_{2h}$$

\overline{G}_s for quadrupole-octupole model

The quadrupole+octupole model.

The intrinsic variables $(\alpha_{20}, \alpha_{21}, \{\alpha_{3\mu}\}, \Omega)$.

The intrinsic frame defined as: $\alpha_{22} = \alpha_{2,-2}$ and $\alpha_{2,\pm 1} = 0$.

The symmetrization group is:

$$g \in \overline{O}$$

Symmetrization for a quadrupole-octupole model

Choice of collective variables:

$$\alpha_{32} = \alpha_{3-2}, \alpha_{30} = \alpha_{3\pm 3} = \alpha_{3\pm 1} = 0$$

$$\alpha_{22} = \alpha_{2,-2}, \quad \alpha_{2,\pm 1} = 0.$$

$$0 = D_{-3-2}^3(g)^* + D_{-32}^3(g)^* \quad (1)$$

$$D_{2-2}^3(g)^* + D_{22}^3(g)^* = D_{-2-2}^3(g)^* + D_{-22}^3(g)^* \quad (2)$$

$$0 = D_{-1-2}^3(g)^* + D_{-12}^3(g)^* \quad (3)$$

$$0 = D_{0-2}^3(g)^* + D_{02}^3(g)^* \quad (4)$$

$$0 = D_{1-2}^3(g)^* + D_{12}^3(g)^* \quad (5)$$

$$0 = D_{3-2}^3(g)^* + D_{32}^3(g)^* \quad (6)$$

The symmetrization group is: $g \in \bar{D}_4$

The symmetrization problem

The physical state space:

$$\mathcal{K} = \{\phi(\alpha, \Omega) : g\phi = \phi, \text{ for all } g \in G_s\}$$

The collective hamiltonians $\hat{\mathcal{H}}$ are generally defined in wider space \mathcal{K}_{coll} consisted of all functions, not only symmetrized.

One needs to restrict $\hat{\mathcal{H}}$ to the physical subspace !

The symmetrization problem

There are 3 possible procedures:

1. Projection

Project the hamiltonian $\hat{\mathcal{H}}$: $\hat{\mathcal{H}}_1 = P_{\mathcal{K}}\hat{\mathcal{H}}P_{\mathcal{K}}$. and solve it in \mathcal{K}

IMPORTANT: $\hat{\mathcal{H}}_1 = P_{\mathcal{K}}\hat{\mathcal{H}}P_{\mathcal{K}}$ has the symmetry of the symmetrization group G_s , e.g. OCTAHEDRAL

2. Selection

Solve $\hat{\mathcal{H}}$ in \mathcal{K}_{coll} and choose solutions belonging to \mathcal{K} (*)

3. Symmetrization

Solve $\hat{\mathcal{H}}$ in \mathcal{K}_{coll} and symmetrize the solutions.

Which procedure is physical ?

The symmetrization problem

Projection operator onto the scalar representation of the symmetrization group \overline{G}_s in \mathcal{K} :

$$P_{\mathcal{K}} = \frac{1}{\text{card}(\overline{G}_s)} \sum_{g \in \overline{G}_s} g,$$

ad. 1. Projection

$$\begin{aligned}\hat{\mathcal{H}}_1 &\equiv P_{\mathcal{K}} \hat{\mathcal{H}} P_{\mathcal{K}} \\ \hat{\mathcal{H}}_1 |\Psi_{1;\nu}\rangle &= E_{1;\nu} |\Psi_{1;\nu}\rangle\end{aligned}$$

then $P_{\mathcal{K}} |\Psi_{1;\nu}\rangle = |\Psi_{1;\nu}\rangle \in \mathcal{K}$.

The symmetrization problem

Spectral form of H_1

$$\hat{\mathcal{H}}_1 = \sum_{\nu} E_{1;\nu} |\Psi_{1;\nu}\rangle \langle \Psi_{1;\nu}|$$

Hamiltonian $\hat{\mathcal{H}}_1$ has the intrinsic symmetry G_s or larger, independently of the symmetry of the original Hamiltonian $\hat{\mathcal{H}}$.

The symmetrization problem

ad. 2. Selection

First, solving the original $\hat{\mathcal{H}}$ in \mathcal{K} :

$$\hat{\mathcal{H}}|\Psi_n\rangle = E_n|\Psi_n\rangle$$

Next, choosing the solutions which fulfil the symmetrization condition

$$P_{\mathcal{K}}|\Psi_n\rangle = |\Psi_n\rangle \equiv |\Psi_n\rangle_{\mathcal{K}}$$

Spectral form of the effective H_2

$$\hat{\mathcal{H}}_2 = \sum_n E_n |\Psi_n\rangle_{\mathcal{K}\mathcal{K}} \langle \Psi_n|$$

The symmetrization problem

Note to the second procedure:

$$\begin{aligned}\hat{\mathcal{H}}|\Psi_n\rangle_{\mathcal{K}} &= E_n|\Psi_n\rangle_{\mathcal{K}} \Rightarrow \\ \hat{\mathcal{H}}_1|\Psi_n\rangle_{\mathcal{K}} &= E_n|\Psi_n\rangle_{\mathcal{K}}.\end{aligned}$$

The solutions for the second procedure are also solutions for the first procedure.

The OPPOSITE property is, in general, not TRUE.

Conclusion

i.e. the projected hamiltonian $\hat{\mathcal{H}}_1$ can provide more solutions $|\Psi\rangle_{\mathcal{K}}$ than $\hat{\mathcal{H}}$ itself.

The symmetrization problem

ad. 3. Symmetrization

First, solving the original $\hat{\mathcal{H}}$ in \mathcal{K} :

$$\hat{\mathcal{H}}|\Psi_n\rangle = E_n|\Psi_n\rangle$$

Next, symmetrizing all solutions

$$|\Psi_n\rangle_S \equiv P_{\mathcal{K}}|\Psi_n\rangle$$

Note that, in general when $[\hat{\mathcal{H}}, \hat{P}_{\mathcal{K}}] \neq 0$:

$${}_S\langle\Psi_{n_1}|\Psi_{n_2}\rangle_S = \langle\Psi_{n_1}|P_{\mathcal{K}}\Psi_{n_2}\rangle \neq 0$$

and cont.

The symmetrization problem

cont.

$$\hat{\mathcal{H}}_3 = \sum_n E_n |\Psi_n\rangle_S \langle \Psi_n|$$

is NOT the spectral decomposition of the effective hamiltonian [error in IJMP E20 (2011) 199].

A formal relation

$$\hat{\mathcal{H}}_1 = P_{\mathcal{K}} \left(\sum_n E_n |\Psi_n\rangle \langle \Psi_n| \right) P_{\mathcal{K}} = \sum_n E_n \{ P_{\mathcal{K}} |\Psi_n\rangle \langle \Psi_n| P_{\mathcal{K}} \} = \hat{\mathcal{H}}_3.$$

does not prove equivalence of 1st and 3rd procedure.

3rd procedure is, in fact, INCORRECT.

CONCLUSIONS:

- concept of constructing collective Hamiltonians already in the intrinsic frame as new way of proceeding,
- symmetrization process can be realized according to, at least, two different schemes,
- symmetrization group depends on the set of collective variables and way of setting the intrinsic frame,
- strength of the EM transitions strongly depends on the group structure of the collective eigenstates