SYMMETRIES IN INTRINSIC FRAME

Andrzej Góźdź,

Institute of Physics, Dep. Math. Phys., UMCS, Lublin, Poland

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Collaboration

Artur Dobrowolski, IF UMCS, Lublin, Poland

Agnieszka Szulerecka, IF UMCS, Lublin, Poland

Jerzy Dudek, IPHC/IReS, Strasbourg, France

> Katarzyna Mazurek IFJ, Kraków, Poland

What is presented ?

Intrinsic frame

Surface collective variables

The symmetrization group

Schematic model

¹⁵⁶Gd vs. ¹⁵⁶Dy

Intuition of intrinsic frame

It is expected that the intrinsic frame:

- excludes contributions from global translational motion;
- introduces rotational degrees of fredom explicitely;
- shows intrinsic symmetries of nuclei;
- separates different kinds of intrinsic motions (sometimes).

Microscopic laboratory frame

DEFINITION: (L.C. Biedernharn, J.D. Louck, Angular Momentum in Quantum Physics)

• Denote by

$$\vec{x}(n) = (x_1(n), (x_2(n), x_3(n)),$$

where n = 1, ..., A the *i*th radius vector of n-th particle in R^{3A} .

• The position vector in the configuration space for A-nucleons is:

$$x = (\vec{x}(1), \vec{x}(2), \vec{x}(3), \dots, \vec{x}(A)).$$

• The laboratory frame basic, orthonormal unit vectors:

$$\vec{l_1}, \vec{l_2}, \vec{l_3}.$$

Microscopic intrinsic frame 1/6

• The orthonormal versors of intrinsic frame:

$$\vec{f}_k(\vec{x}(1),\vec{x}(2),\ldots,\vec{x}(A))$$

where k = 1, 2, 3 are dependent on distribution of nucleons in the space.

 They should satisfy the conditions which allow to interpret the versors as some global vectors fixed to the nucleus (*R* ∈ *O*(3)):

$$ec{f}_k(ec{x}(1)+ec{a},ec{x}(2)+ec{a},\ldots,ec{x}(A)+ec{a}) = \ ec{f}_k(ec{x}(1),ec{x}(2),\ldots,ec{x}(A))$$

$$\vec{f}_k(\hat{\mathcal{R}}\vec{x}(1), \hat{\mathcal{R}}\vec{x}(2), \dots, \hat{\mathcal{R}}\vec{x}(A)) = \hat{\mathcal{R}}\vec{f}_k(\vec{x}(1), \vec{x}(2), \dots, \vec{x}(A)) \\ = \sum_k \mathcal{R}_{ki}\vec{f}_k(\vec{x}(1), \vec{x}(2), \dots, \vec{x}(A))$$

Microscopic intrinsic frame 2/6

• The frame non-singularity condition:

$$(\frac{\partial \vec{f}_i}{\partial x_1(n)}, \frac{\partial \vec{f}_i}{\partial x_2(n)}, \frac{\partial \vec{f}_i}{\partial x_3(n)},) \neq \vec{0},$$

for any i and all n. END of DEFINITION

• The position vectors of the individual particles in the center of mass frame:

$$\vec{y}(n) \equiv \vec{x}(n) - \vec{R}_{CM}.$$

• The laboratory vector components (fixed in the space) of $\vec{y}(n)$ can be calculated by projections onto the laboratory frame are given:

$$\left[\vec{y}(n)\right]_k^{(lab)} = \vec{y}(n) \cdot \vec{l}_k.$$

Microscopic intrinsic frame 3/6

• The intrinsic components of $\vec{y}(n)$ are projections onto the intrinsic versors:

$$y_k(n) \equiv [\vec{y}(n)]_k^{(int)} = \vec{y}(n) \cdot \vec{f}_k(x).$$

- IMPORTANT: the intrinsic coordinates:
 - $y_k(n)$ are not **single particle** coordinates (problem with MF theories))
 - $y_k(n)$ are O(3) invariant.

Microscopic intrinsic frame 4/6

• Intrinsic variables $\{q_s\}$ are functions of O(3) invariants:

 $q_s = h_s(y_1(1), y_2(1), y_3(1), \dots, y_1(A), y_2(A), y_3(A)),$

where s = 1, 2, ..., 3A - 6.

• The center of mass condition

$$\sum_{n=1}^{3A} m_n y_k(n) = 0$$

• Rotational variables Ω determined by scalar products:

$$R_{km}(\Omega) = \vec{f}_k(x) \cdot \vec{l}_m$$

• 3 appropriate conditions for $y_k(n) = \vec{y}(n) \cdot \vec{f}_k(x)$ required.

Microscopic intrinsic frame 5/6

REMARK:

• The above 3 additional conditions for {*y*_k(*n*)} often allow to write the inverse relations (Eckhart, molecular physics):

$$y_k(n) = g_k(n; q_1, q_2, \dots, q_{3A-6})$$

If well defined no SYMMETRIZATION GROUP ! This is not the case of most models in nuclear physics.

Microscopic intrinsic frame 6/6

Example: for fixed $\{\vec{l}_k\}$ the 3 conditions determine the Euler angles Ω between the laboratory and intrinsic frames:

$$x_l(n) = R_l^{CM} + \sum_k D_{kl}(\Omega) y_k(n),$$

$$\vec{l}_k = R(\Omega^{-1}) \vec{f}_k(\vec{y}(1), \dots, \vec{y}(A))$$

IMPORTANT: in general, the rotational variables Ω , for the frames defined by Biedernharn an Louck always determines global rotation (total angular momentum) of the system.

Intrinsic groups $\overline{\mathrm{G}}$

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:

$$\overline{g}S = Sg$$
, 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:

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

The groups G and \overline{G} are antyisomorphic.

Surface collective variables

The equation of nuclear surface in the laboratory frame is:

$$R(heta, \phi) = R_0 \left(1 + \sum_{\lambda \mu} (lpha_{\lambda \mu}^{lab})^* Y_{\lambda \mu}(heta, \phi)
ight)$$

The collective intrinsic variables $\alpha^{\it lab}_{\lambda\mu}$ are spherical tensors in respect to G.

The equation of nuclear surface in the intrinsic frame is:

$${\it R}(heta^{\prime},\phi^{\prime})={\it R}_{0}\left(1+\sum_{\lambda\mu}lpha^{\star}_{\lambda\mu}Y_{\lambda\mu}(heta^{\prime},\phi^{\prime})
ight)$$

The collective intrinsic variables $\alpha_{\lambda\mu}$ are spherical tensors in respect to \overline{G} .

Intrinsic variables

- Laboratory frame $ightarrow \{q_{\lambda\mu}^{lab}\}.$
- Intrinsic frame $\rightarrow q_{\lambda\mu}$

Transformation from laboratory to intrinsic frame:

• N variables to N variables transformation ?

$$q^{lab}
ightarrow (q, \Omega),$$

• Three additional conditions required:

$$F_i(q, \Omega) = 0, \ i = 1, 2, 3.$$

The conditions define physical meaning of Euler angles.

Uniqueness of quantum states

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

$$(q,\Omega) \rightarrow q^{lab}$$

then the states $\hat{g}(q,\Omega) = (q',\Omega') \rightarrow q^{lab}$

$$\hat{g}\Psi(q,\Omega) = \Psi(q')$$

 $\hat{g}\Psi(q,\Omega) = \Psi(q',\Omega') = \Psi(q'^{ab})$

CONTRADICTION; generally $\Psi(q, \Omega) \neq \Psi(q', \Omega')$

 $\{\hat{g}\}\$ form the SYMMETRIZATION GROUP \overline{G}_{sym} . The symmetrization condition. For all $\hat{g} \in \overline{G}_{sym}$:

$$\hat{g}\Psi(q,\Omega)=\Psi(q,\Omega)$$

The group of symmetrization 1/3

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

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

These requirements give the following set of equations:

$$\begin{array}{rcl} D_{20}^2(g) &=& 0\\ D_{\pm 1,-2}^2(g) + D_{\pm 1,2}^2(g) &=& 0\\ D_{-20}^2(g) + D_{-2,-2}^2(g) + D_{-2,2}^2(g) &=& D_{20}^2(g) + D_{2,-2}^2(g) + D_{2,2}^2(g). \end{array}$$

The symmetrization group is:

 $g \in \overline{O}_h$

The group of symmetrization 2/3

2. Another intrinsic variables $(\alpha_{20}, \alpha_{21}, \Omega)$. The intrinsic frame defined as: $\alpha_{2\pm 2} = 0$ and $\alpha_{21} = -\alpha_{2-1}$. It leads to the equations for allowed rotations:

$$egin{array}{rcl} D^2_{\pm 20}(g)&=&0\ D^2_{\pm 2,1}(g)-D^2_{\pm 2,-1}(g)&=&0\ D^2_{10}(g)+D^2_{-1,0}(g)&=&0\ D^2_{11}(g)-D^2_{1,-1}(g)&=&D^2_{-1-1}(g)-D^2_{-11}(g). \end{array}$$

The symmetrization group is:

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

The group of symmetrization 3/3

- 2. 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:

 $g \in \overline{O}$

Maximal realization of $\overline{O}(3)$ group

- $\alpha_{\lambda\mu}$ are $\overline{O}(3)$ tensors.
- The action of $\overline{O}(3)$ group is restricted by the additional conditions required for the intrinsic frame.
- In fact, the appropriate subgroup G ⊂ O(3) is allowed to act in the intrinsic frame.

This subgroup has to leave invariant the conditions

$$F_i(q, \Omega) = 0, \ i = 1, 2, 3.$$

Example: for quadrupole case

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

These conditions allow for $G = \overline{O}_h$. In the case of Bohr's type models the SYMMETRIZATION group and MAXIMAL realization of $\overline{O}(3)$ coincides.

Symmetry operations in the intrinsic frame

The operations allowed in the intrinsic space:

• All operations which fulfil the conditions

$$F_i(\{\alpha_{\lambda\mu}\}, \Omega) = 0, \ i = 1, 2, 3.$$

which save the structure of the intrinsic variables space.

- An example 1.: MAXIMAL realization of $\overline{O}(3)$
- An example 2.: for quadrupole+octupole case and the intrinsic frame

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

the transformations of $\mathrm{SO}(3)_{\mathit{oct}}$ type which ACT only on OCTUPOLE variables:

$$\alpha'_{3\mu} = \sum_{\mu'} D^3_{\mu'\mu}(\xi) \alpha_{3\mu'}$$

fulfil the required conditions.

The schematic model

The model Hamiltonian:

$$\hat{\mathcal{H}}_{2+3} = \hat{\mathcal{H}}_{\textit{vib}} + \hat{\mathcal{H}}_{\textit{rot}}$$

No coupling terms. **The eigenfunctions:**

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

The reduced (in respect to the quantum number M) matrix elements:

$$\langle \Psi_{\Gamma'J'\nu'} || Q_{\lambda} || \Psi_{\Gamma J\nu} \rangle = \sum_{\mu} \langle \phi_{\Gamma'J'} | \bar{Q}_{\lambda\mu} | \phi_{\Gamma J} \rangle \langle R_{J'\nu'} || D_{\cdot\mu}^{\lambda\star} || R_{J\nu} \rangle$$

The reduced probability:

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

Bohr Hamiltonian

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

where

$$\begin{split} \hat{\mathcal{H}}_{\textit{vib};2} &= \frac{1}{2} \left\{ \frac{1}{\beta^4} \frac{\partial}{\partial \beta} \beta^4 \frac{\partial}{\partial \beta} - \frac{1}{\beta^2 \sin(3\gamma)} \frac{\partial}{\partial \gamma} \sin(3\gamma) \frac{\partial}{\partial \gamma} + \beta^2 \right\} + V(\beta,\gamma) \\ \hat{\mathcal{H}}_{\textit{rot}} &= \frac{1}{2} \sum_{k=1,2,3} \frac{J_k^2}{\mathcal{J}_k}. \end{split}$$

Vibrational part $\hat{\mathcal{H}}_{vib;2} \Rightarrow \overline{O}_h - \mathbf{OCTAHEDR}$. Rotational part $\hat{\mathcal{H}}_{rot} \Rightarrow \overline{D}_{2h}$ symmetry.

$$\hat{\mathcal{H}}_{rot} + \hat{\mathcal{H}}_{vr} = \frac{1}{8\beta^4} \sum_{k=1,2,3} \frac{J_k^2}{\sin^2(\gamma - (2\pi/3)k)}.$$
$$G_{ph} = \overline{D}_{2h} \quad \text{because} \quad G_{vib} = \overline{O}_h \quad \text{and} \quad G_{rot} = \overline{D}_{2h}$$

Quadrupole + Octupole model

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_{\textit{vib}}(\beta, \gamma, \alpha_3) + \hat{\mathcal{H}}_{\textit{rot}}(\Omega) + \hat{\mathcal{H}}_{\textit{vr}}(\beta, \gamma, \alpha_3, \Omega)$$

where the vibrational Hamiltonian:

$$\hat{\mathcal{H}}_{\textit{vib}} = \mathcal{T}_{\textit{vib};2}(eta,\gamma) + \mathcal{T}_{\textit{vib};3}(lpha_3) + \mathcal{V}_{\textit{vr}}(eta,\gamma,lpha_3)$$

Here:

$$G_{ph} = \overline{D}_{2h}, \quad G_{vib} = \overline{O}_h, \quad G_{rot} = \overline{D}_{2h}, \quad G_{vr} = \overline{D}_{2h}$$

AGAIN: THE COLLECTIVE VIBRATIONS HAVE OCTAHEDRAL SYMMETRY.

The symmetrization problem 1/2

• The physical state space:

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

- The collective hamiltonians $\hat{\mathcal{H}}$ are defined in wider space \mathcal{K}_{coll} .
- 3 possible procedures:
 - Project the hamiltonian *Ĥ*: *Ĥ*_K = P_K*Ĥ*P_K. and solve it in *K* IMPORTANT: P_K*Ĥ*P_K has the symmetry of the symmetrization group G_{sym}, e.g. OCTAHEDRAL
 - Solve $\hat{\mathcal{H}}$ in \mathcal{K}_{coll} and choose solutions belonging to \mathcal{K} (*)
 - Solve $\hat{\mathcal{H}}$ in \mathcal{K}_{coll} and symmetrize the solutions.

Which procedure is physical ?

The symmetrization problem 2/2

The 3 procedure are not equivalent:

• "Projection". Assume

$$\hat{\mathcal{H}}|\psi
angle=\mathsf{E}|\psi
angle$$

then for $\mathcal{P}_{\mathcal{K}}|\psi
angle=|\psi
angle\in\mathcal{K}$

$$P_{\mathcal{K}}\hat{\mathcal{H}}P_{\mathcal{K}}|\psi\rangle = E|\psi\rangle$$

i.e. the $G_{\textit{sym}}\text{-symmetrical solutions of }\hat{\mathcal{H}}$ are also solutions of $P_{\!\mathcal{K}}\hat{\mathcal{H}}P_{\!\mathcal{K}}$

• $\hat{\mathcal{H}}$ + symmetrical solutions. Assume

$$P_{\mathcal{K}}\hat{\mathcal{H}}P_{\mathcal{K}}|\psi'
angle=E'|\psi'
angle$$

then in general

$$\hat{\mathcal{H}}|\psi'\rangle = E'|\psi'\rangle + |\psi'_{\perp}\rangle \neq |\psi'\rangle.$$

i.e. the projected hamiltonian can provide more solutions than $\hat{\mathcal{H}}$ itself. $$^{25/36}$$

Meaning of intrinsic symmetries 1/2

WEAK vibration+rotation coupling Bohr's type collective models $(\alpha^{lab} \rightarrow (\alpha, \Omega))$.

where due to weak coupling assumption:

$$[\hat{\mathcal{H}}_{vib}, \hat{\mathcal{H}}_{rot}] = 0,$$
$$G_{ph} \sim G' \subset G_{vib} \text{ and } G_{ph} \sim G'' \subset G_{rot}$$

Meaning of intrinsic symmetries 2/2

Example: let $g_v \in G_{vib}$ such that $g_v \alpha = \alpha'$ the meaning of the transformation can be found:

• transformation to the laboratory frame and recognizing the transformation of the nuclear surface.

$$\alpha \to \alpha^{\prime ab}, \quad \alpha' \to \alpha^{\prime (\prime ab)}$$

• using intrinsic frame reprezentation of the nuclear surface directly:

$$R(\theta',\phi') = R_0 \left(1 + \sum_{\lambda\mu} \alpha^{\star}_{\lambda\mu} Y_{\lambda\mu}(\theta',\phi') \right)$$
$$R(\theta',\phi') = R_0 \left(1 + \sum_{\lambda\mu} (g_{\nu}\alpha)^{\star}_{\lambda\mu} Y_{\lambda\mu}(\theta',\phi') \right)$$



SIMPLE DEFORMED QUADRUPOLE-OCTUPOLE HARMONIC MODEL

Vibrational collective functions 1/2 (J.Phys. G: Nucl. Part. Phys. 37 (2010) 064032) The quadrupole state:

$$|q
angle = \mathcal{T}(\check{lpha}_{20},\check{lpha}_{22})|0
angle,$$

where $|0\rangle$ is the quadrupole-octupole vacuum (the Gauss function) and $\mathcal{T}(\{\check{\alpha}_{lm}\})$ is the shift operator in the deformation space:

$$\mathcal{T}(\{\check{\alpha}_{lm}\})f(\{\alpha_{lm}\})=f(\{\alpha_{lm}-\check{\alpha}_{lm}\})$$

The normalization coefficients after projection ont parity:

$$N_0^{(+)} = \sqrt{\frac{2}{1 + \exp(-\eta_3^2 \xi^2)}}$$
$$N_1^{(-)} = \sqrt{\frac{2}{1 + \exp(-\eta_3^2 \xi^2)(1 - 2\eta_3^2 \xi^2)}}$$

Vibrational collective functions 2/2The tetrahedral states – basis of i.r. of T_d :

Vibrational matrix elements 1/2

Static quadrupole-quadrupole:

$$\begin{split} \langle q | Q_{22} | q \rangle &= \frac{3ZR_0^2}{4\pi} (\check{\alpha}_{22} - \frac{20}{7\sqrt{5\pi}} \check{\alpha}_{20} \check{\alpha}_{22}) \\ \langle q | Q_{20} | q \rangle &= \frac{3ZR_0^2}{4\pi} (\check{\alpha}_{20} + \frac{1}{\sqrt{5\pi}} (\frac{10}{7} \check{\alpha}_{20}^2 - \frac{20}{7} \check{\alpha}_{22} - \frac{2}{3\eta_3^2}) \end{split}$$

Here:

$$\eta_2 = \sqrt{\frac{B_2\omega_2}{\hbar}} = \sqrt{\frac{C_2}{\hbar\omega_2}}$$
$$\eta_3 = \sqrt{\frac{B_3\omega_3}{\hbar}} = \sqrt{\frac{C_3}{\hbar\omega_3}}.$$

Vibrational matrix elements 2/2

Static tetrahedr-tetrahedr:

$$\langle A1|Q_{20}|A1\rangle = -\frac{ZR_0^2}{2\pi\sqrt{5\pi}}\frac{1}{\eta_3^2} \langle T1;1|Q_{20}|T1;1\rangle = -\frac{ZR_0^2}{2\pi\sqrt{5\pi}}\frac{1}{\eta_3^2} \langle T2;1|Q_{20}|T2;1\rangle = \frac{ZR_0^2}{2\pi\sqrt{5\pi}}\frac{1}{\eta_3^2}$$

Dependence on zero-point motion only.

Relation between the quadrupole operator diagonal matrix elements:

$$\langle q|Q_{20}|q
angle = rac{3ZR_0^2}{4\pi} \left(\check{lpha}_{20} + rac{10}{7\sqrt{5\pi}} (\check{lpha}_{20}^2 - 2\check{lpha}_{22}^2)
ight) - |\langle t|Q_{20}|t
angle|$$

Spectrum ¹⁵⁶Dy, Argone 2009



Figure: Bands with symmetries ? (Lee Riedinger)

Harmonic model: results for ¹⁵⁶Dy

ARGONE measurements.

- *A* = 156, *Z* = 66
- qudrupole: $\beta=$ 0.293, $\gamma=$ 1 degree, $\eta_{2}=$ 14

• octupole:
$$\xi = 0.12$$
, $\eta_3 = 8$

- Q20 for quadrupole band = 670 $e^2 fm^4$
- $B(E1; T1 \rightarrow q) \sim 5 \cdot 10^{-9}; B(E2; T1 \rightarrow T1) \sim 5 \cdot 10^{-3}$ $B(E2; T1 \rightarrow T1) \sim 2 \cdot 10^{7} c^{-2}$
- $\frac{B(E2;T1 \to T1)}{B(E1;T1 \to q)} \sim 3 \cdot 10^7 \ fm^2$
- $B(E1; T2 \rightarrow q) \sim 1 \cdot 10^{-5}; B(E2; T2 \rightarrow T2) \sim 5 \cdot 10^{-3}$
- $\frac{B(E2;T2\to T2)}{B(E1;T2\to q)} \sim 9 \cdot 10^3 \ fm^2$

where $\mathsf{BE}\lambda$ in W.u.

Harmonic model: results for ¹⁵⁶Gd

GRENOBLE measurements.

- *A* = 156, *Z* = 64
- qudrupole: $\beta=$ 0.23, $\gamma=$ 10 degree, $\eta_{\rm 2}=$ 12

• octupole:
$$\xi = 0.12$$
, $\eta_3 = 0.515$

- Q20 for quadrupole band = 788 $e^2 fm^4$
- $B(E1; T1 \to q) \sim 7 \cdot 10^{-3}; B(E2; T1 \to T1) \sim 298$

•
$$\frac{B(E2;T1 \to T1)}{B(E1;T1 \to q)} \sim 1 \cdot 10^6 \ fm^2$$

- $B(E1; T2 \rightarrow q) \sim 0.2; B(E2; T2 \rightarrow T2) \sim 298$
- $\frac{B(E2;T2\to T2)}{B(E1;T2\to q)} \sim 3.6 \cdot 10^3 \ fm^2$

where $\mathsf{BE}\lambda$ in W.u.

SUMMARY

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