Molecular Symmetries in Atomic Nuclei

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This presentation is based on the theory methods illustrated in the recent articles contributed by our collaboration:

Spectroscopic criteria for identification of nuclear tetrahedral and octahedral symmetries: Illustration on a rare earth nucleus

PHYSICAL REVIEW C 97, 021302(R) (2018)

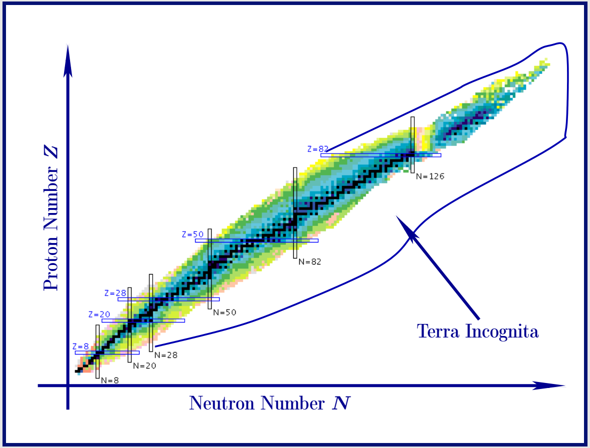
New evidence of interplay between tetrahedral and octahedral symmetries and symmetry breaking: Exotic rotational bands in ^{152}Sm

PHYSICAL REVIEW C 111, 034319 (2025)

Experimental evidence of the molecular H_2O symmetry C_{2v} in the ^{236}U nucleus: Model-independent point-group and combinatorial identification criteria

PHYSICAL REVIEW C 112, 034303 (2025)

The Chart of Nuclides



- Among nearly 3000 systems known experimentally:

→ about 200 nuclei are stable; they are marked in black.

→ more than 80% are strongly deformed, only about 8 'really spherical'

- **Terra Incognita**: Still >6000 nuclei are expected to exist...

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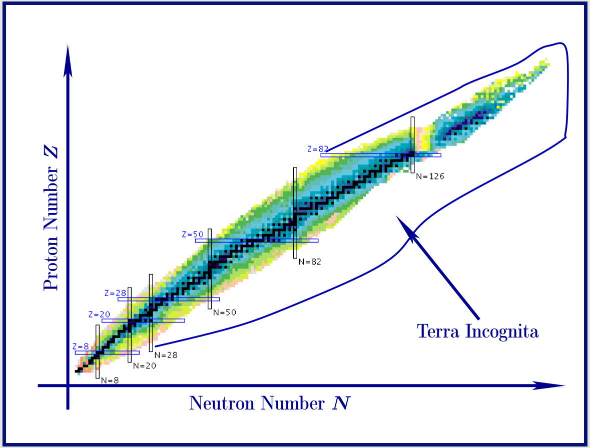

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→ about 200 nuclei are stable; they are marked in black.

→ more than 80% are strongly deformed, only about 8 'really spherical'

- **Terra Incognita**: Still >6000 nuclei are expected to exist...

High chances that they are deformed!

Main Scope of Our Research

- Give the theoretical explanations to the experimental nuclear structure phenomena observed, as well as predicting the still unknown

How do we perform our studies?

- We describe the nuclear interior, i.e. *nuclear structure*, with a simple but very reliable and powerful theory called: **The Nuclear Mean-Field Theory**

- We combine contemporary **mathematical tools** of group theory, inverse problem theory and graph-theory with phenomenological nuclear mean-field theory

- One of the most important strategies: Making sure the theory we use is reliable, offering realistic, experiment comparable results for many nuclei.

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Introductory Remarks and Employed Terminology

Our Definition of the Term: Exotic *(Molecular)* Nuclear Symmetries

- Symmetries which do **not** correspond to prolate, oblate or triaxial quadrupole shapes, neither pear-shape octupole deformations

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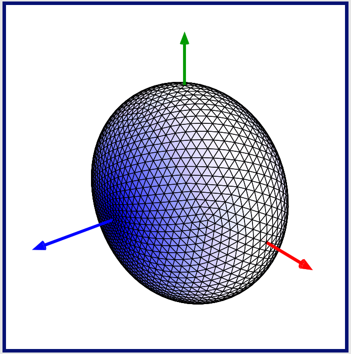
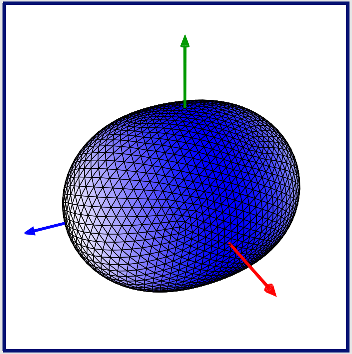
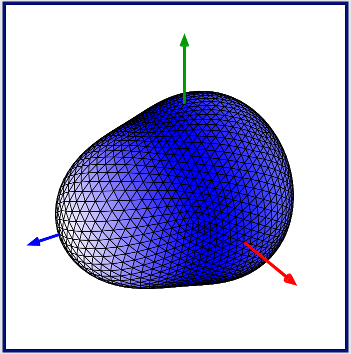
Oblate



Prolate



Pear-shape



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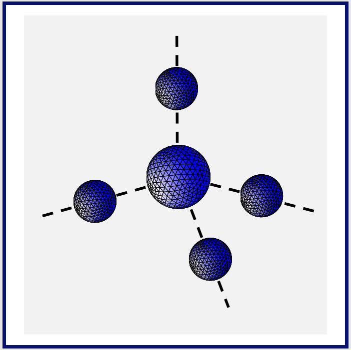
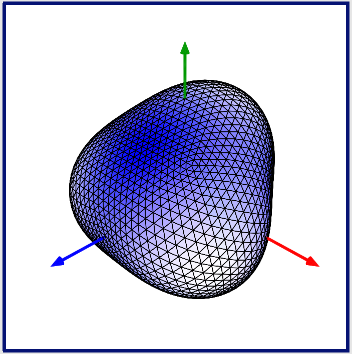
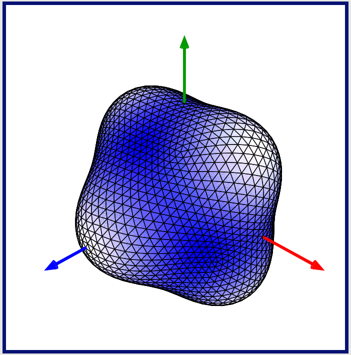
CH_4 Molecule (T_d)



Tetrahedral T_d



Octahedral O_h



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Why Are We Interested in *Molecular Symmetries* in Subatomic Physics ?

• *Observed nearly identical spectra* in totally different objects: ***Molecules*** composed of relatively distant point particles (atoms) and ***Nuclei*** composed of the tightly packed nucleons interacting with the forces among most complex in the universe

• Exotic symmetries generate unprecedented *degeneracies* in both *individual-nucleonic* and *collective-rotation excitations*, new forms of behaviour and unprecedented hindrance factors

Further Consequences for Future Research in This Domain

• New highway towards exotic nuclei: **Nuclear Isomers** living longer than ground-states
• Possible exploration directions in astrophysics: **New magic numbers for nucleosynthesis**

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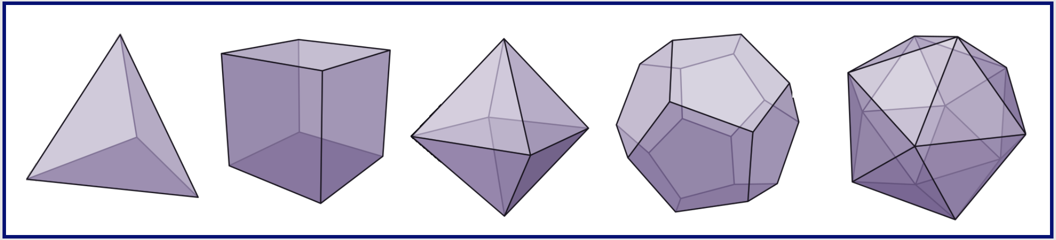
- **Platonic Solids** (Plato, 428-347 bC): Polyhedra whose faces are identical regular convex polygons
- The allowed polygons are: triangles, squares and regular pentagons
- Thus, there are only five Platonic Solids:

Tetrahedron **Cube** **Octahedron** **Dodecahedron** **Icosahedron**



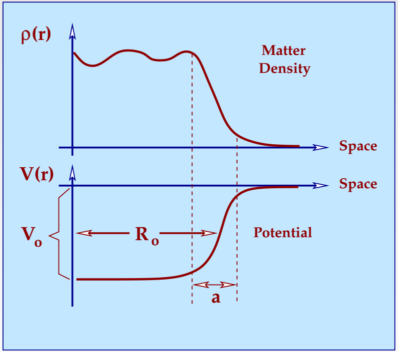
Part 1

Realistic Phenomenological Mean Field Approach

Deformed Universal Woods-Saxon Hamiltonian

Nucleonic Density - vs. - Nuclear Potential

- The short range of the nuclear forces, comparable to the nucleon sizes, imply that the nuclear potential quickly vanishes as soon as the nucleon 'tries to escape' from the nuclear interior [vanishing density]



- A phenomenological [Woods-Saxon] parameterisation of the potential:

$$V(\vec{r}; V_o, r_o, a_o) = \frac{V_o}{1 + \exp[\mathrm{dist}_\Sigma(\vec{r}, R_o)/a_o]}$$

with $R_o = r_o A^{1/3}$

- Each parameter is related to an independent class of experiments:
  - V_o - specific transfer reactions
  - r_o - electron scattering
  - a_o - hadron scattering

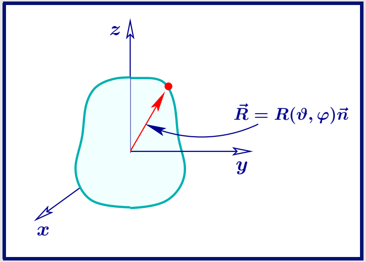
- **$\mathrm{dist}_\Sigma(\vec{r})$** gives the shortest distance between the nuclear surface and a point in space

Description of Nuclear Deformation [or Shapes]

- Given nuclear surface, Σ. It can be expanded in terms of the spherical harmonic basis $\{Y_{\lambda\mu}(\vartheta,\varphi)\}$ (a multipole expansion about the sphere)

$$R(\vartheta,\varphi) = R_o\, c(\{\alpha\}) \left[1 + \sum_{\lambda\mu} \alpha_{\lambda\mu} Y_{\lambda\mu}(\vartheta,\varphi)\right]$$

Given surface Σ



$\vec{n} = \{\cos\varphi \sin\vartheta, \sin\varphi \sin\vartheta, \cos\vartheta\}$

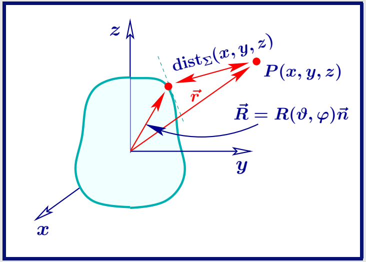
- Parameters $\{\alpha_{\lambda\mu}\}$, are called *deformations*
- The lowest rank deformations:

$\longrightarrow$ $\alpha_{2\mu}$ - quadrupole
$\longrightarrow$ $\alpha_{3\mu}$ - octupole
$\longrightarrow$ $\alpha_{4\mu}$ - hexadecapole

WS Mean-Field is a Functional of $\mathrm{dist}_\Sigma(\vec{r})$

Surface Σ : $R(\vartheta,\varphi) = R_o\, c(\{\alpha\}) \left[1 + \sum_{\lambda\mu} \alpha_{\lambda\mu} Y_{\lambda\mu}(\vartheta,\varphi)\right]$

Given surface $\Sigma \Leftrightarrow \mathrm{dist}_\Sigma(\vec{r})$



$\vec{n} = \{\cos\varphi \sin\vartheta, \sin\varphi\sin\vartheta, \cos\vartheta\}$

- WS Potential [with $R_o = r_o A^{1/3}$]

$$V(\vec{r}; V_o, r_o, a_o) = \frac{V_o}{1 + \exp[\mathrm{dist}_\Sigma(\vec{r}, r_o)/a_o]}$$

- Auxiliary function

$$f(\vartheta,\varphi) \equiv \left[\vec{r} - R(\vartheta,\varphi)\,\vec{n}(\vartheta,\varphi)\right]^2$$

- Distance function

$$\mathrm{dist}_\Sigma(\vec{r}, r) \equiv \min_{\{\vartheta,\varphi\}} f(\vartheta,\varphi)$$

Mean-Field Potential: $\hat{\mathcal{V}}_{\mathrm{m-f}} = \hat{\mathcal{V}}^{\mathrm{WS}}_{\mathrm{cent}} + \hat{\mathcal{V}}^{\mathrm{WS}}_{\mathrm{SO}} + \hat{\mathcal{V}}_{\mathrm{C}}$

Introducing Woods-Saxon Hamiltonian

- We use the phenomenological **Woods-Saxon Hamiltonian** with the **'universal'** parameterisation
  $\Rightarrow$ fixed set of parameters for thousands of nuclei!

- **Central Potential**

$$\mathcal{V}^{\text{WS}}_{\text{cent}} = \frac{V_c}{1 + \exp\left[\text{dist}_\Sigma(\vec{r}; r_c)/a_c\right]}$$

- **Spin-Orbit Potential**

$$\mathcal{V}^{\text{WS}}_{\text{SO}} = \frac{2\hbar\lambda_{so}}{(2mc)^2}\left[(\vec{\nabla}V^{\text{WS}}_{\text{SO}}) \wedge \hat{p}\,\right] \cdot \hat{s}, \;\; \text{with } V^{\text{WS}}_{\text{SO}} = \frac{V_o}{1 + \exp[\text{dist}_\Sigma(\vec{r}, r_{so})/a_{so}]}$$

- **Isospin distinction** ($+ \leftrightarrow$ protons) and ($- \leftrightarrow$ neutrons)

$$V_c = V_o\left[1 \pm \kappa_c \frac{N-Z}{N+Z}\right]; \quad \lambda_{so} = \lambda_o\left[1 \pm \kappa_{so}\frac{N-Z}{N+Z}\right]$$

- **This potential depends *only* on two sets of 6 parameters $\leftrightarrow$ Mass Table**

$$\boxed{\{V_o, \kappa_c, r_c^{\pi,\nu}, a_c^{\pi,\nu}; \lambda_o, \kappa_{so}, r_{so}^{\pi,\nu}, a_{so}^{\pi,\nu}\}}$$

Deformed Mean-Field Hamiltonian

Mean-Field Potential: $\hat{\mathcal{V}}_{\mathrm{m-f}} = \hat{\mathcal{V}}^{\mathrm{WS}}_{\mathrm{cent}} + \hat{\mathcal{V}}^{\mathrm{WS}}_{\mathrm{SO}} + \hat{\mathcal{V}}_{\mathrm{C}}$

↓

Hamiltonian: $\hat{\mathcal{H}}_{\mathrm{m-f}} = \hat{\mathcal{T}} + \hat{\mathcal{V}}_{\mathrm{m-f}}$

↓

Schrödinger Equation: $\hat{\mathcal{H}}_{\mathrm{m-f}}\,\psi_\nu = e_\nu\,\psi_\nu$

↓

SPE as functions of $\alpha_{\lambda\mu}$: $e_\nu = e_\nu(\alpha_{\lambda\mu})$

↓

Total Energy as function of $\alpha_{\lambda\mu}$: $E = E(\alpha_{\lambda\mu})$

Part 2

Selected Molecular Symmetries in Atomic Nuclei

Example: So-called High-Rank*) Symmetries

Tetrahedral T_d and Octahedral O_h

*) They present 4D irreducible spinor representations $\leftrightarrow$ 4-fold nucleonic degeneracies

Tetrahedral Symmetry: Spherical-Harmonic Basis

- **Reminder –** Nuclear surface Σ : $R(\vartheta,\varphi) = R_o\, c(\{\alpha\})\,\left[1 + \sum_{\lambda\mu} \alpha_{\lambda\mu} Y_{\lambda\mu}(\vartheta,\varphi)\right]$

- Only *special combinations* of only odd-order spherical harmonics may form a basis for surfaces with tetrahedral symmetry:

Three Lowest Order Solutions: **Rank $\leftrightarrow$ Multipolarity λ**

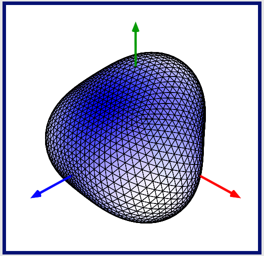
$\lambda = 3$: $t_1 \equiv \alpha_{3,\pm2}$

$\lambda = 5$: **no solution possible**

$\lambda = 7$: $t_2 \equiv \alpha_{7,\pm2}$ and $\alpha_{7,\pm6} = -\sqrt{\frac{11}{13}}\cdot\alpha_{7,\pm2}$

$\lambda = 9$: $t_3 \equiv \alpha_{9,\pm2}$ and $\alpha_{9,\pm6} = +\sqrt{\frac{28}{198}}\cdot\alpha_{9,\pm2}$

$t_1 = 0.2$



- Problem presented in detail in:

J. Dudek, J. Dobaczewski, N. Dubray, A. Góźdź, V. Pangon and N. Schunck,

OBSERVATION:

Tetrahedral symmetry group, T_d, is a sub-group of the octahedral one, O_h

Octahedral Symmetry: Spherical-Harmonic Basis

- **Reminder –** Nuclear surface Σ: $R(\vartheta,\varphi) = R_o\, c(\{\alpha\})\,[1 + \sum_{\lambda\mu} \alpha_{\lambda\mu} Y_{\lambda\mu}(\vartheta,\varphi)]$

- Only *special combinations* of only even-order $\lambda \geq 4$ spherical harmonics may form a basis for surfaces with octahedral symmetry

Three Lowest Order Solutions: Rank ↔ Multipolarity λ

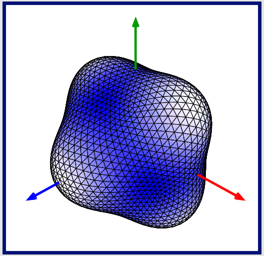
$\lambda = 4:\quad o_1 \equiv \quad \alpha_{40}$ and $\alpha_{4,\pm4} = -\sqrt{\frac{5}{14}} \cdot \alpha_{40}$

$\lambda = 6:\quad o_2 \equiv \quad \alpha_{60}$ and $\alpha_{6,\pm4} = -\sqrt{\frac{7}{2}} \cdot \alpha_{60}$

$\lambda = 8:\quad o_3 \equiv \quad \alpha_{80}$ and $\alpha_{8,\pm4} = \sqrt{\frac{28}{198}} \cdot \alpha_{80}$

and $\alpha_{8,\pm8} = \sqrt{\frac{65}{198}} \cdot \alpha_{80}$

$o_1 = 0.2$



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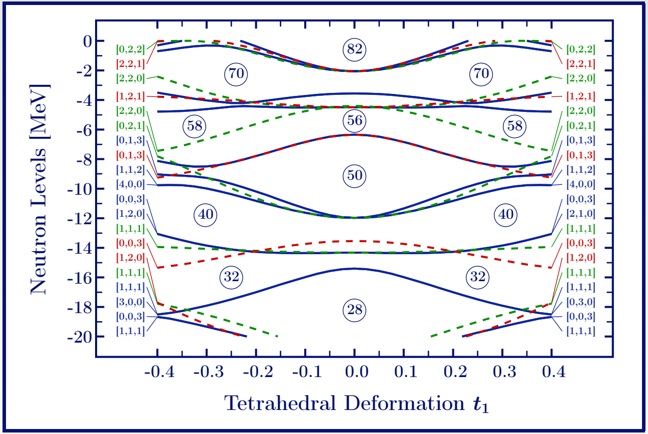
Mean Field Theory: Tetrahedral Gaps – Neutrons

Double group T_d^D has two 2-dimensional and one 4-dimensional irreducible representations (irreps.)

→ Three distinct families of nucleon levels ←

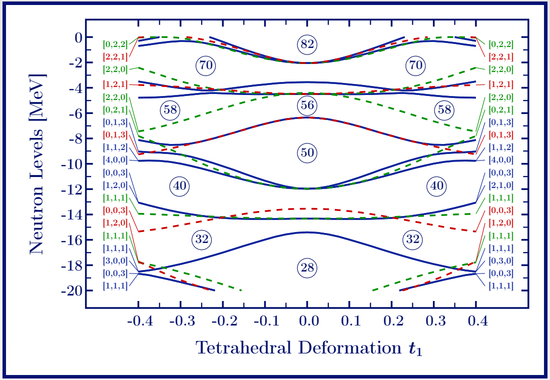


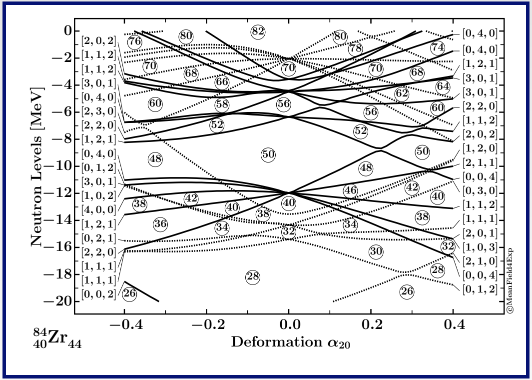
Full lines ↔ one 4D-irreps
Dashed lines ↔ two 2D-irreps

Notice tetrahedral gaps at N = 32, 40, 56, 58 and 70

Mean Field Theory: Tetrahedral vs Quadrupole Gaps

[Reminder: $t_1 = \alpha_{32}$]





- Bigger gaps are open for $t_1 \neq 0.00$ thanks to the unprecedented degeneracies of the T_d^D group, as compared to $\alpha_{20} \neq 0.00$
- Observation: t_1-gaps at $N = 32$, 40, 58 and 70 are very small for α_{20}

Symmetries Are the Factors Determining Stability*) of Atomic Nuclei

Nuclear mean field theory and group representation theory which are used in this research belong to the most powerful tools of nuclear structure theory arsenal

*) ... *by imposing hindrance mechanisms*

Multipole Moments $Q_{\lambda\mu}$ – Theory POV

- Reminder: Surface Σ : $R(\vartheta,\varphi) = R_o\, c(\alpha)\left[1 + \sum_{\lambda\mu} \alpha_{\lambda\mu} Y_{\lambda\mu}(\vartheta,\varphi)\right]$

- Given uniform density $\rho_\Sigma(\vec{r}\,)$ defined using the surface Σ

$$\rho_\Sigma(\vec{r}\,) = \begin{cases} \rho_0 : & \vec{r} \in \Sigma \\ 0 : & \vec{r} \notin \Sigma \end{cases}$$

- **Multipole moments** are defined as

$$Q_{\lambda\mu} = \int \rho_\Sigma(\vec{r}\,)\, r^\lambda\, Y_{\lambda\mu}\, d\vec{r}$$

- We can calculate the **quadrupole moments Q_{20}** as functions of **quadrupole α_{20}**

$$Q_{20} = \rho_0 R_0^5 c^5(\alpha)\left(\alpha_{20} + \frac{2\sqrt{5}}{7\sqrt{\pi}}\alpha_{20}^2\right) \rightarrow Q_0 = \frac{1}{e}\sqrt{\frac{16\pi}{5}}\, Q_{20}$$

- As well as the **Electromagnetic Transition Strength:** $B(E2) = \frac{5}{16\pi}\, Q_0^2$

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Quadrupole Rotational Bands – Experimental POV

- Quadrupole deformed nuclei: (strong) electromagnetic transitions $B(E2) \to Q_{20} \to \alpha_{20}$
- **Rotational Bands:** deformed nuclei present energy spectra where $\boldsymbol{E_{\mathrm{rot}} = \frac{\hbar^2}{2\mathcal{J}} I(I+1)}$

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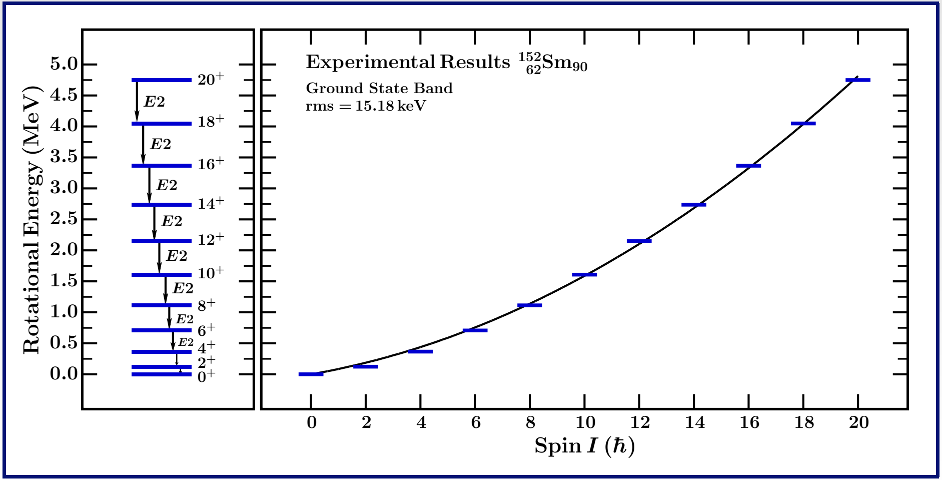

Quadrupole Moments generated by Octupole Shapes

- Reminder I: Surface Σ : $R(\vartheta,\varphi) = R_o\, c(\alpha)\left[1 + \sum_{\lambda\mu} \alpha_{\lambda\mu} Y_{\lambda\mu}(\vartheta,\varphi)\right]$
- Reminder II: express the multipole moments as usual by

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$$\begin{aligned}
\alpha_{30}: \quad Q_{20} &= 4/(3\sqrt{5\pi}) \cdot \rho_0 R_0^5 c^5(\alpha) \cdot \alpha_{30}^2 \\
\alpha_{31}: \quad Q_{20} &= 2/(\sqrt{5\pi}) \cdot \rho_0 R_0^5 c^5(\alpha) \cdot |\alpha_{31}|^2 \\
\alpha_{32}: \quad Q_{20} &= 0 \quad \leftarrow \quad \text{identically vanishing} \\
\alpha_{33}: \quad Q_{20} &= -2\sqrt{5}/(3\sqrt{\pi}) \cdot \rho_0 R_0^5 c^5(\alpha) \cdot |\alpha_{33}|^2
\end{aligned}$$

$$Q_{20}(\alpha_{3\mu}) = \int \rho_\Sigma\, r^2 Y_{20}\, d\vec{r} \Longrightarrow Q_{20}(\alpha_{32}) = 0 \Longrightarrow B(E2) = 0$$

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\alpha_{31}: \quad Q_{20} &= 2/(\sqrt{5\pi})\cdot \rho_0 R_0^5 c^5(\alpha)\cdot |\alpha_{31}|^2 \\
\alpha_{32}: \quad Q_{20} &= 0 \quad \leftarrow \quad \text{identically vanishing} \\
\alpha_{33}: \quad Q_{20} &= -2\sqrt{5}/(3\sqrt{\pi})\cdot \rho_0 R_0^5 c^5(\alpha)\cdot |\alpha_{33}|^2
\end{aligned}$$

$$\boldsymbol{Q_{20}(\alpha_{3\mu}) = \int \rho_\Sigma\, r^2 Y_{20}\, d\vec{r} \implies Q_{20}(\alpha_{32}) = 0 \implies B(E2) = 0}$$

The Notion of Isomeric Bands

Similarly one demonstrates that tetrahedral shapes induce $B(E1) = 0$

One shows that the analogous rules apply for O_h symmetry

Once those symmetries are present one may expect the presence of numerous isomers since $B(E2)$ and $B(E1)$ at the exact T_d and/or O_h symmetry limits – vanish!

As the result, one expects series of long living (isomeric) states with unprecedented parabolic energy-spin relation

Isomeric Bands: $E_I \propto I(I+1)$

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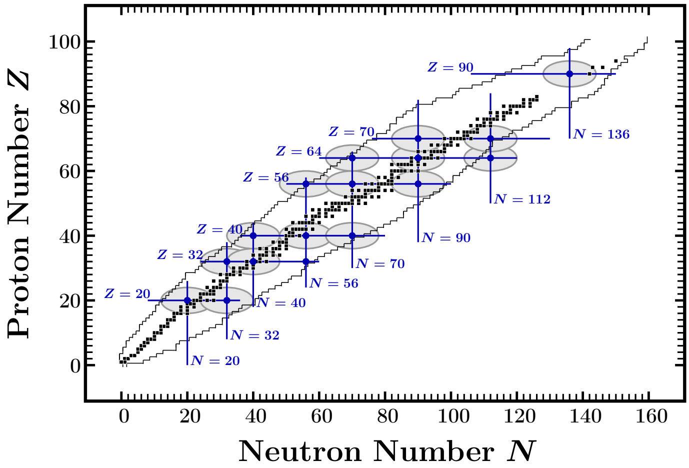
Tetrahedral Symmetry Dominates Mass Table



Tetrahedral doubly-magic nuclei > **Spherical** doubly-magic nuclei

At the exact symmetry limit, T_d nuclei emit neither $E2$ nor $E1$ transitions → ISOMERS

Rotating High-Rank Symmetric Nuclei Seen Through Group-Representation Theory

[Symmetry Properties of Quantum Rotors]

Group and Point Group Theories – In Short

• Consider a point-group symmetry characterised by group G. The SO(3)-group representation of rotor states, $D^{(I\pi)}$, with given I^π, can be decomposed in terms of irreducible representations D_i of the concerned point-group G:

$$D^{(I\pi)} = \sum_{i=1}^{M} a_i^{(I\pi)} D_i,$$

where the so-called multiplicity coefficients, $a_i^{(I\pi)}$, satisfy *)

$$a_i^{(I\pi)} = \frac{1}{N_G} \sum_{R \in G} \chi_{(I\pi)}(R)\chi_i(R) = \frac{1}{N_G} \sum_{\alpha=1}^{M} n_\alpha \chi_{(I\pi)}(g_\alpha)\chi_i(g_\alpha)$$

→ $\chi_{(I\pi)}$ - characters of the reducible representation $D^{(I\pi)}$ of the SO(3)-group;
→ χ_i - characters of the irreducible representation D_i of a point group;
→ N_G - order of the group G;
→ g - group element;
→ n_α - the number of elements in the class α, whose representative element is g_α.

---

*) M. Hamermesh, *Group Theory and Its Application to Physical Problems*, Addison-Wesley Publishing Company, Inc., 1962

*) Tagami, Shimizu, Dudek, Phys. Rev. C**87**, 054306 (2013), DOI: `https://doi.org/10.1103/PhysRevC.87.054306`

Tetrahedral T_d-Group – In Short

- Tetrahedral group has 5 irreducible representations, and 5 classes
- The representative elements $\{g\}$ are: $E, C_2\,(= S_4^2), C_3, \sigma_d, S_4$
- The characters of irreducible representations of T_d are listed below

T_d	E	$C_3(8)$	$C_2(3)$	$\sigma_d(2)$	$S_4(6)$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
E	2	−1	2	0	0
F_1	3	0	−1	−1	1
F_2	3	0	−1	1	−1

- The characters $\chi_{(I\pi)}(g_\alpha)$ for the SO(3) representations are as follows:

$$\chi_{(I\pi)}(E) = 2I+1, \quad \chi_{(I\pi)}(C_n) = \sum_{K=-I}^{I} e^{\frac{2\pi K}{n} i}, \quad \chi_{(I\pi)}(\sigma_d) = \pi \times \chi_{(I\pi)}(C_2), \quad \chi_{(I\pi)}(S_4) = \pi \times \chi_{(I\pi)}(C_4)$$

- Multiplicity coefficients can be calculated in an elementary fashion

$$a_i^{(I\pi)} = \frac{1}{N_G}\sum_{g\in G}\chi_{(I\pi)}(g)\chi_i(g) = \frac{1}{N_G}\sum_{\alpha=1}^{M} n_\alpha \chi_{(I\pi)}(g_\alpha)\chi_i(g_\alpha);$$

Attention: Resulting Prediction of the Structure of T_d-Bands

- The number of states $a_i^{(I\pi)}$ within five irreducible representations. If $a_i^{(I\pi)} = 0 \rightarrow$ states not allowed; $a_i^{(I\pi)} = 2 \rightarrow$ doubly degenerate, etc.

I^+	0^+	1^+	2^+	3^+	4^+	5^+	6^+	7^+	8^+	9^+	10^+
A_1	1	0	0	0	1	0	1	0	1	1	1
A_2	0	0	0	1	0	0	1	1	0	1	1
E	0	0	1	0	1	1	1	1	2	1	2
F_1	0	1	0	1	1	2	1	2	2	3	2
F_2	0	0	1	1	1	1	2	2	2	2	3
I^-	0^-	1^-	2^-	3^-	4^-	5^-	6^-	7^-	8^-	9^-	10^-
A_1	0	0	0	1	0	0	1	1	0	1	1
A_2	1	0	0	0	1	0	1	0	1	1	1
E	0	0	1	0	1	1	1	1	2	1	2
F_1	0	0	1	1	1	1	2	2	2	2	3
F_2	0	1	0	1	1	2	1	2	2	3	2

- In this way we find the spin-parity sequence for A_1-representation

$$\mathbf{A_1: \quad 0^+, 3^-, 4^+, 6^+, 6^-, 7^-, 8^+, 9^+, 9^-, 10^+, 10^-, 11^-, 2\times 12^+, 12^-, \cdots}$$

- This is the group-theory prediction of the spin-parity structure of the tetrahedral g.s.b.

Tetrahedral Bands Are Not Like the Others!

One can demonstrate, using the methods of
the point-group representation theory
that rotational bands based on 0^+ "T_d ground-state" have the structure:

$$\mathbf{A_1:}\quad 0^+, 3^-, 4^+, 6^+, 6^-, 7^-, 8^+, 9^+, 9^-, 10^+, 10^-, 11^-, 2\times 12^+, 12^-, \cdots$$

and NOT

$$I^\pi:\quad 0^+, 2^+, 4^+, 6^+, 8^+, 10^+, 12^+, \cdots$$

Similarly there are **no analogies** of the "octupole bands"

$$I^\pi:\quad 3^-, 5^-, 7^-, 9^-, 11^-, 13^-, 15^-, \cdots$$

Quantum Rotors: Tetrahedral vs. Octahedral

- The **tetrahedral $\mathbf{T_d}$** symmetry group has 5 irreducible representations
- The ground-state $I^\pi = 0^+$ belongs to A_1 representation given by:

$$\mathrm{A}_1: \quad \underbrace{0^+, 3^-, 4^+, \underbrace{(6^+, 6^-)}_{\text{doublet}}, 7^-, 8^+, \underbrace{(9^+, 9^-)}_{\text{doublet}}, \underbrace{(10^+, 10^-)}_{\text{doublet}}, 11^-, \underbrace{2\times 12^+, 12^-}_{\text{triplet}}, \cdots}_{\text{Forming a common parabola}}$$

- There are no states with spins $I = 1, 2$ and 5. We have parity doublets: $I = 6, 9, 10\ \ldots$, at energies: $E_{6^-} \approx E_{6^+}$, $E_{9^-} \approx E_{9^+}$, etc.

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- There are no states with spins $I = 1, 2$ and 5. We have parity doublets: $I = 6, 9, 10 \ldots$, at energies: $E_{6^-} \approx E_{6^+}$, $E_{9^-} \approx E_{9^+}$, etc.
- One shows the analogue structures for the **octahedral $\mathbf{O_h}$** symmetry

$$\underbrace{A_{1g}:\; 0^+, 4^+, 6^+, 8^+, 9^+, 10^+,\; \ldots,\; I^\pi = I^+}_{\textbf{Forming a common parabola}}$$

$$\underbrace{A_{2u}:\; 3^-, 6^-, 7^-, 9^-, 10^-, 11^-, \ldots,\; I^\pi = I^-}_{\textbf{Forming a common parabola}}$$

Experimental Data Selection for T_d

Criteria for the experimental data search

- Central condition followed: Nuclear states with exact high-rank symmetries produce neither dipole, nor quadrupole moments
- Such states neither emit any collective/strong $E1/E2$ transitions nor can be fed by such transitions $\longrightarrow$ focus on the population by nuclear processes
- Therefore we decided to focus first of all on the nuclei which can be populated with a big number of nuclear reactions since we may expect that - in such nuclei - the states sought exist in the literature
- We had verified that the nucleus ^{152}Sm can be produced by about 25 nuclear reactions, whereas surrounding nuclei can be produced typically with about a dozen, usually much fewer reactions only
- Energy-wise – tetrahedral bands form regular "parabolic" or "rotor-like" sequences

$$E_I \propto AI^2 + BI + C$$

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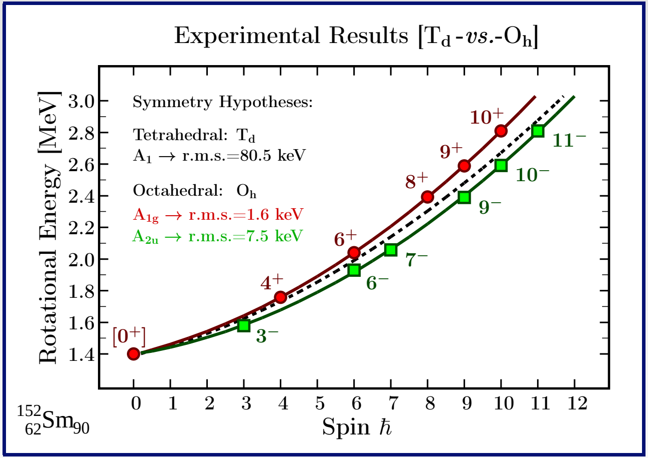
PHYSICAL REVIEW C VOLUME 97, 021302(R) FEBRUARY 2018

Spectroscopic criteria for identification of nuclear tetrahedral and octahedral symmetries: Illustration on a rare earth nucleus

J. Dudek, D. Curien, I. Dedes, K. Mazurek, S. Tagami, Y. R. Shimizu and T. Bhattacharjee

We formulate criteria for identification of the nuclear tetrahedral and octahedral symmetries and illustrate for the first time their possible realization in a rare earth nucleus ^{152}Sm. We use realistic nuclear mean-field theory calculations with the phenomenological macroscopic-microscopic method, the Gogny-Hartree-Fock-Bogoliubov approach, and general point-group theory considerations to guide the experimental identification method as illustrated on published experimental data. Following group theory the examined symmetries imply the existence of exotic rotational bands on whose properties the spectroscopic identification criteria are based. These bands may contain simultaneously states of even and odd spins, of both parities and parity doublets at well-defined spins. In the exact-symmetry limit those bands involve no E2 transitions. We show that coexistence of tetrahedral and octahedral deformations is essential when calculating the corresponding energy minima and surrounding barriers, and that it has a characteristic impact on the rotational bands. The symmetries in question imply the existence of long-lived shape isomers and, possibly, new waiting point nuclei-impacting the nucleosynthesis processes in astrophysics – and an existence of 16-fold degenerate particle-hole excitations.

Perfect Parabolas Represent Experimental Results

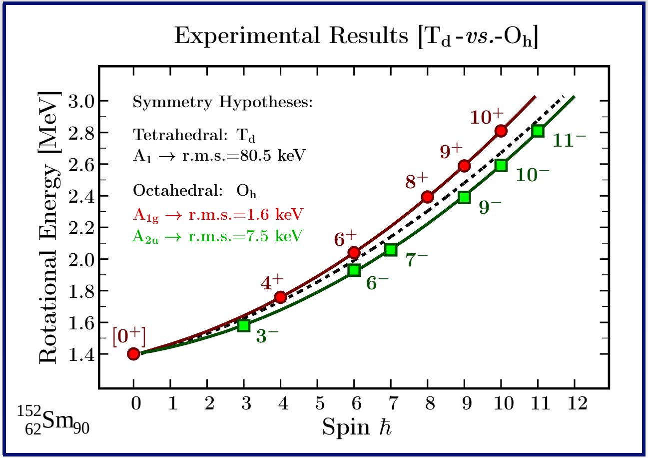


- Parabolic looking sequences are interpreted as **coexistence of tetrahedral and octahedral symmetries.**

Curves represent the parabolic fit and are *not* meant to guide the eye.

This is the first evidence of T_d(dashed) and O_h based on the experimental data

Perfect Parabolas Represent Experimental Results



From the article: **Spectroscopic criteria for identification of nuclear tetrahedral and octahedral symmetries: Illustration on a rare earth nucleus**

J. Dudek et al., PHYSICAL REVIEW C 97, 021302(R) (2018)

[DOI: https://doi.org/10.1103/PhysRevC.97.021302]

World-First Announcement of the Discovery – Part II

PHYSICAL REVIEW C VOLUME 111, 034319 MARCH 2025

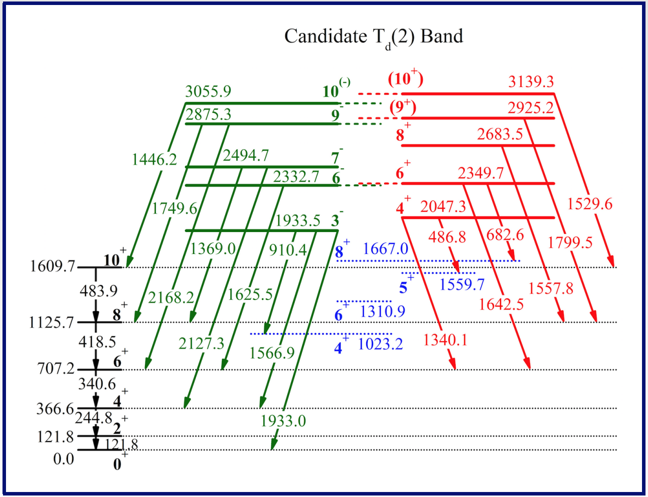
New evidence of interplay between tetrahedral and octahedral symmetries and symmetry breaking: Exotic rotational bands in ^{152}Sm

S. Basak, D. Kumar, T. Bhattacharjee, I. Dedes, J. Dudek, A. Pal, S. S. Alam, A. Saha, A. K. Sikdar, et al.

We report on experimental evidence for a new, second tetrahedral band in $^{152}_{62}$Sm$_{90}$. It was populated via fusion evaporation reaction ^{150}Nd$(\alpha, 2n)^{152}$Sm, employing a 26 MeV beam of α particles from the K-130 cyclotron at the Variable Energy Cyclotron Centre, Kolkata, India. The newly observed possible mixed parity sequence with absence of $E2$ and strong indication of $E3$ transitions is consistent with the spectroscopic criteria for a tetrahedral-symmetry rotational band that could be constructed from the allowed spin-parity assignments. This structure differs from the structure of the band previously found in the same nucleus, the new one manifesting tetrahedral symmetry not accompanied by the octahedral one. Our new experimental results are interpreted in terms of group representation theory and the collective nuclear-motion theory of Bohr. We propose to generalize the notion of the tetrahedral vibrational bands and believe that our new experimental results support a number of theory predictions related to nuclear tetrahedral symmetry published earlier and bring a new light into the issue of spontaneous symmetry breaking in heavy nuclei.

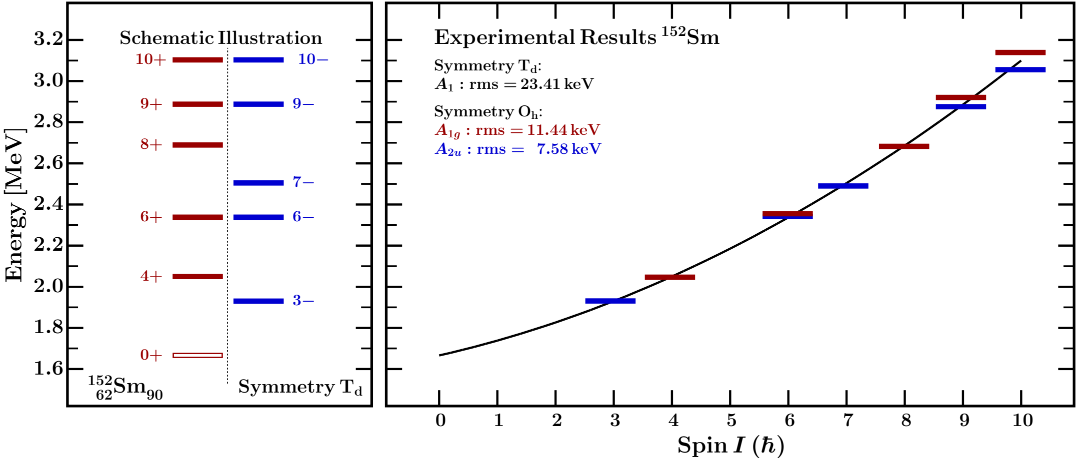
New Tetrahedral/Octahedral Rotational Band Evidence in ^{152}Sm

- Newly measured rotational band in ^{152}Sm; the energy levels satisfy the T_d spin-parity sequence



- Reminder $\Longrightarrow$ A_1: 0^+, 3^-, 4^+, 6^+, 6^-, 7^-, 8^+, 9^+, 9^-, 10^+, 10^-, 11^-, $2 \times 12^+$, 12^-, $\cdots$

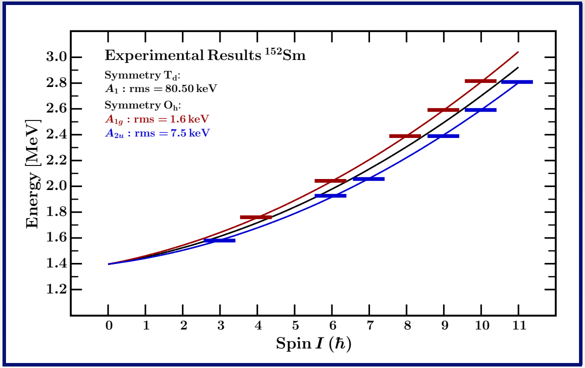
New Tetrahedral Rotational Band Evidence in ^{152}Sm



- **The R.M.S. of the ground-state band is 15.18 keV – same order of magnitude as for T_d (1)**

Comparing the two T_d Rotational Bands in ^{152}Sm

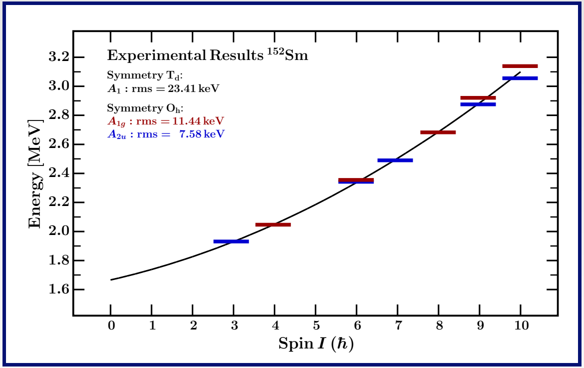
PHYSICAL REVIEW C **97**, 021302(R) (2018)



T_d(1): Significant splitting of the two parity branches, manifesting the breaking of T_d symmetry

The Oh symmetry spontaneously breaks Td symmetry

PHYSICAL REVIEW C **111**, 034319 (2025)



T_d(2): Near degeneracy of two parity branches – signifies nearly exact symmetry conditions

Qualitative Discussion of Symmetry Breaking: Example of T_d

- Exact symmetry present ↔ the positive and negative parity T_d "parabolas" practically coincide

- Breaking degeneracies between two parity branches ↔ manifests tetrahedral symmetry breaking

- Physicist's question: What are the possible ways of symmetry breaking? Where do parabolas go?

- Suppose tetrahedral symmetry is replaced by octahedral one → positive and negative parity branches "receive a freedom" to displace arbitrarily in the vertical space ↔ both bands get arbitrarily distant

- But this is NOT what we observe: The average position of the two branches remains in the "old" tetrahedral position ↔ INTERPRETATION: not removing the symmetry but rather gradual breaking

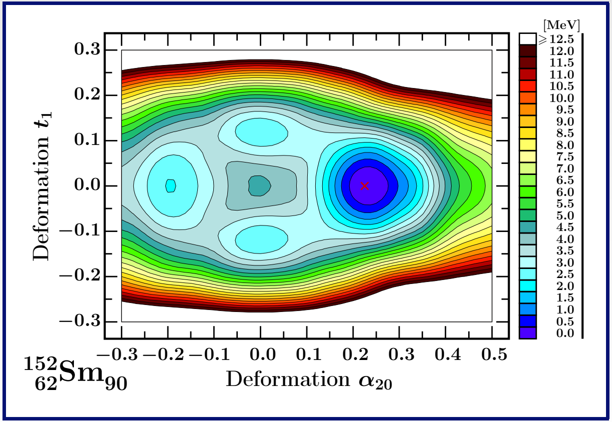
- Attention: Both parity sequences resemble structure in the octahedral case ↔ INTERPRETATION: Not just any symmetry breaking → TETRAHEDRAL broken by OCTAHEDRAL one.

- Question: Is it a "spontaneous symmetry breaking"? Since we do not know of any theory reasons for this particular behaviour → It is often referred to in the literature as s p o n t a n e o u s breaking

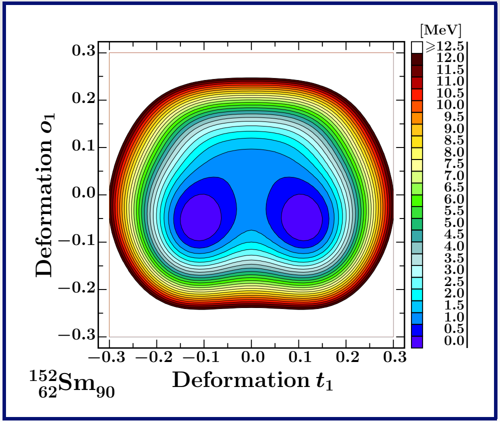
^{152}Sm: Coexistence or Competition of T_d and O_h Symmetries

Potential Energy Surfaces projected on

(α_{20},t_1): quadrupole g.s.



(t_1,o_1): coexistence of both shapes



Collective Schrödinger Equation

• Our collaboration has developed new concepts of adiabaticity within collective model of Bohr and related approach to collective inertia tensor

PHYSICAL REVIEW C 99, 041303(R) (2019)

D. Rouvel and J. Dudek

• Using the newly re-formulated concept of adiabaticity and perturbation theory a new method of calculating collective inertia tensor $B_{\alpha_{\lambda\mu},\alpha_{\lambda'\mu'}}(\alpha)$ is obtained → new approach based on Bohr theory

• The new expression is free from destructive divergencies contained in all the preceding formulations of this theory based on perturbation approach ← Particularly important new result $(q^m \leftrightarrow \alpha_{\lambda\mu})$

$$
\begin{aligned}
B_{nm}(q;t) &= 2\hbar^2 \sum_{j=1}^{N} \langle\phi_{\mathrm{mb};j}(x;q)|\frac{\partial}{\partial q^n}|\phi_{\mathrm{mb};0}(x;q)\rangle \times \langle\phi_{\mathrm{mb};j}(x;q)|\frac{\partial}{\partial q^m}|\phi_{\mathrm{mb};0}(x;q)\rangle^* \\
&\times \frac{\mathcal{N}_{0j}(q;\tau)}{E_{\mathrm{mb};j}(q) - E_{\mathrm{mb};0}(q)}
\end{aligned}
$$

← **This factor gives 1 at the crossings – not ∞**

• *Nota bene:* Collective excitations in ^{208}Pb are well reproduced without parameter adjustments

Collective Schrödinger Equation

- It follows that collective Hamiltonian takes the form:

$$\hat{H}_{\text{coll}} = -\frac{\hbar^2}{2}\Delta + V(\alpha) \;\leftrightarrow\; \Delta \overset{df.}{=} \sum_{m,n=1}^{d} \frac{1}{\sqrt{|B|}} \frac{\partial}{\partial q^n}\left(\sqrt{|B|}B^{nm}\frac{\partial}{\partial q^m}\right); \quad (q^m \leftrightarrow \alpha_{\lambda,\mu})$$

where $|B|$- determinant of the mass tensor, with the resulting collective Schrödinger equation

$$\boxed{\hat{H}_{\text{coll}}\Psi_{\text{coll}} = E_{\text{coll}}\Psi_{\text{coll}}}$$

- All details, illustrations, comparisons with experiment, together with references can be found in:

A New Approach to Adiabaticity Concepts in Collective Nuclear Motion: Impact for the Collective-Inertia Tensor and Comparisons with Experiment

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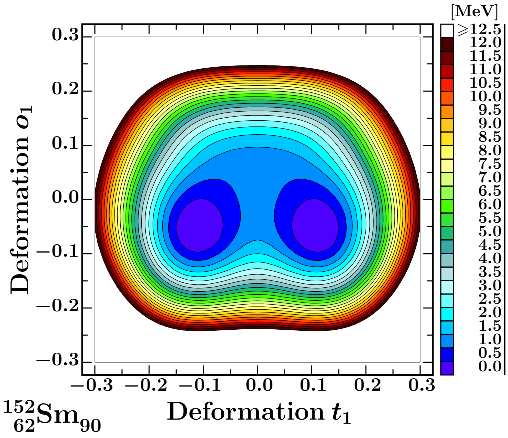
PHYSICAL REVIEW C 99, 041303(R) (2019)

D. Rouvel and J. Dudek

^{152}Sm: Coexistence or Competition of T_d and O_h Symmetries

- Potential Energy Surface projected on (t_1, o_1) showing the coexistence of both shapes



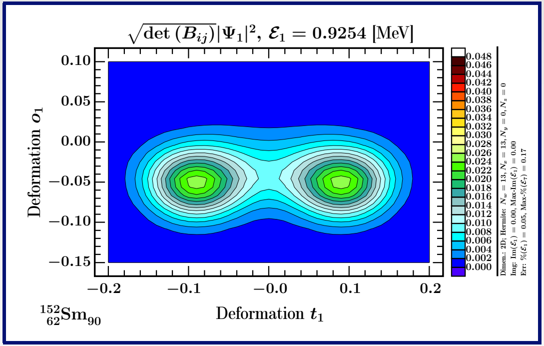
- Solving the Collective Schrödinger Equation we may calculate most probable deformations ↔ and learn which one dominates

$$\langle q_n^2 \rangle = \int \Psi^*(q) q_n^2 \Psi(q) \sqrt{\det(B)}\, dV$$

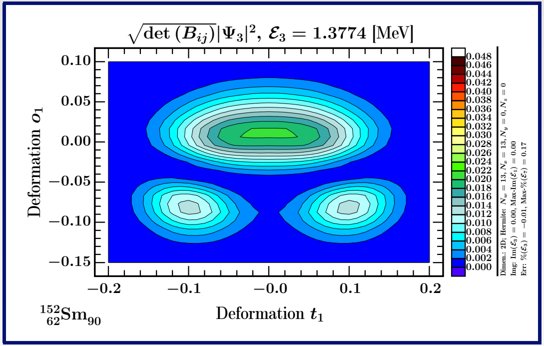
with $n = 1, 2$ and $(q_1, q_2) = (t_1 - ?,\ o_1 - ?)$

We Already Know the Experimental Answer: Breaking of T_d by O_h

Probability Density Distributions: Tetrahedral Shapes Dominate No Matter What

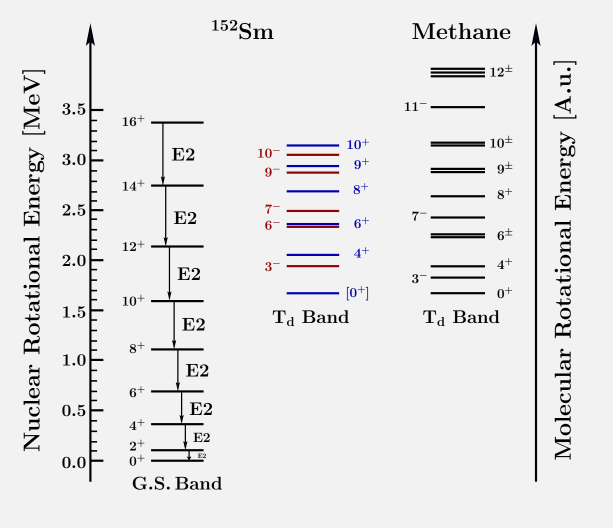


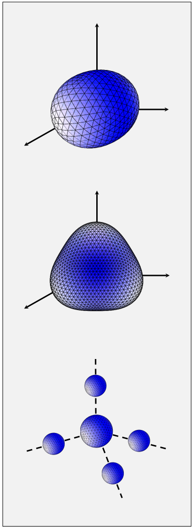
- The lowest energy solution showing most probable distribution at $\sqrt{\langle t_1^2\rangle} = \pm 0.084$ and $\sqrt{\langle o_1^2\rangle} = -0.041$
  $\Rightarrow$ Identified as $T_d(1)$



- The second excited state strongly tetrahedral shaped $\sqrt{\langle t_1^2\rangle} = \pm 0.069$, centred at $\sqrt{\langle o_1^2\rangle} = -0.010$
  $\Rightarrow$ Identified as $T_d(2)$

^{152}Sm: Nuclear vs Molecular Symmetry





Hunt for Molecular Symmetries Throughout the Nuclear Chart

World First Experimental Evidence of C_{2v} in $^{236}U^{*)}$

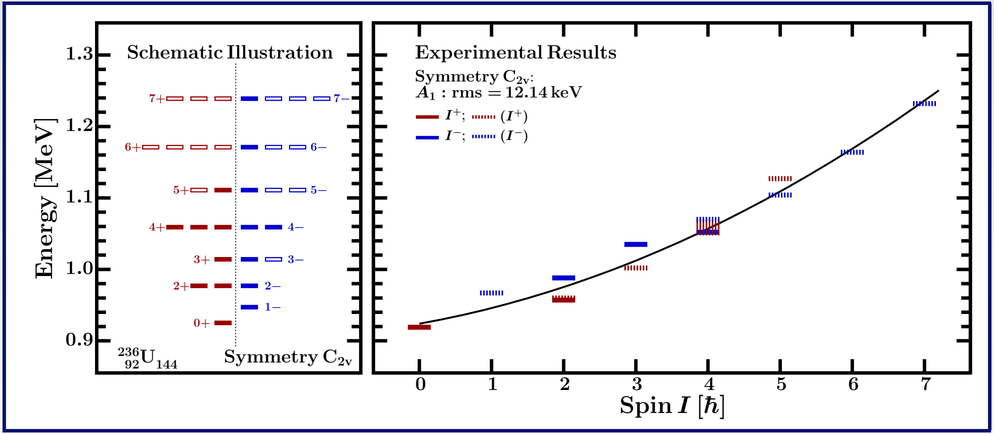
I. Dedes, J. Dudek, A. Baran *et al.*, Phys. Rev. C 112, 034303 (2025)

After a series of publications:

- J. Yang, J .Dudek, I. Dedes *et al.*, Phys. Rev. C **105**, 034348 (2022)
- J. Yang, J .Dudek, I. Dedes *et al.*, Phys. Rev. C **106**, 054314 (2022)
- J. Yang, J .Dudek, I. Dedes *et al.*, Phys. Rev. C **107**, 054304 (2023)

Experimental Identification - Recent Results : ^{236}U

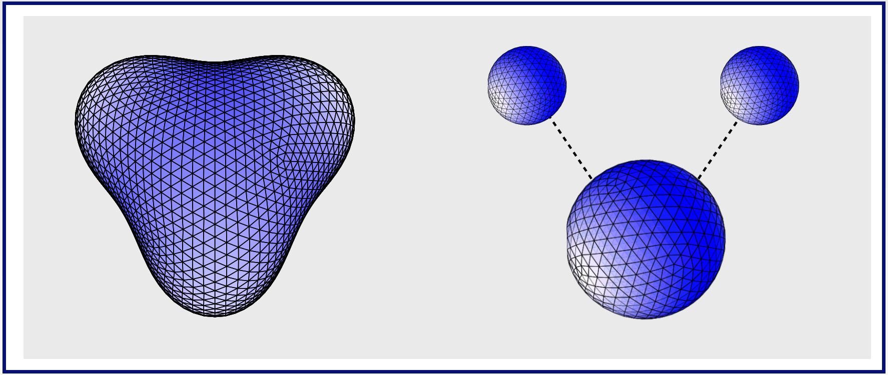
- **Rotational band structure of a nucleus according to a C_{2v}-symmetric configuration**



$$C_{2v} \rightarrow A_1 : 0^+, 1^-, \underbrace{2\times 2^+, 2^-}_{\text{triplet } I=2}, \underbrace{3^+, 2\times 3^-}_{\text{triplet } I=3}, \underbrace{3\times 4^+, 2\times 4^-}_{\text{quintuplet } I=4}, \underbrace{2\times 5^+, 3\times 5^-}_{\text{quintuplet } I=5}, \underbrace{4\times 6^+, 3\times 6^-}_{\text{septuplet } I=6}, \ldots$$

Exotic Symmetries: Nuclei vs. Molecules

- **Rotational band structure of a nucleus according to a C_{2v}-symmetric configuration**
- **Nuclei vs. Molecules: C_{2v} is the symmetry of the water molecule**



^{236}U Nucleus **H_2O Molecule**

Summary and Conclusions

• Recent ‘new spectroscopy rules’ related to **exotic point group nuclear symmetries** have been presented, based on group representation theory ↔ they address isomerism and new rotational band properties

• Analysing existing experimental data, a **first Tetrahedral / Octahedral Rotational Band was found in ^{152}Sm**

• Thanks to the collaboration with experimental teams, a **second Tetrahedral Rotational Band in ^{152}Sm was identified**

• Comparison of these two bands allowed for addressing spontaneous symmetry breaking and a new interpretations related to the **Tetrahedral Symmetry Spontaneously Broken by Octahedral one**

• We constructed the experimental identification criteria of exotic point-group symmetries in nuclei employing group-, and group representation theories – which lead to the bands with degenerate states

• We have presented the world first identification of the exotic C_{2v} point group symmetry in ^{236}U