Exotic 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

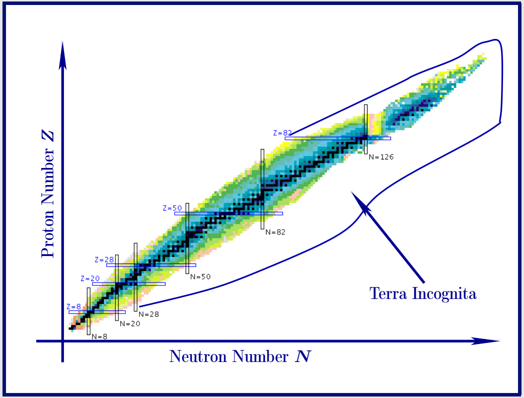
PHYSICAL REVIEW C 111, 034319 (2025)

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)

There Are Nearly 3000 Nuclei Observed So Far

The Chart of Nuclides



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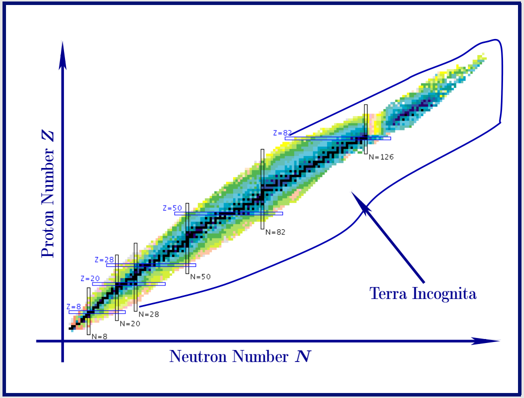

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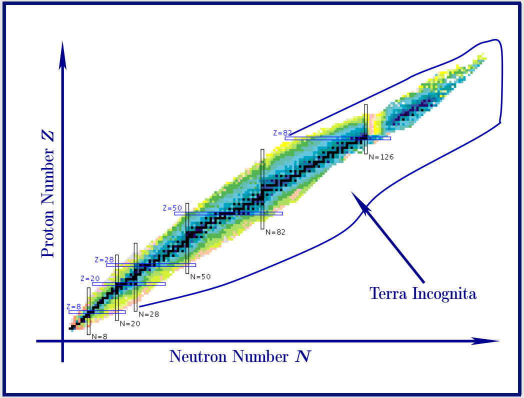

• Among nearly 3000 systems known experimentally:

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

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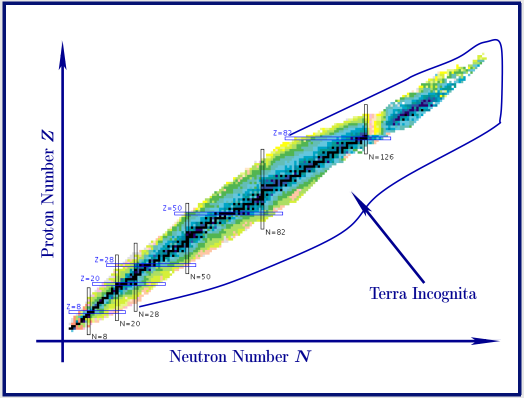

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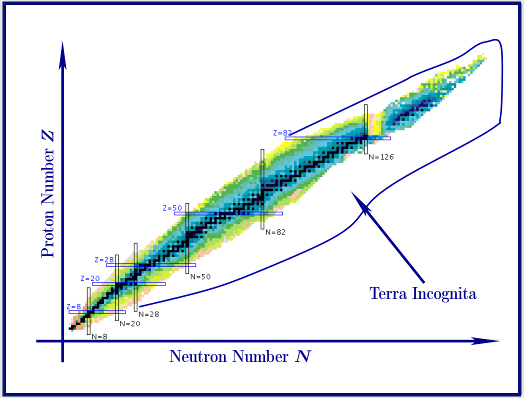

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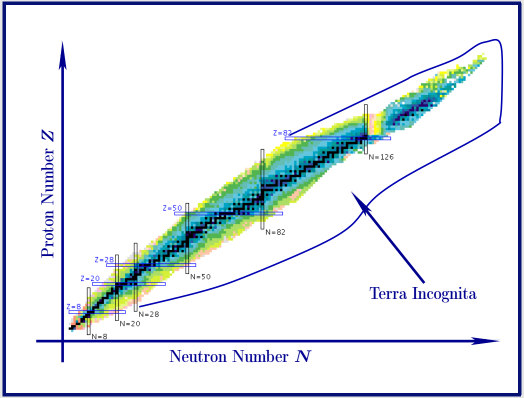

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• **Terra Incognita**: Still >6000 nuclei are expected to exist...

High chances that they are deformed!

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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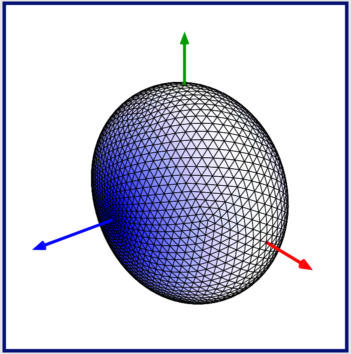
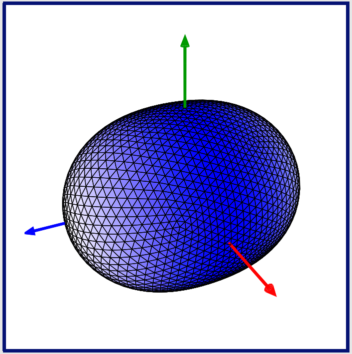
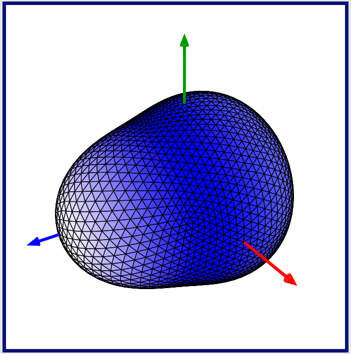
Oblate



Prolate



Pear-shape



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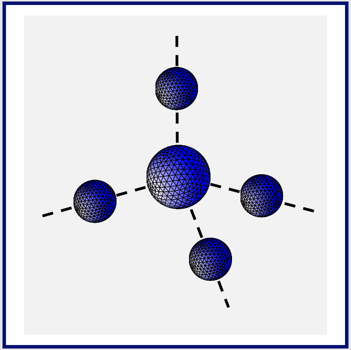
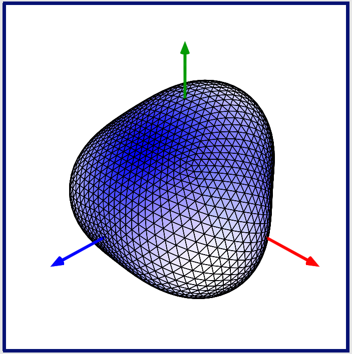
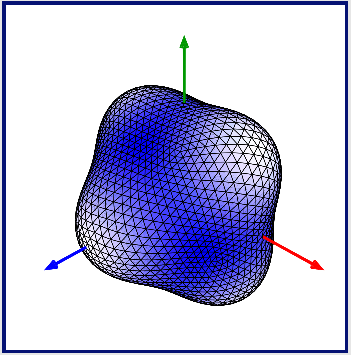
CH_4 Molecule (T_d)



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**

Non-Trivial Exotic Nuclear Shapes: Historical Perspective

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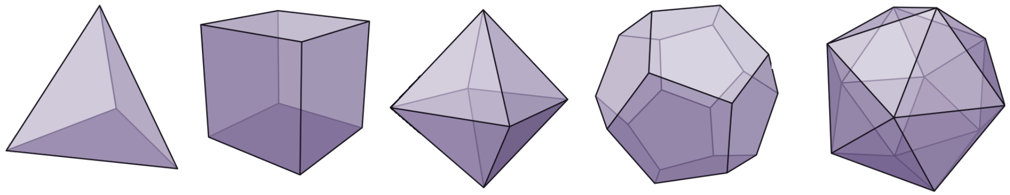
- **Platonic Solids** (Plato, 428-347 bC): Polyhedra whose faces are identical regular convex polygons
- The allowed polygons are: triangles, squares and regular pentagons
- Thus, there are only five Platonic Solids:

Tetrahedron	Cube	Octahedron	Dodecahedron	Icosahedron



Principal Goals and Strategy of Presented Research

• Large scale mean-field theory calculations addressing the presence of various exotic shape symmetries, their competition and evolution throughout the Mass Table

Principal Methods Used

• We calculate and analyse nuclear energies using one of the most powerful nuclear structure techniques: **Realistic Phenomenological Nuclear Mean-Field Theory**

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

• Our modelling employs parameter optimisation based on recent experimental data – **using Inverse Problem & Monte Carlo methods** to remove parametric correlations

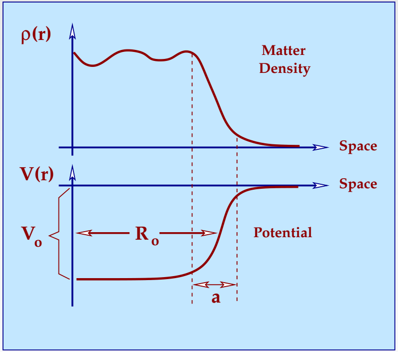
Part 1

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:

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

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

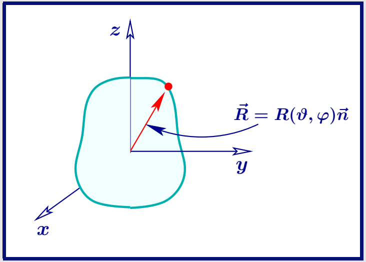
- Function $\mathbf{dist}_\Sigma(\vec{r})$ gives the shortest distance between the nuclear surface and a point in space (see next slides)

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



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

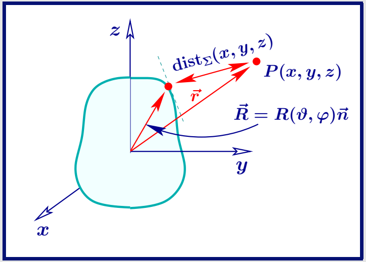
- Parameters $\{\alpha_{\lambda\mu}\}$, are called *deformations*
- The lowest rank deformations:

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

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

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

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**

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

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 ↔ 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**

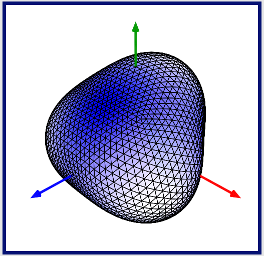
$\lambda = 3:\quad t_1 \equiv \alpha_{3,\pm2}$

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

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

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

$t_1 = 0.2$



- 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**

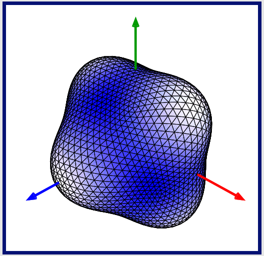
$$\lambda = 4: \quad o_1 \equiv \quad \alpha_{40} \quad \text{and} \quad \alpha_{4,\pm4} = -\sqrt{\tfrac{5}{14}} \cdot \alpha_{40}$$

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

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

$$\text{and} \quad \alpha_{8,\pm8} = \sqrt{\tfrac{65}{198}} \cdot \alpha_{80}$$

$o_1 = 0.2$



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Mean Field Theory: Tetrahedral Gaps – Protons

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

→ Three distinct families of nucleon levels ←

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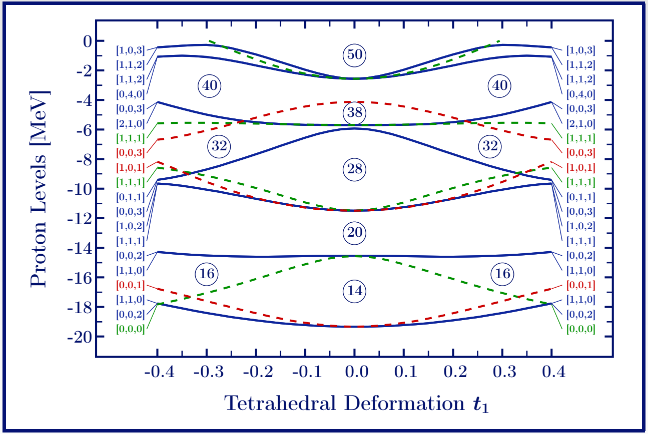

Full lines ↔ one 4D-irreps
Dashed lines ↔ two 2D-irreps

Notice tetrahedral gaps at $Z = 16, 32$ and 40

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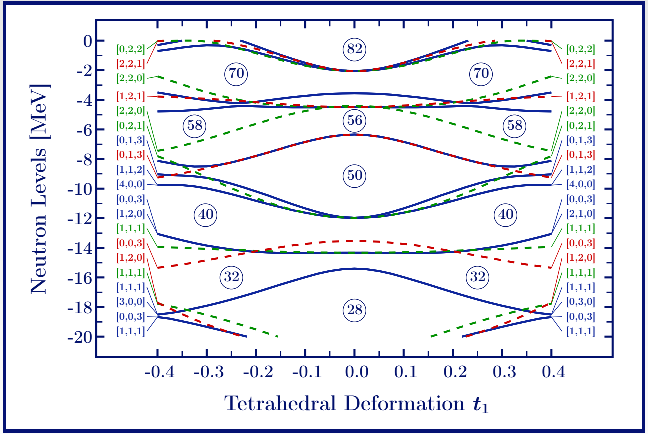

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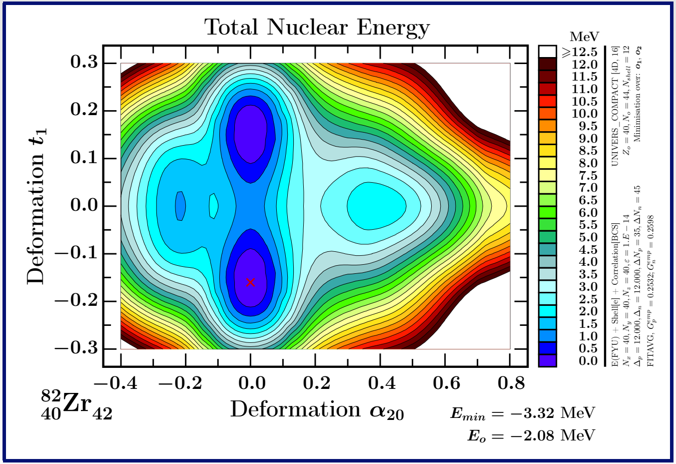
Notice tetrahedral gaps at N = 32, 40, 56, 58 and 70

Mean Field Theory: Total Nuclear Surfaces

- Total Nuclear Energy of ^{82}Zr projected onto the $(\alpha_{20}, \alpha_{32})$-plane $[t_1 \equiv \alpha_{32}]$



- Big gaps on the single particle spectra may translate into deep potential energy minima

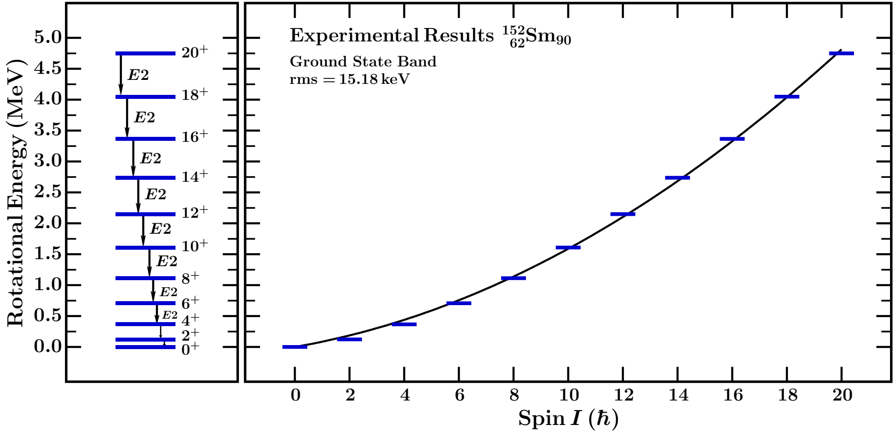
Symmetries Are the Factors Determining Stability*) of Atomic Nuclei

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*

Quadrupole Rotational Bands

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



Quadrupole Moments Generated by Octupole Shapes

- Express the multipole moments as usual by $[\Sigma: \; R(\vartheta,\varphi) = R_o\, c(\alpha)\,[1+\sum_{\lambda\mu}\alpha_{\lambda\mu}Y_{\lambda\mu}(\vartheta,\varphi)]]$

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

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

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

- We can calculate the **quadrupole moments** Q_{20} as functions of **octupole** $\alpha_{3\mu}$

$$\alpha_{30}: \quad Q_{20} = 4/(3\sqrt{5\pi}) \cdot \rho_0 R_0^5 c^5(\alpha) \cdot \alpha_{30}^2$$

$$\alpha_{31}: \quad Q_{20} = 2/(\sqrt{5\pi}) \cdot \rho_0 R_0^5 c^5(\alpha) \cdot |\alpha_{31}|^2$$

$$\alpha_{32}: \quad Q_{20} = 0 \quad \leftarrow \quad \text{identically vanishing}$$

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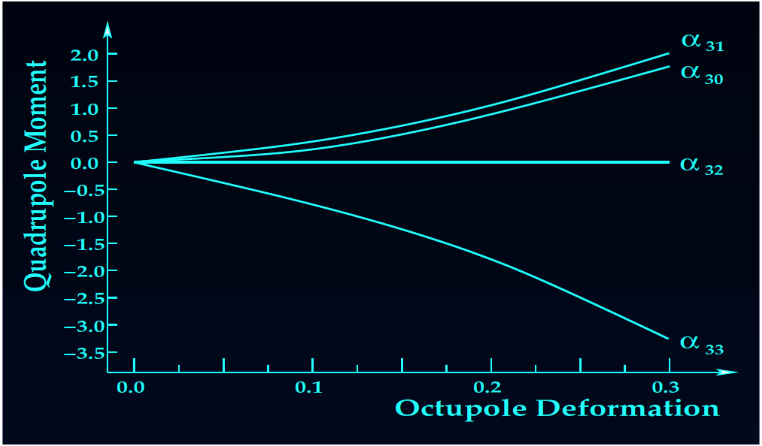
\end{aligned}$$

Quadrupole Moments vs. Pure Octupole Shapes

- For microscopically calculated quadrupole moments (W.S.):

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



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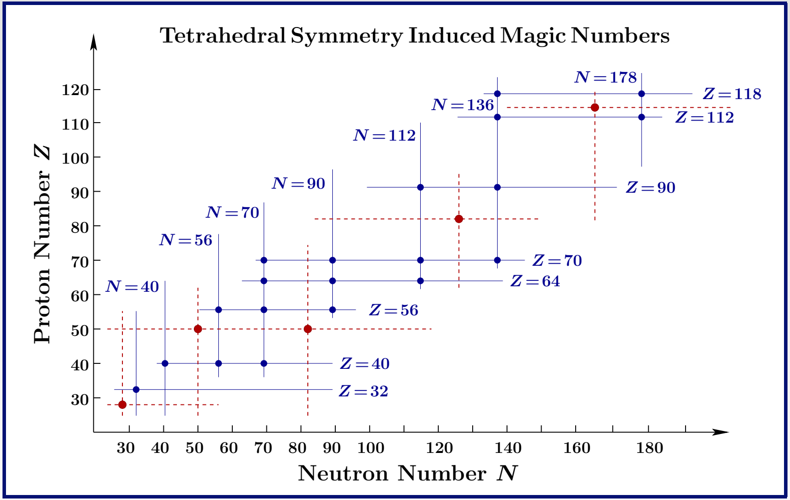
Once those symmetries are present one may expect the presence of numerous isomers since $B(E2)$ and $B(E1)$ at the exact T_d and/or O_h symmetry limits – vanish!

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

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

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:

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

$$\chi_{(I\pi)}(\sigma_d) = \pi \times \chi_{(I\pi)}(C_2), \; \chi_{(I\pi)}(S_4) = \pi \times \chi_{(I\pi)}(C_4)$$

- 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
$F_1(T_1)$	0	1	0	1	1	2	1	2	2	3	2
$F_2(T_2)$	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

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

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

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

Quantum Rotors: Tetrahedral vs. Octahedral

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

$$A_1 : \quad \underbrace{0^+, 3^-, 4^+, \underbrace{(6^+, 6^-)}_{\text{doublet}}, 7^-, 8^+, \underbrace{(9^+, 9^-)}_{\text{doublet}}, \underbrace{(10^+, 10^-)}_{\text{doublet}}, 11^-, \underbrace{2\times 12^+, 12^-}_{\text{triplet}}, \cdots}_{\text{Forming a common parabola}}$$

- 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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- One shows the analogue structures for the **octahedral O_h** symmetry

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

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

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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World-First Announcement of the Discovery – Part I

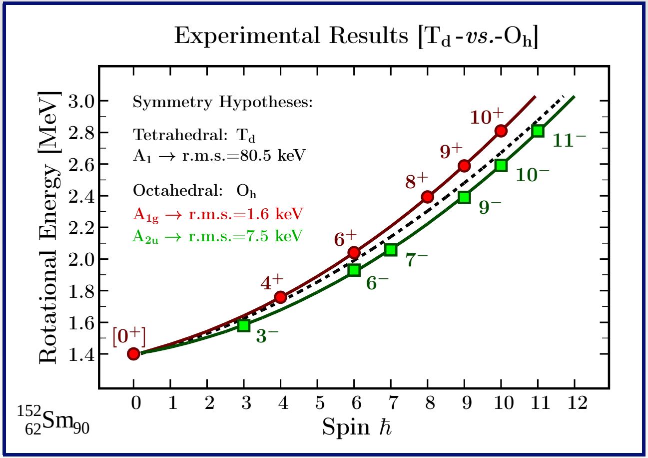
PHYSICAL REVIEW C VOLUME 97, 021302(R) FEBRUARY 2018

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

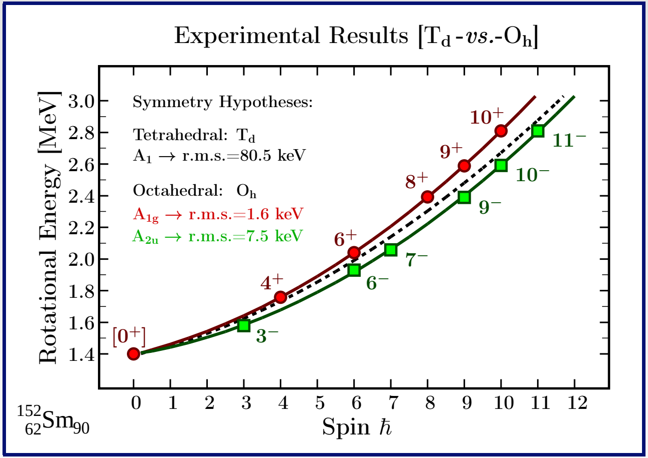


- Parabolic looking sequences are interpreted as **coexistence of tetrahedral and octahedral symmetries.**

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

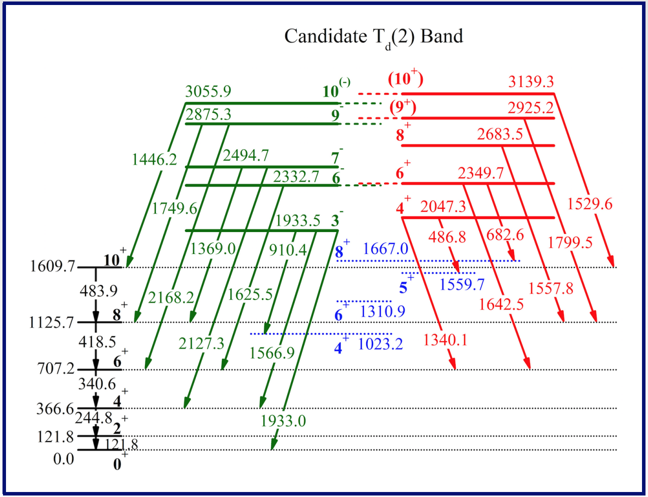
New evidence of interplay between tetrahedral and octahedral symmetries and symmetry breaking: Exotic rotational bands in ^{152}Sm

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 $^{152}_{62}\mathrm{Sm}_{90}$. It was populated via fusion evaporation reaction $^{150}\mathrm{Nd}(\alpha, 2n)^{152}\mathrm{Sm}$, 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.

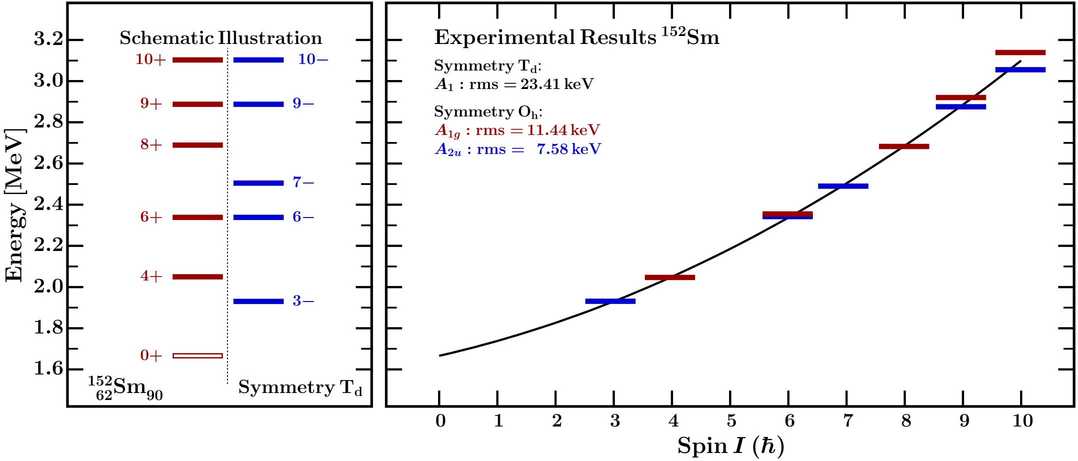
New Tetrahedral/Octahedral Rotational Band Evidence in ^{152}Sm

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



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

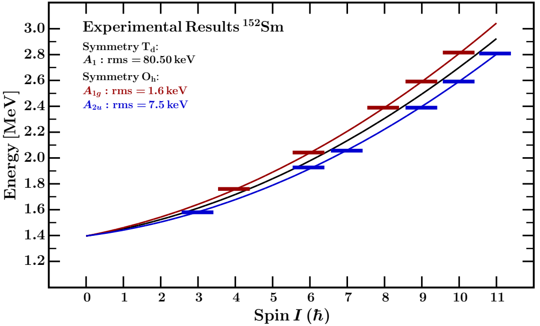
New Tetrahedral Rotational Band Evidence in ^{152}Sm



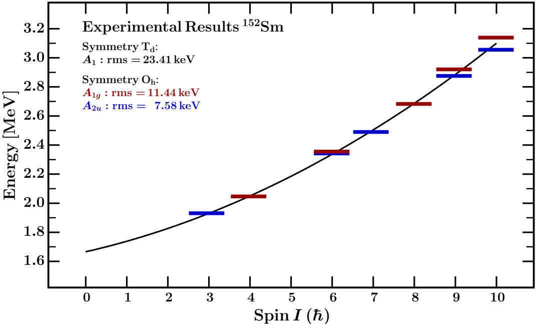
- **The R.M.S. of the ground-state band is 15.18 keV – same order of magnitude as for T$_d$ (1)**

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

- Comparison shows distinct differences in the splitting-size of nearly degenerate sequences



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



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

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

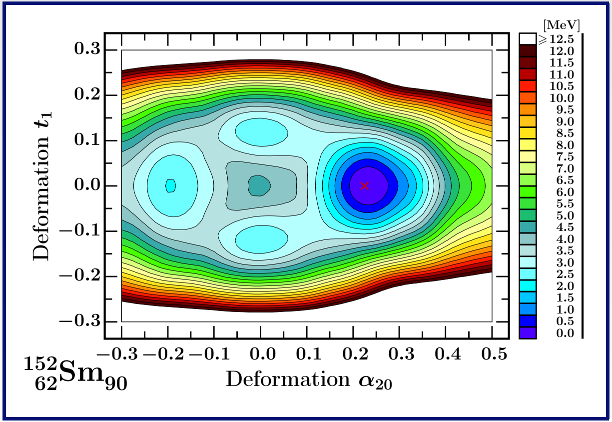
- Attention: Both parity sequences resemble structure in the octahedral case ↔ INTERPRETATION: Not just any symmetry breaking → TETRAHEDRAL broken by OCTAHEDRAL one.

- 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

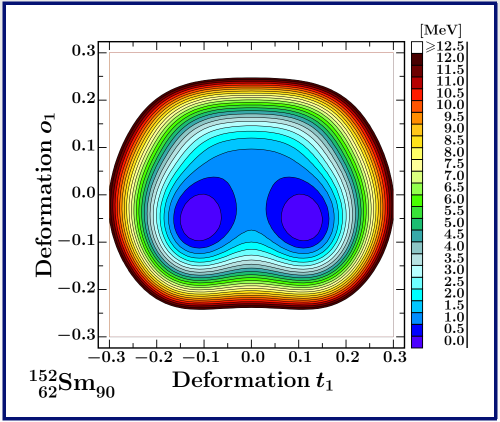
^{152}Sm: Coexistence or Competition of T_d and O_h Symmetries

Potential Energy Surfaces projected on

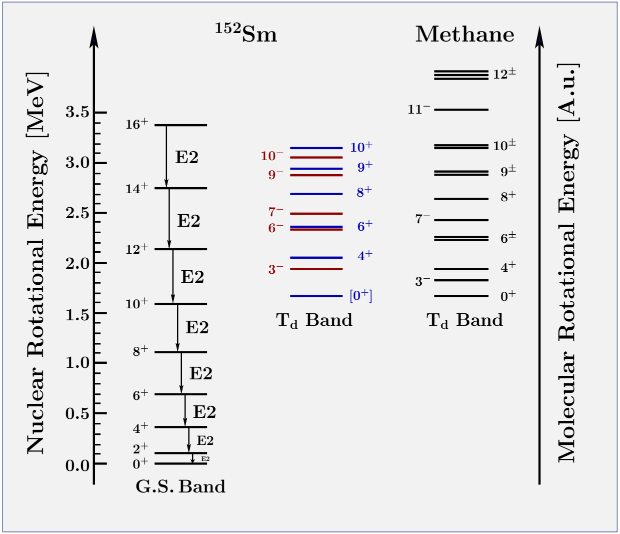
(α_{20}, t_1): quadrupole g.s.

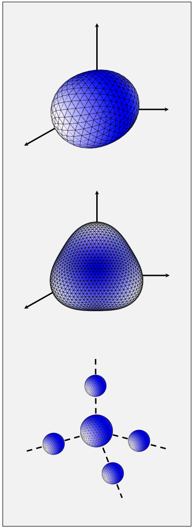


(t_1, o_1): coexistence of both shapes



^{152}Sm: Nuclear vs Molecular Symmetry





Hunt for Molecular Symmetries Throughout the Nuclear Chart

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

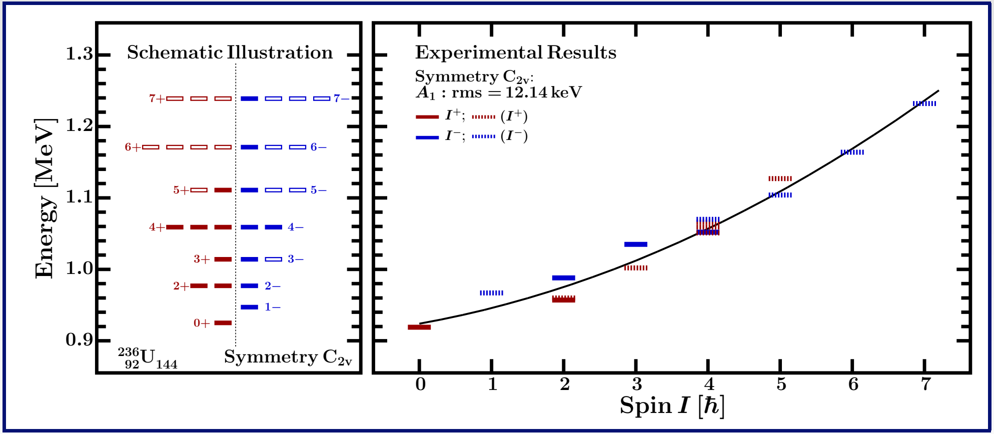
I. Dedes, J. Dudek, A. Baran *et al.*, Phys. Rev. C 112, 034303 (2025)

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

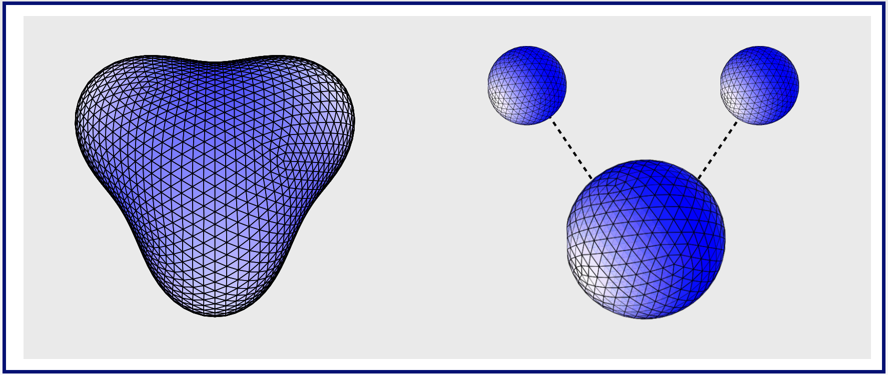
- **Rotational band structure of a nucleus according to a C_{2v}-symmetric configuration**



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

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

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