Theory Predictions of Exotic Nuclear Symmetries and Spontaneous Symmetry Breaking: Identification Methods

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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)

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

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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Interests in High-Rank Symmetries (T_d and O_h)

- Theory predicts numerous total energy minima manifesting exotic symmetries in many regions of the Mass Table
- These symmetries may lead to well pronounced potential energy minima generating unprecedented, new nuclear quantum mechanisms in terms of spectroscopy and isomerism
- For instance: High-rank symmetry groups have 4D irreducible representations – it follows that some levels are 4-fold degenerate – in contrast to the usual 2-fold (Kramers) degeneracy
- It follows: Existence of exotic (16-fold) degeneracies of 2p-2h excitations built out of 4-fold degenerate levels – similarly 32-fold degeneracies in the more complex 4p-4h excitations
- For instance: Exotic degeneracies in rotational bands with positive and negative parities
- For instance: unprecedented forms of the nuclear rotational behaviour - rotational bands without 'rotational $E2$-transitions'
- ... and many more

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About Physics and Mathematics Tools Used

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

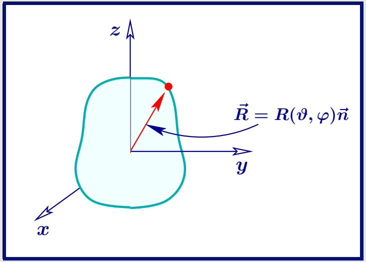
Deformed Universal Woods-Saxon Hamiltonian

Reminding standard definitions

Deformed Universal Woods-Saxon Hamiltonian

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 Σ



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

- Woods-Saxon Central Potential, traditional spherical form:

$$\mathcal{V}_c^{\rm WS}(\vec{r}; V_c, R_c, a_c) = \frac{V_c}{1 + \exp[(r - R_c)/a_c]}$$

- Spin-Orbit Potential

$$\mathcal{V}_{so}^{\rm WS} = \mathcal{V}_{so}^{\rm WS}(\vec{r}; \lambda_{so}, R_{so}, a_{so})$$

- **Universal Parametrisation: fixed set of 12 parameters for the whole Nuclear Chart!**

$$\{V_c, r_c, a_c; \lambda_{so}, r_{so}, a_{so}\}_{\pi,\nu}$$

Part 2

Selected Molecular Symmetries in Atomic Nuclei

Example: So-called High-Rank*) Symmetries

Tetrahedral T_d and Octahedral O_h

*) The only ones with 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

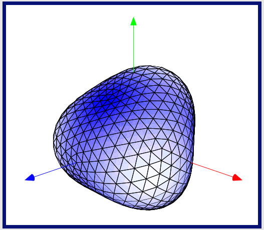
$\lambda = 3:$ $\quad t_1 \equiv \alpha_{3,\pm 2}$

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

$\lambda = 7:$ $\quad t_2 \equiv \alpha_{7,\pm 2}$ and $\alpha_{7,\pm 6} = -\sqrt{\frac{11}{13}}\cdot\alpha_{7,\pm 2}$

$\lambda = 9:$ $\quad t_3 \equiv \alpha_{9,\pm 2}$ and $\alpha_{9,\pm 6} = +\sqrt{\frac{28}{198}}\cdot\alpha_{9,\pm 2}$

$t_1 = 0.2$



- Problem presented in detail in:

J. Dudek, J. Dobaczewski, N. Dubray, A. Góźdź, V. Pangon and N. Schunck, Int. J. Mod. Phys. E16, 516 (2007) [516-532].

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

- 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 $\leftrightarrow$ Multipolarity λ**

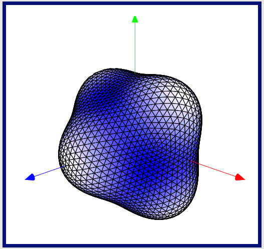
$\lambda = 4:\quad o_1 \equiv \quad \alpha_{40}$ and $\alpha_{4,\pm 4} = -\sqrt{\frac{5}{14}} \cdot \alpha_{40}$

$\lambda = 6:\quad o_2 \equiv \quad \alpha_{60}$ and $\alpha_{6,\pm 4} = -\sqrt{\frac{7}{2}} \cdot \alpha_{60}$

$\lambda = 8:\quad o_3 \equiv \quad \alpha_{80}$ and $\alpha_{8,\pm 4} = \sqrt{\frac{28}{198}} \cdot \alpha_{80}$

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

$o_1 = 0.2$



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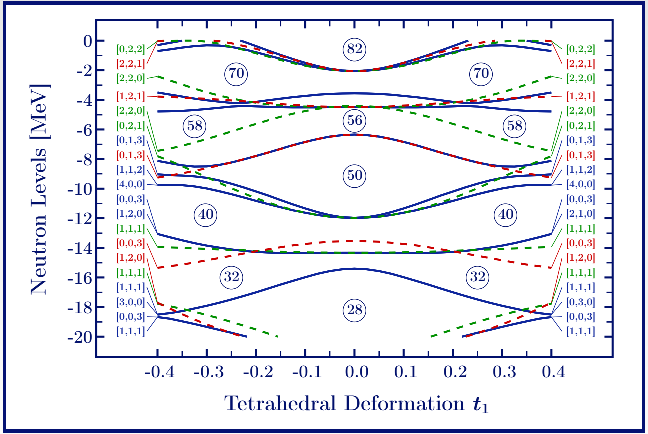
Mean Field Theory: Tetrahedral Gaps – Neutrons

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

→ Three distinct families of nucleon levels ←

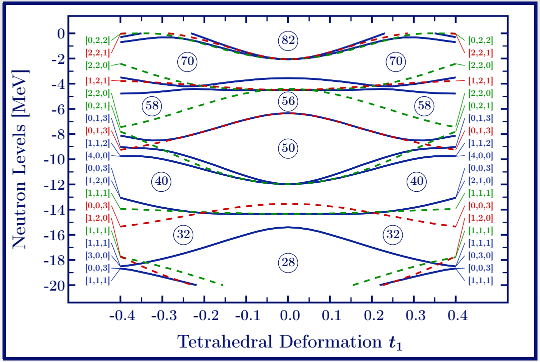


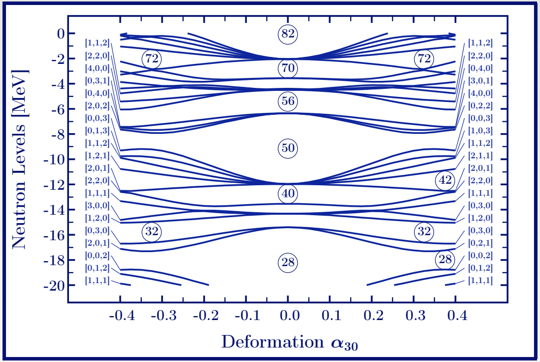
Full lines ↔ one 4D-irreps
Dashed lines ↔ two 2D-irreps

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

Mean Field Theory: Tetrahedral vs Pear-Shape 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 $\alpha_{30} \neq 0.00$
- Observation: t_1-gaps at $N = 32$, 40, 58 and 70 are (almost) inexistent or very small for α_{30}

Symmetries Are the Factors Determining Stability*) of Atomic Nuclei

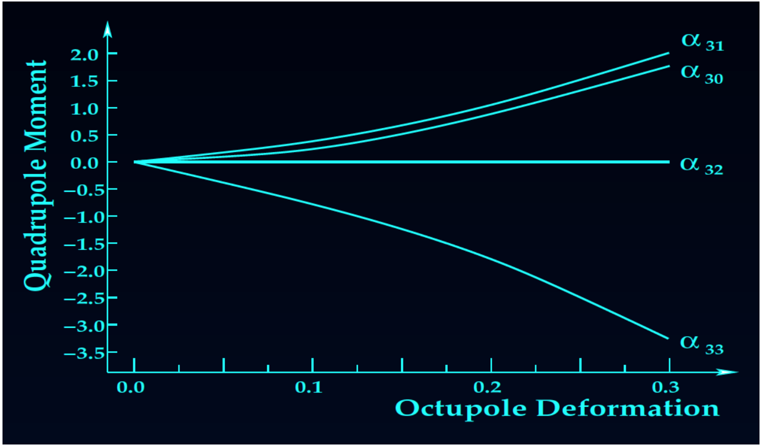
Nuclear mean field theory and group representation theory which are used in this research belong to the most powerful tools of nuclear structure theory arsenal

*) ... *by imposing hindrance mechanisms*

Quadrupole Moments vs. Pure Octupole Shapes

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

$$Q_{20}(\alpha_{3\mu}) = \int \Psi^*_{WS}(\tau)\hat{Q}_{20}\Psi_{WS}(\tau)d\tau \Longrightarrow Q_{20}(\alpha_{32}) = 0 \Longrightarrow B(E2) = 0 \, !$$



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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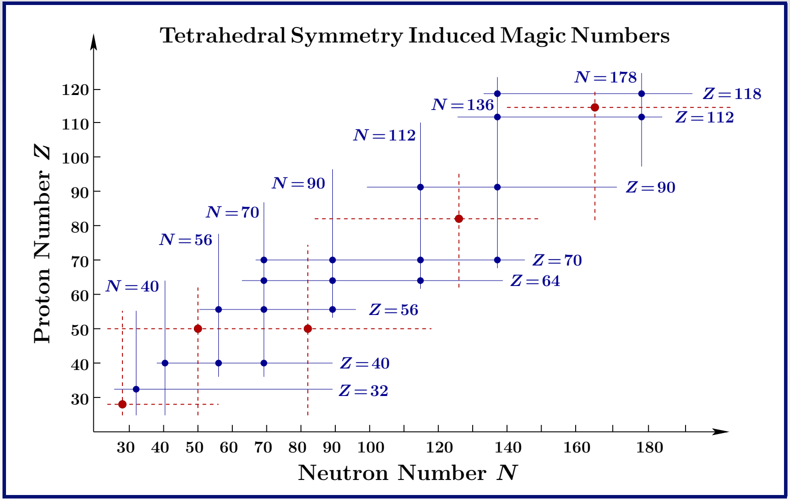
Tetrahedral Symmetry Dominates Mass Table



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

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

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:

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

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:

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

- 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

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

$$\underbrace{A_{2u}: \; 3^-, 6^-, 7^-, 9^-, 10^-, 11^-, \ldots, \; I^\pi = I^-}$$

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

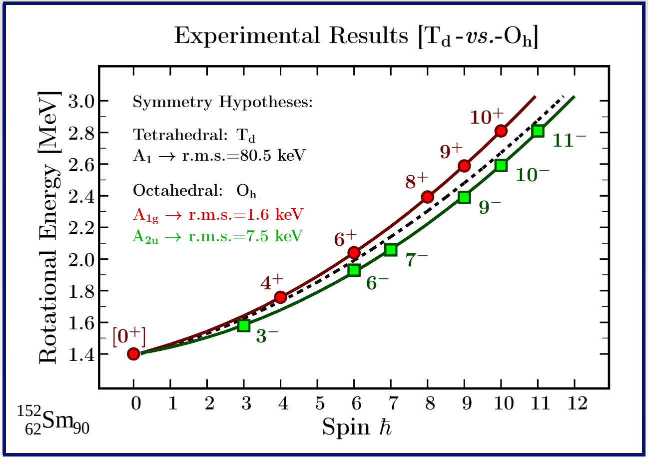
PHYSICAL REVIEW C VOLUME 97, 021302(R) FEBRUARY 2018

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

World-First Announcement of the Discovery – Part II

PHYSICAL REVIEW C VOLUME 111, 034319 MARCH 2025

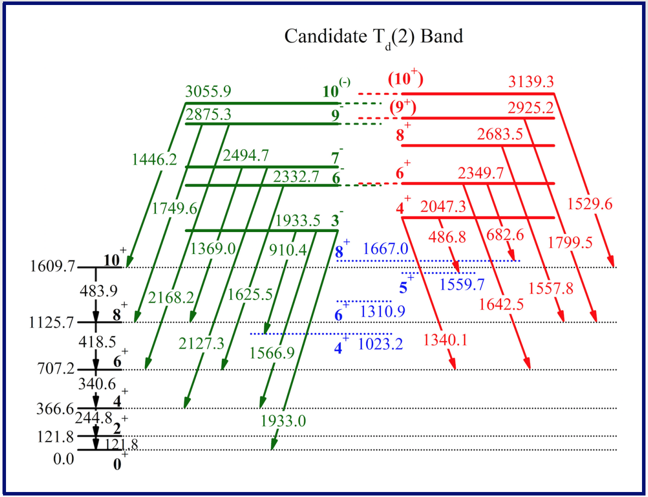
New evidence of interplay between tetrahedral and octahedral symmetries and symmetry breaking: Exotic rotational bands in ^{152}Sm

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.

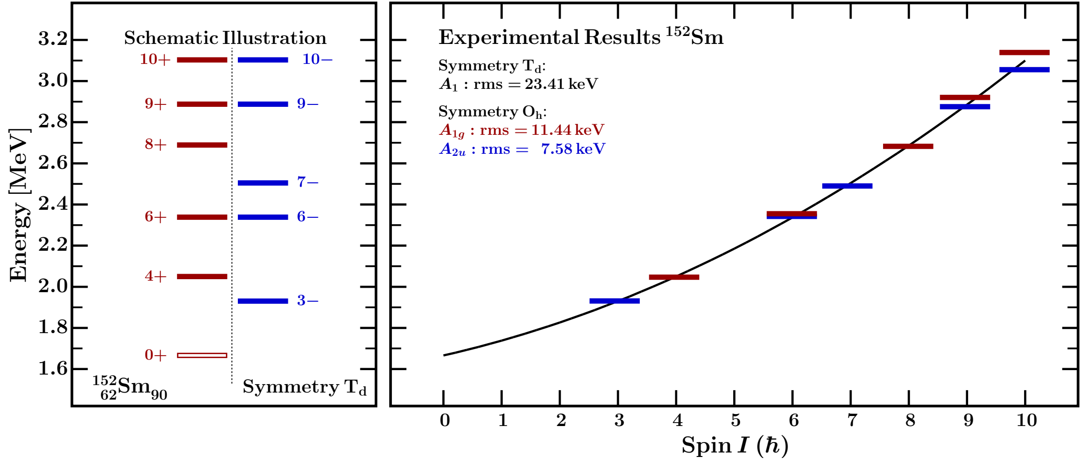
New Tetrahedral/Octahedral Rotational Band Evidence in ^{152}Sm

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



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

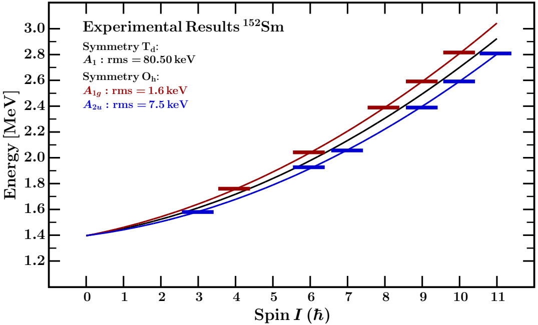
New Tetrahedral Rotational Band Evidence in ^{152}Sm



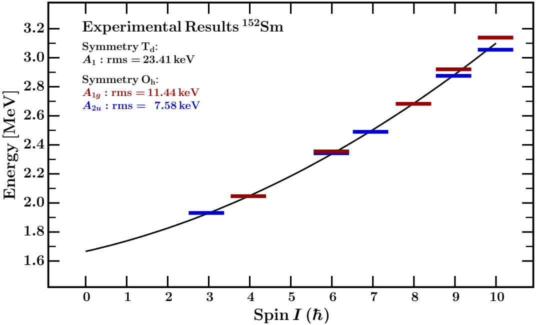
- **The R.M.S. of the ground-state band is 15.18 keV – same order of magnitude as for T_d (1)**

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

Hunt for Molecular Symmetries Throughout the Nuclear Chart

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

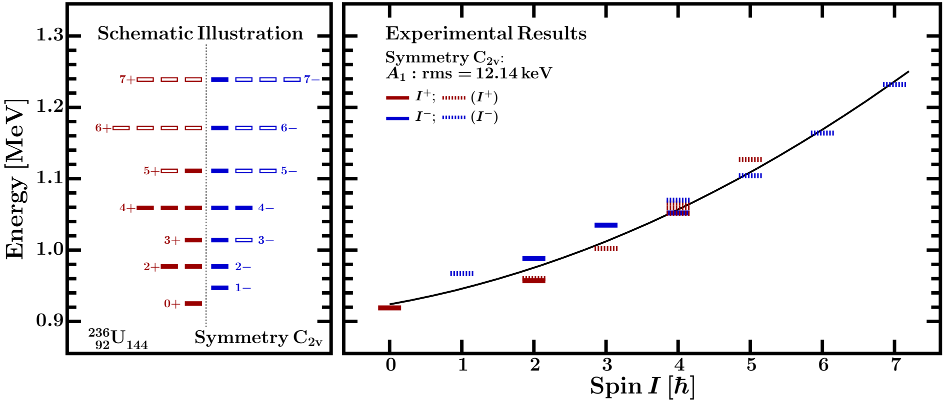
I. Dedes, J. Dudek, A. Baran *et al.*, Phys. Rev. C 112, 034303 (2025)

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

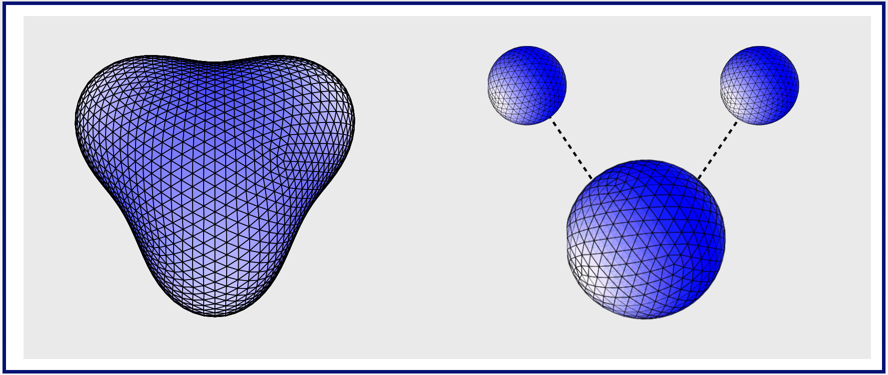
- **Rotational band structure of a nucleus according to a C_{2v}-symmetric configuration**



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

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**

World-First Identifications of 3 Molecular Symmetries in Nuclei

- **Only the beginning. What now? Should we look for yet another symmetry?**
- How to do better: Get profit for nuclear structure domain? **Address new physics?**

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Round tables: experiment - theory

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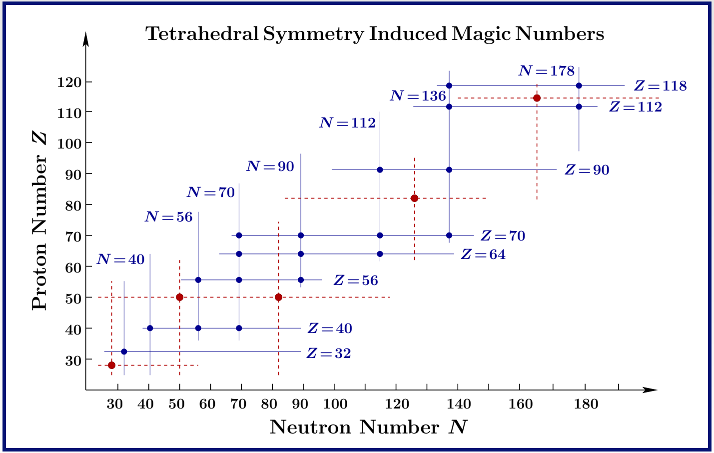
Examples of something new to think about →

“World-First” Hides Surprises: Specific Difficulties to Think About 1

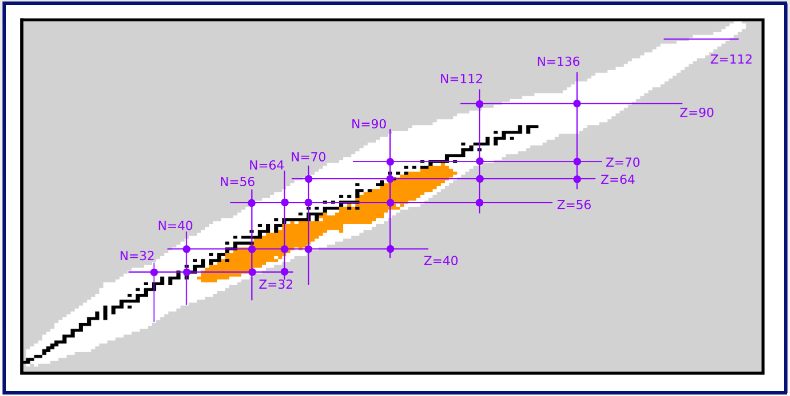
Difficulty No. 1: T_d symmetry ↔ $B(E1) = 0$ and $B(E2) = 0$ ⇔ The strongest feeding and decay out transitions are out ⇔ The majority of states never seen – Worse: Never sought



“World-First” Hides Surprises: Specific Difficulties to Think About 2

Difficulty No. 1: Follow up. $B(E1) = 0$ and $B(E2) = 0 \Leftrightarrow$ The strongest γ-ray detectors are not of the first help $\Leftrightarrow$ How about alternatives e.g. high-resolution mass spectrometry?

Fromt GSI colleagues: Mass overlap in terms of fission fragments of their ^{256}Cf source



EPJ Web of Conferences **223**, 01014 (2019)

"World-First" Hides Surprises: Specific Difficulties to Think About 2

Difficulty No. 2: We encourage totally new experimental efforts (and imagination). For theorists it is not obvious how to combine the instrumental and human readiness and interests

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• The first tools which come to one's mind are 4π detection systems: Gammasphere? AGATA? GRETA? But measuring transition multipolarities may require long beam-times...

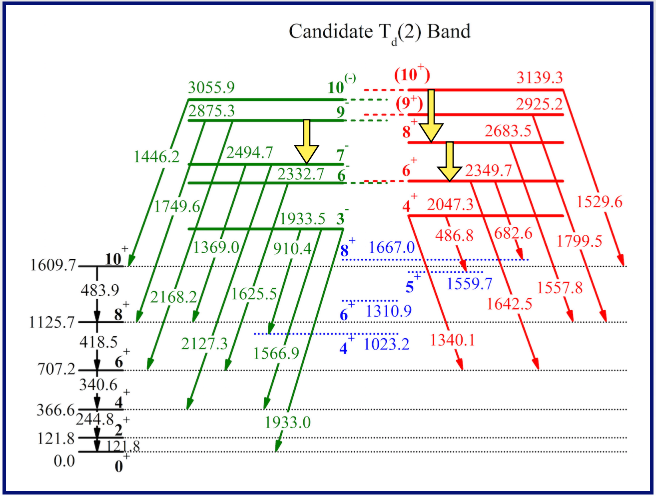
• Before measuring we will need to populate – Example: ENSDF table of reactions leading to ^{152}Sm tetrahedral case ⇔ How about the accelerators and surrounding instrumentation?

A	^{152}Pm β^- decay (4.12 min)	J	^{152}Sm(n,n$'\gamma$)	S	^{155}Gd(n,α)
B	^{152}Pm β^- decay (7.52 min)	K	Coulomb excitation	T	^{154}Sm(^{12}C,^{14}C)
C	^{152}Pm β^- decay (13.8 min)	L	^{152}Sm(x,x$'$)	U	^{152}Sm(γ,γ'):Mossbauer
D	^{152}Eu ε decay (13.517 y)	M	^{153}Eu(t,α)	V	^{154}Sm(α,^{6}He)
E	^{152}Eu ε decay (9.3116 h)	N	^{154}Sm(p,t)	W	^{154}Sm(^{208}Pb,Xγ),(^{176}Yb,Xγ)
F	^{150}Nd(α,2nγ)	O	Muonic atom	X	^{152}Sm(α,α'):giant resonances
G	^{151}Sm(n,γ) E=thermal	P	^{252}Cf SF decay	Y	^{151}Sm(n,γ) E=resonance
H	^{151}Sm(d,p)	Q	^{150}Sm(t,p)		

For ^{152}Sm out preferred reaction is Case F

Example 1: Clarify the Quadrupole Hindrance in T_d Nuclei

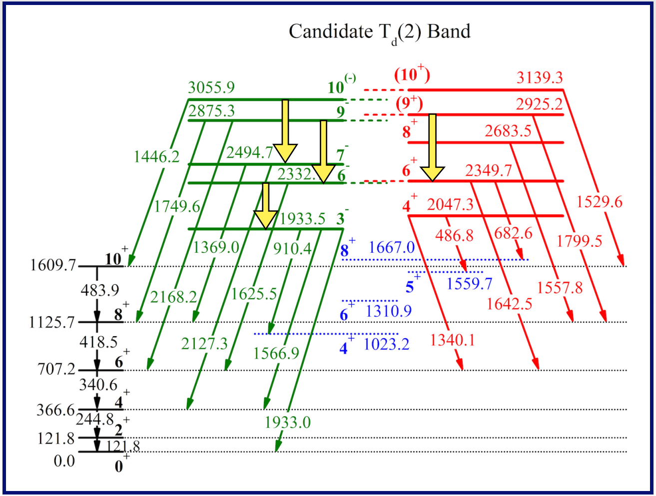
- Forbidden $E2$ transitions in the T_d bands $(10^+ \to 8^+)$, $(9^- \to 7^-)$, $(8^+ \to 6^+)$



- Production of the discussed states by alpha-fusion evaporation reaction
- Discuss optimal choice and use of gamma multi-detector system
- Address measuring both the angular distributions and polarisations
- Attract attention of colleagues using instrumentation with high efficiency gamma detection, multi-gating (type γ, γ, γ)
- Address extracting $B(E2)$ – but equally instructive, estimate upper limits of the hindrance

Example 2: Address Octupole $B(E3)$ Strength: $T_d \leftrightarrow \alpha_{\lambda=3,2}$

• Since tetrahedral deformation α_{32} has multipolarity $\lambda = 3$ – all the octupole transition properties known in the literature – play the same role in this case – except population



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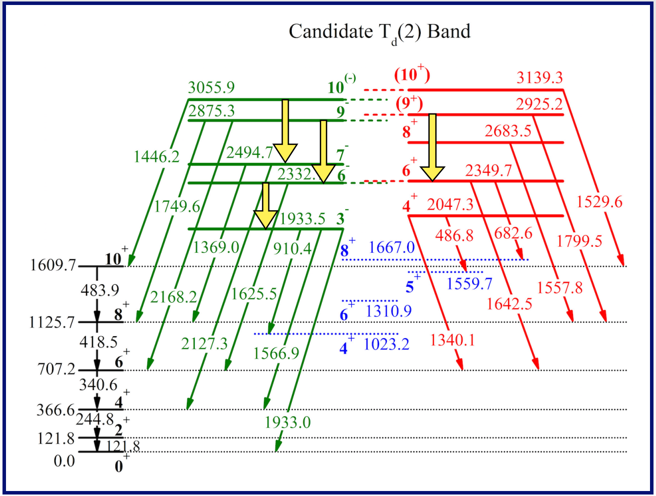
• Address extracting $B(E3)$: On theory side we can provide contributions from all 4 components $\alpha_{3,\mu}$ – not only pear-shapes

Example 3: Address Higher Spins with $I > 10\hbar$



- At higher spins the measuring conditions get cleaner / facilitate obtaining new information
- Using predictive power: from the parabolic fit give predictions estimates for $I > 10\hbar$ states
- This could give new hints for new dedicated experiments for decays from these predicted states

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

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