From T<sub>d</sub> to C<sub>2v</sub>: Water Molecule Symmetry Identified in an Actinide Nucleus – <sup>236</sup>U

## **Irene Dedes**

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Shape and Symmetries in Nuclei: from Experiment to Theory 4 – 8 November 2024 IJCLab, Orsay, France

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## **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 ?

• *Similarities* in the observed 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

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• New highway towards exotic nuclei: Nuclear Isomers living longer than the ground-states

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- 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'
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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 technique: **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

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Our Choice of Theory Approach: Phenomenological Mean Field Deformed Woods-Saxon Hamiltonian

# Introducing Deformed Universal Woods-Saxon Hamiltonian

 Phenomenological Woods-Saxon Hamiltonian with the so-called 'universal' parameterisation ⇒ fixed set of parameters for thousands of nuclei!

• Central Potential

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

• Spin-Orbit Potential

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

• **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 ↔ Mass Table ~ 3 000 nuclei

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

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



• WS potential respects the surface- $\Sigma$  symmetries:

$$V(\vec{r}; V_o, R, a) = \frac{V_o}{1 + \exp[\operatorname{dist}_{\Sigma}(\vec{r})/a]}$$

• Auxiliary function

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

• Distance function

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**Mean-Field Potential** 

$$\hat{\mathcal{V}}_{m-f} = \hat{\mathcal{V}}_{cent}^{WS} + \hat{\mathcal{V}}_{SO}^{WS} + \hat{\mathcal{V}}_{C}$$

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

From T<sub>d</sub> to C<sub>2v</sub>: Water Molecule Symmetry Identified in <sup>236</sup>U

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# **A Short Historical Perspective**

The hunt for exotic high-rank symmetries started several years ago ...

- Already in Ancient Greece, they were interested in the beauty in symmetry
- **Platonic Solids** (Plato, 428-347 bC): Polyhedra whose faces are identical regular convex polygons  $\implies$  triangles, squares and regular pentagons
- Thus, there are only five Platonic Solids:

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### Nuclear Tetrahedral Symmetry: Possibly Present throughout the Periodic Table

#### J. Dudek, A. Góźdź, N. Schunck, and M. Miśkiewicz

More than half a century after the fundamental, spherical shell structure in nuclei had been established, theoretical predictions indicate that the **shell gaps comparable or** even stronger than those at spherical shapes may exist. Group-theoretical analysis supported by realistic mean-field calculations indicate that the corresponding nuclei are characterized by the  $T_d^D$  ("double-tetrahedral") symmetry group.

**Strong shell-gap structure is enhanced by the existence of the four-fold degenerate levels;** *it can be seen as a geometrical effect that does not depend on a particular realization of the mean field. Possibilities of discovering the*  $T_d^D$  *symmetry in experiment are discussed.* 

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> [This was a follow-up of an earlier pilot project: X. Li and J. Dudek, Phys. Rev. C 94, R1250 (1994)]

#### 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 <sup>152</sup>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.

### This article announces the discovery – Culmination

Selected Molecular Symmetries in Atomic Nuclei Example: So-called High-Rank<sup>\*)</sup> Symmetries Tetrahedral T<sub>d</sub> and Octahedral O<sub>h</sub>

\*) The ones with 4D irreducible spinor representations – 4-fold nucleonic degeneracies

# **Tetrahedral Symmetry:** Spherical-Harmonic Basis

- **Reminder:** nuclear surface,  $\Sigma$ :  $R(\vartheta, \varphi) = R_o c(\{\alpha\}) \left[1 + \sum_{\lambda \mu} \alpha_{\lambda \mu} Y_{\lambda \mu}(\vartheta, \varphi)\right]$
- Only *special combinations* of only odd-order spherical harmonics may form a basis for surfaces with tetrahedral symmetry:



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].

I. DEDES, IFJ Polish Academy of Sciences From T<sub>d</sub> to C<sub>2v</sub>: Water Molecule Symmetry Identified in <sup>236</sup>U

# **OBSERVATION:**

# Tetrahedral symmetry group, $T_d$ , is a sub-group of the octahedral one, $O_h$
#### **Octahedral Symmetry:** Spherical-Harmonic Basis

- **Reminder:** nuclear surface,  $\Sigma$ :  $R(\vartheta, \varphi) = R_o c(\{\alpha\}) \left[1 + \sum_{\lambda \mu} \alpha_{\lambda \mu} Y_{\lambda \mu}(\vartheta, \varphi)\right]$
- Only *special combinations* of only even-order  $\lambda \ge 4$  spherical harmonics may form a basis for surfaces with octahedral symmetry

#### **Three Lowest Order Solutions:**



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

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

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

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

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### Mean Field Theory: Tetrahedral Gaps – Shape Stabilisation I

Double group  $T_d^D$  has two 2-dimensional and one 4-dimensional irreducible representations (irreps.)  $\rightarrow$  Three distinct families of nucleon levels  $\leftarrow$ 



### Mean Field Theory: Tetrahedral Gaps – Shape Stabilisation II

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#### Numerous Tetrahedral Doubly-Magic Nuclei



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• Doubly-Magic Tetrahedral Nuclei are more numerous than Doubly-Magic Spherical Nuclei

• Recall: at the exact symmetry limit tetrahedral nuclei emit neither E2 nor E1 transitions → ISOMERS

#### Numerous Tetrahedral Doubly-Magic Nuclei



Doubly-Magic Tetrahedral Nuclei are more numerous than Doubly-Magic Spherical Nuclei

• Recall: at the exact symmetry limit tetrahedral nuclei emit neither E2 nor E1 transitions → ISOMERS Tetrahedral (octahedral) symmetries generate bands without rotational electromagnetic transitions "bands of isomers"

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

[Symmetry Properties of Quantum Rotors]

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1

[Symmetry Properties of Quantum Rotors]

#### **Reminders for Theorists: Group and Point Group Theories**

• Consider a point-group symmetry characterised by group G. The SO(3)-group representation which mathematically describes rotor wave functions,  $D^{(I\pi)}$ , with given  $I^{\pi}$ , can be decomposed in terms of irreducible representations  $D_i$  (*irreps.*) 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<sup>\*)</sup>

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

- $\rightarrow \chi_{(I\pi)}$  characters of the reducible representation  $D^{(I\pi)}$  of the SO(3)-group;
- $\rightarrow \chi_i^{(1R)}$  characters of the irreducible representation  $D_i$  of a point group;
- $\rightarrow N_G$  order of the group G;
- $\rightarrow g$  group element;
- $\rightarrow n_{\alpha}$  the number of elements in the class  $\alpha$ , whose representative element is  $g_{\alpha}$ .

\*) Tagami, Shimizu, Dudek, Phys. Rev. C87, 054306 (2013)

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

#### **Reminders for Theorists – Example: Tetrahedral T<sub>d</sub>-Group**

- T<sub>d</sub>-group has 5 irreps.:  $A_1, A_2, E, F_1, F_2$ , and 5 classes:  $E, C_3, C_2 (= S_4^2), \sigma_d, S_4$
- The characters of irreducible representations  $\chi_i$  of T<sub>d</sub> are listed below \*)

T <sub>d</sub>	Ε	$C_{3}(8)$	$C_{2}(3)$	$\sigma_d(6)$	$S_4(6)$
$A_1$	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) reducible representations are as follows <sup>\*</sup>):  $\chi_{(I\pi)}(E) = 2I + 1, \quad \chi_{(I\pi)}(C_n) = \sum_{K=-I}^{I} e^{\frac{2\pi K}{n}i}, \quad \chi_{(I\pi)}(\sigma_d) = \pi \times \chi_{(I\pi)}(C_2), \quad \chi_{(I\pi)}(S_4) = \pi \times \chi_{(I\pi)}(C_4)$ 

• Multiplicity coefficients can be calculated in an elementary fashion

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

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#### **Reminders: Resulting Prediction of the Structure of T<sub>d</sub>-Bands**

• The number of states  $a_i^{(I\pi)}$  within five irreps

• If  $a_i^{(I\pi)} = 0 \rightarrow$  states not allowed;  $a_i^{(I\pi)} = 2 \rightarrow$  doubly degenerate, etc.

<i>I</i> <sup>+</sup>	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
Ē	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>I</i> <sup>-</sup>	0-	1-	2-	3-	4-	5-	6-	7-	8-	9-	10-
$I^-$ $A_1$	<b>0</b> - 0	<b>1</b> <sup>-</sup> 0	<b>2</b> - 0	3 <sup>-</sup> 1	<b>4</b> <sup>-</sup> 0	<b>5</b> - 0	6 <sup>-</sup> 1	7 <sup>-</sup> 1	<b>8</b> - 0	9- 1	10 <sup>-</sup>
$\frac{I^-}{A_1}$	<b>0</b> - 0 1	1 <sup>-</sup> 0 0	<b>2</b> <sup>-</sup> 0 0	<b>3</b> - <b>1</b> 0	<b>4</b> <sup>-</sup> 0 1	5- 0 0	6 <sup>-</sup> 1 1	7 <sup>-</sup> 1 0	<b>8</b> - 0 1	9- 1 1	<b>10</b> <sup>-</sup> <b>1</b> 1
$ \frac{I^-}{A_1} \\ \frac{A_2}{E} $	<b>0</b> - 0 1 0	1- 0 0 0	<b>2</b> - 0 0 1	<b>3</b> - <b>1</b> 0 0	<b>4</b> - 0 1 1	<b>5</b> - 0 0 1	6 <sup>-</sup> 1 1 1	7 <sup>-</sup> 1 0 1	<b>8</b> - 0 1 2	<b>9</b> - <b>1</b> 1 1	<b>10</b> <sup>-</sup> <b>1</b> 1 2
$ \frac{I^-}{A_1} \\ \frac{A_2}{E} \\ F_1 $	<b>0</b> - 0 1 0 0	1- 0 0 0 0	<b>2</b> <sup>-</sup> 0 0 1 1	<b>3</b> - <b>1</b> 0 0 1	<b>4</b> - 0 1 1 1	<b>5</b> - 0 0 1 1	<b>6</b> - <b>1</b> 1 1 2	<b>7</b> - <b>1</b> 0 1 2	<b>8</b> - 0 1 2 2	<b>9</b> - <b>1</b> 1 1 2	<b>10</b> - <b>1</b> 1 2 3

• In this way we find the  $I^{\pi}$ -sequence for  $A_1$ -representation

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

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

#### **Tetrahedral Bands Are Not Like the Others!**

As we have shown using the methods of the point-group representation theory that, for instance, rotational bands based on  $0^+$  "T<sub>d</sub> ground-state" have the structure:

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

and NOT "ellipsoidal like"

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

#### **Tetrahedral Bands Are Not Like the Others!**

As we have shown using the methods of the point-group representation theory that, for instance, rotational bands based on  $0^+$  "T<sub>d</sub> ground-state" have the structure:

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

and NOT "ellipsoidal like"

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

Similarly there are no analogies of the "octupole bands"

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

#### **Quantum Rotors: Tetrahedral vs. Octahedral**

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



#### **Quantum Rotors: Tetrahedral vs. Octahedral**

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



Forming another (common) parabola

#### **Perfect Parabolas Represent Experimental Results**

Physical Review C 97, 021302(R) (2018)



• 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  $O_h$  (two branches) based on the experimental data

## Molecular Symmetries in Subatomic Physics: Methane vs. <sup>152</sup>Sm



• Left: The world first experimental identification of the tetrahedral-rotor band in <sup>152</sup>Sm

• Right: tetrahedral rotor band associated with the methane CH<sub>4</sub> molecule\*)

\*) G. Herzberg, *Molecular Spectra And Molecular Structure*, Vol II, (D.van Nostrand Company Inc., 1945)

### Continuing the Hunt for Molecular Symmetries Throughout the Nuclear Chart

## Possible World First Experimental Evidence of $C_{2v}$ in <sup>236</sup>U

After a series of publications
J. Yang, J. Dudek *et al.*, Phys. Rev. C 105, 034348 (2022)
J. Yang, J. Dudek *et al.*, Phys. Rev. C 106, 054314 (2022)
J. Yang, J. Dudek *et al.*, Phys. Rev. C 107, 054304 (2023)

 $\rightarrow$  See next talk by **J. Yang**,

Exotic Nuclear Symmetries and New Concepts of Magic Numbers: Focus on Heavy Nuclear

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- $\rightarrow$  See next talk by **J. Yang**,

Exotic Nuclear Symmetries and New Concepts of Magic Numbers: Focus on Heavy Nuclei

#### Synthetic View of Octupole Instabilities

• Our calculations show octupole shape instabilities for N = 136, with big shell gaps and pronounced energy surface minima

• The octupole-shape deformations include  $\alpha_{\lambda=3,\mu=0,1,2,3}$  thus leading to 4 independent shape degrees of freedom

• They generate Point-Group Symmetries:

$$\alpha_{30} \Rightarrow C_{\infty v}, \quad \alpha_{31} \Rightarrow C_{2v}, \quad \alpha_{32} \Rightarrow T_d, \quad \alpha_{33} \Rightarrow D_{3h}$$

• It turns out that octupole static or dynamic equilibrium configurations are expected to generate specific rotational band structures mixing both parities  $\Rightarrow$  What are these structures?

#### Molecular (Point-Group) Symmetry - $C_{2v} \Leftrightarrow \alpha_{31}$

#### • Symmetry induced by either $(\alpha_{31} \neq 0)$ or $(\alpha_{20} \neq 0, \alpha_{31} \neq 0)$



Nuclear C<sub>2v</sub> Point Group Symmetry Shapes

#### Molecular (Point-Group) Symmetries - $T_d \& D_{2d} \Leftrightarrow \alpha_{32}$

• Symmetries induced by  $(\alpha_{32} \neq 0 \rightarrow T_d)$  or  $(\alpha_{20} \neq 0, \alpha_{32} \neq 0 \rightarrow D_{2d})$ 



 $T_d$ :  $\alpha_{32} = 0.25$ 

**D**<sub>2d</sub>:  $\alpha_{20} = 0.15, \alpha_{32} = 0.25$ 

Nuclear T<sub>d</sub> and D<sub>2d</sub> Point Group Symmetry Shapes

#### Molecular (Point-Group) Symmetries - $D_{3h} \Leftrightarrow \alpha_{33}$

#### • Symmetry induced by both $(\alpha_{33} \neq 0)$ and $(\alpha_{20} \neq 0, \alpha_{33} \neq 0)$



Nuclear D<sub>3h</sub> Point Group Symmetry Shapes

How to proceed to experimental identification once we know the point group symmetry of interest?

#### How to proceed to experimental identification once we know the point group symmetry of interest?

## **Suggestion:** Formulate the identification criteria with the help of the group representation theory

### **Resulting Prediction of the Structure of C<sub>2v</sub>-Bands**

#### • Multiplicity factors for the 4 irreducible representations of C<sub>2v</sub>-group

$I^+$	0+	1+	2+	3+	4+	5+	6+	7+	8+	9+	10+
$A_1$	1	0	2	1	3	2	4	3	5	4	6
$A_2$	0	1	1	2	2	3	3	4	4	5	5
$\boldsymbol{B}_1$	0	1	1	2	2	3	3	4	4	5	5
$\boldsymbol{B}_2$	0	1	1	2	2	3	3	4	4	5	5
<i>I</i> <sup>-</sup>	0-	1-	2-	3-	4-	5-	6-	7-	8-	9-	10-
$I^-$ $A_1$	<b>0</b> - 0	1 <sup>-</sup> 1	2- 1	3 <sup>-</sup> 2	4 <sup>-</sup> 2	5- 3	6 <sup>-</sup> 3	7 <sup>-</sup> 4	8 <sup>-</sup> 4	9- 5	10 <sup>-</sup> 5
$\frac{I^-}{A_1}$	<b>0</b> - 0 1	1 <sup>-</sup> 1 0	2- 1 2	3 <sup>-</sup> 2 1	<b>4</b> <sup>-</sup> <b>2</b> 3	5- 3 2	6 <sup>-</sup> 3 4	7- 4 3	8- 4 5	9- 5 4	<b>10</b> <sup>-</sup> <b>5</b> 6
$\frac{I^-}{\begin{array}{c} A_1\\ A_2\\ B_1 \end{array}}$	<b>0</b> - 0 1 0	1- 1 0 1	<b>2</b> - <b>1</b> 2 1	<b>3</b> - <b>2</b> 1 2	<b>4</b> - <b>2</b> 3 2	5- 3 2 3	6 <sup>-</sup> 3 4 3	7- 4 3 4	<b>8</b> - <b>4</b> 5 4	<b>9</b> - <b>5</b> 4 5	<b>10</b> <sup>-</sup> <b>5</b> 6 5

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

 $A_1: 0^+, 1^-, 2 \times 2^+, 2^-, 3^+, 2 \times 3^-, 3 \times 4^+, 2 \times 4^-, 2 \times 5^+, 3 \times 5^-, 4 \times 6^+, 4 \times 6^-, \cdots$ 

• Group-theory prediction of the spin-parity structure of the  $C_{2v}$  g.s.b.

. . . similarly can be done for  $D_{2d}$  and  $D_{3h}$ 

#### **Experimental Data Selection for C<sub>2v</sub>**

#### About criteria for the experimental data search

 $C_{2v} \to A_1: 0^+, 1^-, 2 \times 2^+, 2^-, 3^+, 2 \times 3^-, 3 \times 4^+, 2 \times 4^-, 2 \times 5^+, 3 \times 5^-, 4 \times 6^+, 4 \times 6^-, \cdots$ 

## • Avoid rotational bands generated by leading ellipsoidal geometry and characterised by strong $\Delta I = 2$ quadrupole transitions

• Identified yrast-trap or *K*-isomers and related axial symmetry non-collective particle-hole excitations should be eliminated

• Energy-wise  $-C_{2v}$  bands form regular sequences

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

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 $C_{2v} \to A_1: 0^+, 1^-, 2 \times 2^+, 2^-, 3^+, 2 \times 3^-, 3 \times 4^+, 2 \times 4^-, 2 \times 5^+, 3 \times 5^-, 4 \times 6^+, 4 \times 6^-, \cdots$ 

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#### **Experimental Data Selection for C<sub>2v</sub>**

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## Experimental Identification - Recent Results : <sup>236</sup>U

• Rotational band structure of a nucleus according to a C<sub>2v</sub>-symmetric configuration Attention: Experimental degeneracies for  $^{236}$ U according to NNDC



## Experimental Identification - Recent Results : <sup>236</sup>U

• Rotational band structure of a nucleus according to a C<sub>2v</sub>-symmetric configuration Attention: Experimental degeneracies for  $^{236}$ U according to NNDC



• Rotational band constructed employing 16 states; we find r.m.s. deviation 12.14 keV [rms(gsb)=3.79 keV]

#### Exotic Symmetries: Nuclei vs. Molecules

• Rotational band structure of a nucleus according to a C<sub>2v</sub>-symmetric configuration Attention: Experimental degeneracies for <sup>236</sup>U according to NNDC

• Notice similarities in the observed spectra (see below) in totally different objects: Molecules are 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



•  $\alpha_{31} = 0.25$ 

• H<sub>2</sub>O has C<sub>2v</sub>-symmetry:



## Exotic Symmetries for <sup>236</sup>U – Suspects for C<sub>2v</sub>



• We associate the prolate minimum at  $\alpha_{20}^{\text{th}} \sim 0.25 \text{ [r.m.s.}(\alpha_{20}^{\text{exp}}) = 0.2821(18)]^{*}$  with the ground-state, ...

• ... and enlarging the scales around the prolate minimum,  $\alpha_{31} \neq 0$  is worth noticing

 $\implies$  associated with the C<sub>2v</sub> symmetry

Atomic Data and Nuclear Data Tables, Vol. 78, No. 1, May 2001

I. DEDES, IFJ Polish Academy of Sciences From T<sub>d</sub> to C<sub>2</sub>:

From Td to C2v: Water Molecule Symmetry Identified in 236U

<sup>\*)</sup> S. Raman, C. W. Nestor, JR., and P. Tikkanen

We have argued that the potential energy landscapes may only give qualitative suggestions about equilibrium deformations → shapes & symmetries We have argued that the potential energy landscapes may only give qualitative suggestions about equilibrium deformations → shapes & symmetries

# We will turn to the solutions of the collective Schrödinger equation!!

## **Collective Schrödinger Equation**

A New Approach to Adiabaticity Concepts in Collective Nuclear Motion: Impact for the Collective-Inertia Tensor and Comparisons with Experiment PHYSICAL REVIEW C **99**, 041303(R) (2019)

#### D. Rouvel and J. Dudek

• New concepts of adiabaticity within collective model of Bohr, employing new microscopic method of calculations of collective inertia tensor

• It follows that collective Hamiltonian takes the form:

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

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

$$\hat{H}_{\rm coll}\Psi_{\rm coll} = E_{\rm coll}\Psi_{\rm coll}$$

• The most probable  $\alpha_{\lambda\mu}$  deformation  $\leftrightarrow$  the so-called "dynamic equilibrium"

$$\alpha_{\lambda\mu}^{\rm dyn} \leftrightarrow \langle \alpha_{\lambda\mu}^2 \rangle = \int \Psi^*(\alpha_{\lambda\mu}) \alpha_{\lambda\mu}^2 \Psi(\alpha_{\lambda\mu}) d\alpha_{\lambda\mu}$$
### 2D Collective Schrödinger Equation for C<sub>2v</sub>

• The most probable deformation  $\leftrightarrow$  ("dynamic equilibrium") deduced from the following solutions



- Left: Probability density distribution corresponding to the ground-state
- Right: Similar, corresponding to the first excited state with two C2v-symmetry maxima
- Resulting dynamical equilibrium values are close to typical values of the secondary deformations such as the hexadecapole one reported in many nuclei  $\leftrightarrow$  a typical numerical estimate  $\alpha_{\lambda>2,\mu} \approx 0.10$

#### Collaboration between IFJ PAN and IPHC Strasbourg

https://meanfield4exp.ifj.edu.pl

Woods-Saxon phenomenological mean-field calculations, developed by J. Dudek *et al.* 

Currently four (almost six) services:

- Single Particle Energies
- Macroscopic-Microscopic Energy
- (3D Cranking, preliminary stage)

- Nuclear Energy Diagrams
- Shape Evolution with Spin
- (3D Nuclear Surface, preliminary stage)

• **Registration** required through  $\rightarrow$  https://iam-eurolabs.ijclab.in2p3.fr/login

- Contact us: meanfield4exp@ifj.edu.pl
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### **EURO-LABS Project – MeanField4Exp**



I. DEDES, IFJ Polish Academy of Sciences From T<sub>d</sub> to C<sub>2v</sub>: Water Molecule Symmetry Identified in <sup>236</sup>U

### **EURO-LABS Project – MeanField4Exp**



# **Summary and Conclusions**

• 'Spectroscopy rules' related to point group nuclear symmetries have been presented, based on group representation theory  $\leftrightarrow$  they address isomerism and new rotational band properties

• Analysis used for the first Tetrahedral Rotational Band found in <sup>152</sup>Sm allowed for addressing spontaneous symmetry breaking and a new interpretations related to **Tetrahedral Symmetry Spontaneously Broken by Octahedral one** 

• Presence of universal magic gaps at N = 136 and another one at N = 198 generating strong shell effects/minima in heavy nuclei for  $\alpha_{30}$ ,  $\alpha_{31}$ ,  $\alpha_{32}$  and  $\alpha_{33}$  deformations – simultaneously

• 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

- Exotic symmetries associated with  $\alpha_{30}$ ,  $\alpha_{31}$ ,  $\alpha_{32}$  or  $\alpha_{33}$  are given by groups  $C_{\infty v}$ ,  $C_{2v}$ ,  $T_d$  and  $D_{3h}$
- We have presented the world first identification of the exotic  $C_{2v}$  point group symmetry in  $^{236}U$

• By solving the collective Schrödinger equation in the framework of the theory of Bohr we have been able to establish the most probable dynamical deformations for exotic symmetry configurations