Tetrahedral and Octahedral Symmetries in Nuclei

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Part I

Introduction: Symmetry and Nuclear Stability

Gaps and Stability Symmetry and Gaps

Nuclear Stability and Gaps in the Spectra [1]

- Here and in the following we use the nuclear mean-field approach
- The deformation-parameter axis represents often *many independent* deformations of the mean field
- The presence of the sufficiently strong gaps at Fermi levels leads to shape coexistence
- In what follows we focus on shell effects generated by high symmetry point-groups (see below)





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- One of the first mechanisms used in nuclear physics is related to the Harmonic Oscillator 'rule': $\omega_x : \omega_y : \omega_z = k : m : n$
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- How to optimise the mathematical conditions so that the degeneracies are the strongest possible?
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Use the group- and the group-representation theory!

- Given Hamiltonian H and a group: $\mathcal{G} = \{\mathcal{O}_1, \mathcal{O}_2, \dots, \mathcal{O}_f\}$
- Assume that $\mathcal G$ is a symmetry group of H i.e

 $[M, C_{ij}] = 0$ with $k = 1, 2, \dots, \ell$

- Let irreducible representations of G be $\{\mathcal{R}_1, \mathcal{R}_2, \ldots, \mathcal{R}_r\}$
- Let their dimensions be $\{d_1, d_2, \ldots, d_r\}$, respectively
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Gaps and Stability Symmetry and Gaps

What Are the Nuclear High-Level Symmetry Groups?

32 Point Groups: Subgroups



Figure: *Cubic group structure*

Dashed lines indicate that the subgroup marked is not invariant

Trivial groups: $C_1 \equiv \{\mathbb{I}\}, C_s \equiv \{\mathbb{I}, \hat{\sigma}\}$ and $C_i \equiv \{\mathbb{I}, \hat{\pi}\}$

Only the double groups O_h^D and T_d^D lead to <u>four-fold</u> degeneracies in the nucleonic spectra - all the others cause <u>merely two-fold</u> degeneracies. This is why the former are called *high-level* ...

Irreducible Representations and Gaps - Nuclear Context

- The nuclear potential depth is approximately constant it depends only weakly on the particle numbers and on deformation
- The higher the dimensions of the irreps. \rightarrow the higher the degeneracies of s.p. levels \rightarrow the larger the gaps, on the average
- The highest dimensions of the irreducible representations correspond to the *Double* Tetrahedral & Octahedral Groups (d = 4)

Three 'repartitions' of single particle levels into various irreducible repres.: Left: one two-dimensional irrep. Middle: two two-dimensional irreps. Right: one two-dimensional and 2 four-dimensional irreps.



Tetrahedral and Octahedral Symmetries in Nuclei

Symmetries and Gaps in Nuclear Context: Summary

To increase the chances of having big gaps in the spectra we either look for point groups with high dimension irreps or with many irreps

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Mean Field with O and T Symmetries

Part II

Octahedral and Tetrahedral Nuclei

Introducing Nuclear Octahedral Symmetry

Let us recall one of the magic forms introduced long time by Plato. The implied symmetry leads to the *octahedral group* denoted O_h

An octahedron has 8 equal walls. Its shape is invariant with respect to 48 symmetry elements that include inversion. However, the nuclear surface cannot be represented in the form of a diamond $\rightarrow \rightarrow \rightarrow \rightarrow \rightarrow \rightarrow \rightarrow \rightarrow$



... but rather in a form of a regular spherical harmonic expansion:

$$\mathcal{R}(\vartheta, arphi) = \mathcal{R}_0 \, c(\{lpha\}) [1 + \sum_{\lambda}^{\lambda_{max}} \sum_{\mu = -\lambda}^{\lambda} lpha_{\lambda,\mu} \, Y_{\lambda,\mu}(\vartheta, arphi)]$$

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Tetrahedral and Octahedral Symmetries in Nuclei

A Basis for Octahedral Symmetry

Only special combinations of spherical harmonics may form a basis for surfaces with octahedral symmetry:



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Mean Field with O and T Symmetries

Octahedral Symmetry Tetrahedral Symmetry

Nuclear Octahedral Shapes - 3D Examples

Illustrations below show the octahedral-symmetric surfaces at three increasing values of rank $\lambda = 4$ deformations o_4 : 0.1, 0.2 and 0.3:



Figure: $o_4 = 0.1$ Figure: $o_4 = 0.2$ Figure: $o_4 = 0.3$ Recall: $\alpha_{40} \equiv o_4;$ $\alpha_{4,\pm 4} \equiv \pm \sqrt{\frac{5}{14}} \cdot o_4$

Mean Field with O and T Symmetries

Octahedral Symmetry Tetrahedral Symmetry

Among the Highest Symmetries in Molecular Physics

Group T_d - Molecule: [CH₄]



Group O_h - Molecule: [SF₆]



Group D_{6d} - Mol.: [Cr(C₆H₆)₂]



From J. Goss, University of Newcastle

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Group I_h - Molecule: $[C_{60}]$



Tetrahedral and Octahedral Symmetries in Nuclei

Nuclear Octahedral Shapes - Neutron Spectra

Double group O_h^D has four 2-dimensional and two 4-dimensional irreducible representations \rightarrow six distinct families of levels



Figure: Full lines correspond to 4-dimensional irreducible representations - they are marked with double Nilsson labels. Observe huge gap at N=114.

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Nuclear Octahedral Shapes - Proton Spectra

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Figure: Full lines correspond to 4-dimensional irreducible representations - they are marked with double Nilsson labels. Observe huge gap at Z=70.

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Discrete Symmetries in Nuclei

Let us recall one of the magic forms introduced long time by Plato. The implied symmetry leads to the *tetrahedral group* denoted T_d

A tetrahedron has four equal walls. Its shape is invariant with respect to 24 symmetry elements. Tetrahedron is <u>not</u> invariant with respect to the inversion. Of course nuclei cannot be represented by a sharp-edge pyramid



... but rather in a form of a regular spherical harmonic expansion:

$$\mathcal{R}(artheta,arphi) = \mathsf{R}_{\mathsf{0}} \, \mathsf{c}(\{lpha\}) [1 + \sum_{\lambda}^{\lambda_{max}} \sum_{\mu=-\lambda}^{\lambda} lpha_{\lambda,\mu} \, Y_{\lambda,\mu}(artheta,arphi)]$$

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Tetrahedral Symmetry in Heavy Zr Nuclei

The Table below shows the HFB energies relative to the energy of the tetrahedral minimum. Calculations with SLy4 parametrisation. Energy in MeV.

Nucleus	¹⁰⁴ Zr	¹⁰⁶ Zr	¹⁰⁸ Zr	¹¹⁰ Zr	¹¹² Zr
Tetrahedral	+0.00	+0.00	+0.00	+0.00	+0.00
Spherical	+0.22	+0.29	+0.39		
Oblate	-1.57	-1.52	-1.10	+0.07	+0.30
Prolate	-2.07	-1.76	-0.68		+1.01

Conclusion: In some exotic nuclei the ground-state energies may correspond to the tetrahedral minima

Part III

Tetrahedral Rare Earths - A Test-Ground

- The tetrahedral/octahedral symmetric nuclei are predicted around magic closures $\{Z_t, N_t\} = \{32, 40, 56, 64, 70, 90, 132 136\}$
- ... and more precisely around the following nuclei:
- The majority of these are either proton-rich or neutron-rich
- An important exception is the God's gift: Rare Earth Region around Gd and Yb mass A~150-160 nuclei
- Therefore after having examined this 'easier' range the majority of the physics in question corresponds to the realm of Spiral 2

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Total Energies Experiment

Tetrahedral vs. Ground-State Configurations

Tetrahedral minima compete with the prolate ground-state minima Tetrahedral Symmetry / Instability



Figure: Barriers between the tetrahedral and quadrupole-deformed minima.

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Tetrahedral Shapes in Rare Earth Nuclei - Stability

The chances to observe the new symmetries in experiment increase with the increasing heights of the barriers surrounding these minima



Figure: Barriers between the tetrahedral and quadrupole-deformed minima. Brick size 100 keV; this corresponds to the highest barriers \sim 2.5 MeV.

• Conclusion: The highest barriers correspond to the Gadolinum and Ytterbium nuclei with $N \sim 90$.

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Tetrahedral and octahedral deformations combine lowering energies Tetrahedral Symmetry / Instability



Figure: The octahedral deformation may provide down to 1 MeV extra.

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Total Energies Experiment

Tetrahedral vs. Normal-Deformed Energy Differences

The chances to observe the new symmetries in experiment increase with the decreasing energy difference: $(E_t - E_{nd})$



Figure: Energy difference $\Delta E = (E_t - E_{nd})$. Brick size 1 MeV.

Conclusion: The best chances correspond to the N~90-92 isotones.

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About Enormous Instability of Spherical Shapes

Let us examine the energy gain in spherical nuclei by allowing them to get tetrahedral and/or octahedral deformed



Figure: Energy difference $\Delta E \equiv (E_{sph} - E_t)$ between the spherical and tetrahedral minima. Brick-size 500 keV.

• Conclusion: *The majority of the Rare Earth area has 'unstable sphericity'*! In other words: tetrahedral/prolate coexisting minima.

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Tetrahedral/Octahedral Shapes Have No Q₂-Moments

At the exact tetrahedral symmetry the quadrupole moments vanish.





Figure: Equilibrium shape $t_1 = 0.15$.

Total Energies Experiment

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However, the induced dipole moments are calculated to be sizeable.

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Comparison Theory - Experiment: Alignments

Three hypotheses: 1. Tetrahedral and Octahedral \leftrightarrow (microscopic); 2. Tetrahedral and Octahedral + Zero-Point Motion ($\alpha_{20}^{pol.} = 0.07$); 3. Prolate ('standard')



Total Energies Experiment

Comparison Theory - Experiment: B(E2)/B(E1)

Comparison between the mean-field predictions and experiment



Total Energies Experiment

Possible Further Signs of Tetrahedral Symmetry

Table: Experimental ratios $B(E2)_{in}/B(E1)_{out} \times 10^6$

Spin	¹⁵² Gd	¹⁵⁶ Gd	¹⁵⁴ Dy	¹⁶⁰ Er	¹⁶⁴ Er	¹⁶² Yb	¹⁶⁴ Yb
19-	-	50	-	-	-	-	-
17-	-	16		-	-		-
15-	-	6		60	24		-
13-	14	7	15	18	23		17
11-	4	15	5	9	0	10	11
9-	4	0		0	-	11	10
7-	0	0	0	-	-	0	0

Above: Branching ratios related to the negative parity bands interpreted as tetrahedral, inter-band transitions to g.s.band

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Conclusion: The suspected bands in Rare Earth nuclei behave very differently as compared e.g. to 'classical' octupole ²²²Th band!

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Part IV

Spatial Representation of Nuclear Shells

3D Diagrams

Spherical Nuclei Tetrahedral Nucle

Spatial Structure of Orbitals (Spherical ¹³²Sn) ($|\psi(\vec{r})|^2$)



Density distribution $|\psi_{\pi}(\vec{r})|^2 \geq \text{Limit}$, for $\pi = [2, 0, 2]1/2$ orbital

3D Diagrams

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Spherical Nuclei Tetrahedral Nucle

Spatial Structure of N=3 Spherical Shell $(|\psi_{\nu}(\vec{r})|^2)$





¹³²Sn: Distributions $|\psi_{\nu}(\vec{r})|^2$ for single proton orbitals. Top \mathcal{O}_{xz} , bottom \mathcal{O}_{yz} . Proton $e_{\nu} \leftrightarrow [\nu=30, 32, \dots 38]$ for spherical shell

Spherical Nuclei Tetrahedral Nucle

Spatial Structure of N=3 Spherical Shell $(|\psi_{\nu}(\vec{r})|^2)$





¹³²Sn: Distributions $|\psi_{\nu}(\vec{r})|^2$ for single proton orbitals. Top \mathcal{O}_{xz} , bottom \mathcal{O}_{yz} . Proton $e_{\nu} \leftrightarrow [\nu=40, 42, \dots 48]$ for spherical shell

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Spherical Nuclei Tetrahedral Nuclei

The First Octahedral Shell (20 Nucleons)) $(|\psi(\vec{r})|^2)$



Left: accumulating image of all orbitals; Right: Single Orbital (No.1)

Spherical Nuclei Tetrahedral Nuclei

The First Octahedral Shell (20 Nucleons)) $(|\psi(\vec{r})|^2)$



Left: accumulating image of all orbitals; Right: Single Orbital (No.2)

Spherical Nuclei Tetrahedral Nuclei

The First Octahedral Shell (20 Nucleons)) $(|\psi(\vec{r})|^2)$



Left: accumulating image of all orbitals; Right: Single Orbital (No.3)

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Spherical Nuclei Tetrahedral Nuclei

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Left: accumulating image of all orbitals; Right: Single Orbital (No.9)

Spherical Nuclei Tetrahedral Nuclei

The First Octahedral Shell (20 Nucleons)) $(|\psi(\vec{r})|^2)$



Three space perspectives of the full octahedral shell (n=20 nucleons)

Part V

Nuclear Quantum Rotor

Energy Spectra Electromagnetic Transitions

Quantum Systems and Rotation: Preliminaries [1]

Microscopic 'True' H -> All Solutions

Energy Spectra Electromagnetic Transitions

Quantum Systems and Rotation: Preliminaries [1]

Microscopic 'True' H -> All Solutions

Alternative:

Mean Field H -> Individual Nucleons

Energy Spectra Electromagnetic Transitions

Quantum Systems and Rotation: Preliminaries [1]

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Alternative:

Collective Rotor H -> Rotational Bands

Energy Spectra Electromagnetic Transitions

Quantum Systems and Rotation: Preliminaries [2]

Collective Rotor Hamiltonian

Jerzy DUDEK Tetral

Tetrahedral and Octahedral Symmetries in Nuclei

Energy Spectra Electromagnetic Transitions

Quantum Systems and Rotation: Preliminaries [2]



Energy Spectra Electromagnetic Transitions

Quantum Systems and Rotation: Preliminaries [2]



- Suppose a system manifests a spontaneous symmetry breaking
- We find it convenient to describe it with the help of $H_{mf}(\{6A\})$
- We wish to stress rotational degrees of freedom by introducing

 $H_{eff}(\{6A\}) = H_{rot} + H_{mf}(\{6A\})$

Thus the symmetries of H_{eff}({6A}) and of H_{mf}({6A}) coincide
 Thus symmetries of H_{rot} and of H_{mf}({6A}) should be the same

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What Must - and What Must Not be Attempted

The only direct observables are <u>energy and angular momentum</u> Refusing:

- No use of the classical concepts such as 'inertia' or 'rigid body'
- No use of derived concepts as VMI or Harris parametrisations

Accepting:

Nuclear modelling focuses on the mechanism under interest

- To study individual-nucleonic features ightarrow Basis of \hat{x}_k & \hat{p}_k
- For collective rotation $\ o \underline{\mathsf{Basis}}$ of $\{\hat{l}_+, \hat{l}_-, \hat{l}_0\}$ & $\{lpha, eta, \gamma\}$

Basis
$$\{\hat{l}_+, \hat{l}_-, \hat{l}_0\}$$
 : $\hat{\mathcal{T}}_{\lambda\mu}(n) \stackrel{df.}{=} [(\hat{l} \otimes \hat{l}) \otimes \ldots \otimes \hat{l}]_{\lambda\mu}$

n factors

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Nuclear Rotor: Collective vs. Intrinsic Hamiltonians

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• Neglecting the interaction term as an approximation leads to

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Nuclear Rotor: Collective vs. Intrinsic Hamiltonians

• To compare the rotor spectra with experiment, we must shift every band upwards, introducing the band-head energies



• Setting all band-head energies to zero we obtain the so-called <u>reduced</u> form of rotor spectra allowing to discuss properties of H^{rot.}

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Energy Spectra Electromagnetic Transitions

Ellipsoidal Rotor: Energy Spectrum at $\gamma = 0^o$



To facilitate reading, the spectrum is normalised to the yrast line

Energy Spectra Electromagnetic Transitions

Ellipsoidal Rotor: Energy Spectrum at $\gamma = 10^o$



To facilitate reading, the spectrum is normalised to the yrast line

Energy Spectra Electromagnetic Transitions

Ellipsoidal Rotor: Energy Spectrum at $\gamma = 20^o$



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Energy Spectra Electromagnetic Transitions

Ellipsoidal Rotor: Energy Spectrum at $\gamma = 30^o$



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Energy Spectra Electromagnetic Transitions

Ellipsoidal Rotor: Energy Spectrum at $\gamma = 40^o$



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Energy Spectra Electromagnetic Transitions

Ellipsoidal Rotor: Energy Spectrum at $\gamma = 50^o$



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Energy Spectra Electromagnetic Transitions

Ellipsoidal Rotor: Energy Spectrum at $\gamma = 60^o$



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Energy Spectra Electromagnetic Transitions

Stretched Qudrupole Transitions in the D₂ Rotor



Observe the domination of $\Delta I = 2$ stretched E2 \rightarrow g.s. transitions

Energy Spectra Electromagnetic Transitions

Reduced Spectrum of the Tetrahedral-Symmetric Rotor



Spectrum is normalised to 99 % of the yrast line

Jerzy DUDEK

Energy Spectra Electromagnetic Transitions

Electro-Magnetic E2 Transitions from $I_{[9]}[C2]=4$ State



Stretched and non-stretched E2 transitions: observe retardation of the $C2 \rightarrow C2$ transitions

Energy Spectra Electromagnetic Transitions

Electro-Magnetic E2 Transitions from I_[5][C2] State



Stretched and non-stretched E2 transitions: observed retarded $C1 \rightarrow C1$ transitions

Energy Spectra Electromagnetic Transitions

Electro-Magnetic E2 Transitions from I_[1][C2] State



Stretched and non-stretched E2 transitions: observed retarded $C3 \rightarrow C3$ transitions

Energy Spectra Electromagnetic Transitions

Electro-Magnetic E2 Transitions - Comparison



Observe the <u>domination</u> of $Ci \rightarrow C(k \neq i)$ transitions and <u>retardation</u> of the $Ci \rightarrow Ci$ type transitions

- We expect a competition between the minima of tetrahedral and quadrupole-deformed (prolate and/or oblate) shapes
- The decay patterns of the quadrupole bands are very neat; stretched E2-transitions dominate ↔ a distinct feature
- The tetrahedral minima are expected to be 'contaminated' with quadrupole deformation. Contamination with $\beta \sim 0.03$ implies already a significant E1-E2 competition
- There is a degeneracy pattern different in the D₂ and T-symmetry cases: tetrahedral symmetry implies three-fold degeneracies

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E2 Selection - Detailed Predictions [2]

- E2-transitions connect C1, C2 and C3 symmetry states among themselves and T1-symmetry states among themselves!
- Quadrupole transitions of the type C1 \rightarrow C1, C2 \rightarrow C2 and C3 \rightarrow C3 are vanishing/negligible
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Energy Spectra Electromagnetic Transitions

Statistical Wobbling in Space: O_h-Case



Spin-Orientation Probability I=9, n=1, Representation A2

Energy Spectra Electromagnetic Transitions

Statistical Wobbling in Space: O_h-Case



Spin-Orientation Probability I=9, n=2, T2 (3-fold degenerate)

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Energy Spectra Electromagnetic Transitions

Statistical Wobbling in Space: O_h-Case



Spin-Orientation Probability I=9, n=3, T2 (3-fold degenerate)

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Energy Spectra Electromagnetic Transitions

Statistical Wobbling in Space: O_h-Case



Spin-Orientation Probability I=9, n=4, T2 (3-fold degenerate)

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Energy Spectra Electromagnetic Transitions

Statistical Wobbling in Space: O_h-Case



Spin-Orientation Probability I=9, n=5, T1 (3-fold degenerate)

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Energy Spectra Electromagnetic Transitions

Statistical Wobbling in Space: O_h-Case



Spin-Orientation Probability I=9, n=6, T1 (3-fold degenerate)

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Energy Spectra Electromagnetic Transitions

Statistical Wobbling in Space: O_h-Case



Spin-Orientation Probability I=9, n=7, T1 (3-fold degenerate)

Jerzy DUDEK

Energy Spectra Electromagnetic Transitions

Statistical Wobbling in Space: O_h-Case



Spin-Orientation Probability I=9, n=8, A1 (1-fold degenerate)

Jerzy DUDEK Tet

Energy Spectra Electromagnetic Transitions

Statistical Wobbling in Space: O_h-Case



Spin-Orientation Probability I=9, n=9, T1 (3-fold degenerate)

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Energy Spectra Electromagnetic Transitions

Statistical Wobbling in Space: O_h-Case



Spin-Orientation Probability I=9, n=10, T1 (3-fold degenerate)

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Energy Spectra Electromagnetic Transitions

Statistical Wobbling in Space: O_h-Case



Spin-Orientation Probability I=9, n=11, T1 (3-fold degenerate)

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Energy Spectra Electromagnetic Transitions

Statistical Wobbling in Space: O_h-Case



Spin-Orientation Probability I=9, n=12, E (2-fold degenerate)

Energy Spectra Electromagnetic Transitions

Statistical Wobbling in Space: O_h-Case



Spin-Orientation Probability I=9, n=13, E (2-fold degenerate)

Part VI

Summary & Perspectives

- Tetrahedral symmetry in nuclei is predicted as an abundant phenomenon in numerous islands throughout the Periodic Table
- seen already with 'old' non-existing facilities not realising it!
- The tetrahedral Rare-Earth nuclei are about the only non-exotic nuclei that can be studied with relatively modest facilities
- The latter can be seen as a cadeau du ciel: allowing to learn the new physics 'inexpensively'

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A few points about the TETRANUC collaboration:

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