Nuclear Structure Theory Modelling
for
Large Scale Comparisons with Experiment

Jerzy DUDEK

UdS/IN$_2$P$_3$/CNRS, France

NUSTAR Week 2021

COLLABORATORS

Irene Dedes

IFJ, Polish Academy of Sciences, Cracow, Poland

Andrzej Baran, Andrzej Góźdź and Jie Yang

UMCS, Lublin, Poland

Dominique Curien and David Rouvel

IPHC and University of Strasbourg, France

Rami Gaamouci

University of Algiers, Algiers, Algeria

Aleksandra Pędrak

National Centre for Nuclear Research, Warsaw, Poland

Hua-Lei Wang

Zhengzhou University, Zhengzhou, China

About This Presentation

NUCLEAR STRUCTURE COLLABORATION

EXPERIMENT

THEORY

We already have results

INTERPRETATION?

We have new predictions

A COMMON PROPOSAL?

How to optimise efforts,
combine the newest instrumentation
with the newest, unprecedented
theory perspectives

Recent common publications →

PHYSICAL REVIEW LETTERS **127,** 112501 (2021)

Mass Measurements of Neutron-Deficient Yb Isotopes and Nuclear Structure at the Extreme Proton-Rich Side of the $N = 82$ Shell

Sönke Beck,[1,2,*] Brian Kootte,[3,4] Irene Dedes,[5,6] Timo Dickel,[1,2] A. A. Kwiatkowski,[3,7] Eleni Marina Lykiardopoulou,[8,3] Wolfgang R. Plaß,[1,2] Moritz P. Reiter,[1,3,9] Corina Andreoiu,[10] Julian Bergmann,[1] Thomas Brunner,[11] Dominique Curien,[12] Jens Dilling,[3,8] Jerzy Dudek,[12,6] Eleanor Dunling,[3,13] Jake Flowerdew,[14] Abdelghafar Gaamouci,[15] Leigh Graham,[3] Gerald Gwinner,[4] Andrew Jacobs,[8,3] Renee Klawitter,[3] Yang Lan,[8] Erich Leistenschneider,[8,3] Nikolay Minkov,[16] Victor Monier,[3] Ish Mukul,[3] Stefan F. Paul,[3] Christoph Scheidenberger,[1,2,17] Robert I. Thompson,[14] James L. Tracy, Jr.,[3] Michael Vansteenkiste,[3] Hua-Lei Wang,[18] Michael E. Wieser,[14] Christian Will,[1] and Jie Yang[6,18]

Recent common publications →

Physics Letters B 802 (2020) 135200

Contents lists available at ScienceDirect

Physics Letters B

www.elsevier.com/locate/physletb

Isomer studies in the vicinity of the doubly-magic nucleus ^{100}Sn: Observation of a new low-lying isomeric state in ^{97}Ag

Christine Hornung[a,*], Daler Amanbayev[a], Irene Dedes[b], Gabriella Kripko-Koncz[a], Ivan Miskun[a], Noritaka Shimizu[c], Samuel Ayet San Andrés[a,d], Julian Bergmann[a], Timo Dickel[a,d], Jerzy Dudek[e,b], Jens Ebert[a], Hans Geissel[a,d], Magdalena Górska[d], Hubert Grawe[d], Florian Greiner[a], Emma Haettner[d], Takaharu Otsuka[f], Wolfgang R. Plaß[a,d], Sivaji Purushothaman[d], Ann-Kathrin Rink[a], Christoph Scheidenberger[a,d], Helmut Weick[d], Soumya Bagchi[a,d,g], Andrey Blazhev[h], Olga Charviakova[i], Dominique Curien[e], Andrew Finlay[j], Satbir Kaur[g], Wayne Lippert[a], Jan-Hendrik Otto[a], Zygmunt Patyk[i], Stephane Pietri[d], Yoshiki K. Tanaka[d], Yusuke Tsunoda[c], John S. Winfield[d]

These Lines of Thinking Were Tested ...

Recent common experiment proposals / LoI's $\rightarrow$

... we can quote 5 recent initiatives in these categories

This presentation →

We discuss a selection of Physics Themes

which could provide platforms

for Experiment & Theory Collaborations

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K-isomers,
Yrast trap isomers and yrast lines,
Shape isomers,
In particular fission isomers, etc.;

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New/Improved measurements of nuclear masses

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2. **Nuclear Masses**

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3. **Rotational band properties**

Bands – in particular – bands based on isomers,
Quasi-particle band structures,
Band crossings and interactions,
Shape evolution with spin,
So-called pairing phase transitions, etc.;

4. Exotic symmetries and shapes

Tetrahedral and octahedral symmetries (freshly discovered)
Super-deformation, Hyper-deformation,
Toroidal shapes,
Shapes leading to tripartition, etc.;

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Competing fission paths,
Local-minimum to local-minimum transitions, etc.;

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Competing fission paths,
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6. Specific nuclear excitations modes

Modes involving increasing temperatures,
Modes involving increasing spins,
Giant Dipole Resonances,
Jacobi and Poincaré shape transitions, etc.;

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EUROPEAN LABORATORIES FOR ACCELERATOR BASED SCIENCES

EUROPEAN LABORATORIES FOR ACCELERATOR BASED SCIENCE

SHORT NAME: **EURO-LABS**

DEPOSITED PROJECT*)

MeanField4Exp: User-Friendly Interface to the Advanced Nuclear-Structure Theory Calculations

[Spokesperson: J. DUDEK, Université de Strasbourg, IPHC/IN$_2$P$_3$/CNRS, France]

Collaborators:

Adam MAJ, Piotr BEDNARCZYK, Irene DEDES, Bogdan FORNAL
IFJ PAN Cracow, Poland

Paweł NAPIÓRKOWSKI, Krzysztof RUSEK
HIL Warsaw University Warsaw, Poland

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*) Even if proponents hope for the best, the project may (or may not) be funded

EUROpean Laboratories for Accelerator Based Science

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• About MeanField4Exp Proposal

– Providing Research Infrastructure users a mean-field theory based universal-use software allowing a non-expert to produce state-of-the-art and standard today theory results comparable with experiment

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Theory Results with Theoretical Uncertainties

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– Large spectrum of nuclear structure subfields covers many mechanisms of potential interest at GSI/FAIR, GANIL/SPIRAL2, LNL/SPES, ALTO, ISOLDE, JYFL, HIL Warsaw, CCB Cracow, and, and, and ...

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– The subjects covered in this European Project cover nearly the full list just shown

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But does your theory have predictive power?

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→ He added:

Did you read the special Editorial of Physical Review requesting analysis of uncertainties of theoretical calculations?

Editorial: Uncertainty Estimates, PHYSICAL REVIEW **A 83**, 040001 (2011)

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→ We answered:

Elementary! We have been doing this type of estimates*) for quite some time by now !!!

*) *Open Problems in Nuclear Theory*, J Dudek and collaborators, J. Phys. G: Nucl. Part. Phys. 37 (2010) 064031

PHYSICAL REVIEW A **83**, 040001 (2011)

Editorial: Uncertainty Estimates

The purpose of this Editorial is to discuss the importance of including uncertainty estimates in papers involving theoretical calculations of physical quantities.

It is not unusual for manuscripts on theoretical work to be submitted without uncertainty estimates for numerical results. In contrast, papers presenting the results of laboratory measurements would usually not be considered acceptable for publication in *Physical Review A* without a detailed discussion of the uncertainties involved in the measurements. For example, a graphical presentation of data is always accompanied by error bars for the data points. The determination of these error bars is often the most difficult part of the measurement. Without them, it is impossible to tell whether or not bumps and irregularities in the data are real physical effects, or artifacts of the measurement. Even papers reporting the observation of entirely new phenomena need to contain enough information to convince the reader that the effect being reported is real. The standards become much more rigorous for papers claiming high accuracy.

The question is to what extent can the same high standards be applied to papers reporting the results of theoretical calculations. It is all too often the case that the numerical results are presented without uncertainty estimates. Authors sometimes say that it is difficult to arrive at error estimates. Should this be considered an adequate reason for omitting them? In order to answer this question, we need to consider the goals and objectives of the theoretical (or computational) work being done. Theoretical papers can be broadly classified as follows:

1. Development of new theoretical techniques or formalisms.
2. Development of approximation methods, where the comparison with experiment, or other theory, itself provides an assessment of the error in the method of calculation.
3. Explanation of previously unexplained phenomena, where a semiquantitative agreement with experiment is already significant.
4. Proposals for new experimental arrangements or configurations, such as optical lattices.
5. Quantitative comparisons with experiment for the purpose of (a) verifying that all significant physical effects have been taken into account, and/or (b) interpolating or extrapolating known experimental data.
6. Provision of benchmark results intended as reference data or standards of comparison with other less accurate methods.

It is primarily papers in the last two categories that require a careful assessment of the theoretical uncertainties. The uncertainties can arise from two sources: (a) the degree to which the numerical results accurately represent the predictions of an underlying theoretical formalism, for example, convergence with the size of a basis set, or the step size in a numerical integration, and (b) physical effects not included in the calculation from the beginning, such as electron correlation and relativistic corrections. It is of course never possible to state precisely what the error is without in fact doing a larger calculation and obtaining the higher accuracy. However, the same is true for the uncertainties in experimental data. The aim is to estimate the uncertainty, not to state the exact amount of the error or provide a rigorous bound.

There are many cases where it is indeed not practical to give a meaningful error estimate for a theoretical calculation; for example, in scattering processes involving complex systems. The comparison with experiment itself provides a test of our theoretical understanding. However, there is a broad class of papers where estimates of theoretical uncertainties can and should be made. Papers presenting the results of theoretical calculations are expected to include uncertainty estimates for the calculations whenever practicable, and especially under the following circumstances:

1. If the authors claim high accuracy, or improvements on the accuracy of previous work.
2. If the primary motivation for the paper is to make comparisons with present or future high precision experimental measurements.
3. If the primary motivation is to provide interpolations or extrapolations of known experimental measurements.

These guidelines have been used on a case-by-case basis for the past two years. Authors have adapted well to this, resulting in papers of greater interest and significance for our readers.

The Editors

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PACS number(s): 01.30.Ww

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The question is to what extent can the same high standards be applied to papers reporting the results of theoretical calculations. It is all too often the case that the numerical results are presented without uncertainty estimates. Authors sometimes say that it is difficult to arrive at error estimates. Should this be considered an adequate reason for omitting them? In order to answer this question, we need to consider the goals and objectives of the theoretical (or computational) work being done. Theoretical papers can be broadly classified as follows:

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Part I

Nuclear Theories Linked with Experiments: Predictive-Power Perspective

Our research projects are formulated within the following

Stochastic Interpretation of Predictive Power *)

*) **Introduced in "Open Problems in Nuclear Theory", J Dudek and collaborators, J. Phys. G: Nucl. Part. Phys. 37 (2010) 064031**

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Stochastic Interpretation of Predictive Power[*)]

- Given theory $\mathcal{T}$, of a quantum phenomenon $\mathcal{P}$, employing observables
$$\hat{\mathcal{F}}_1, \hat{\mathcal{F}}_2, \ldots \hat{\mathcal{F}}_p$$

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- Observables will be characterised not only by related eigenvalues i.e. $\{f_j\}$
$$\big[\hat{\mathcal{F}}_1 \to \{f_1\}, \quad \hat{\mathcal{F}}_2 \to \{f_2\}, \quad \ldots\ \hat{\mathcal{F}}_p \to \{f_p\}\big]$$

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but also by distributions of probability of their validity - or applicability
$$\mathcal{P}_1 = \mathcal{P}_1(f_1), \;\; \mathcal{P}_2 = \mathcal{P}_2(f_2), \; \ldots \; \mathcal{P}_p = \mathcal{P}_1(f_p)$$

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Predictive Power of Theories: Stochastic Approach

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but also by distributions of probability of their validity - or applicability
$$\mathcal{P}_1 = \mathcal{P}_1(f_1),\ \ \mathcal{P}_2 = \mathcal{P}_2(f_2),\ \ldots\ \mathcal{P}_p = \mathcal{P}_1(f_p)$$
- These distributions are obtained using stochastic methods on the basis of **uncertainties known-, or possible to estimate today**

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Theory-Errors Limit Theory's Predictive Power

- **There exist effective means of limiting the negative impact of the ignorance originating from incompleteness of information**

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- **In other words: We estimate which answer is more,- and which less-likely 'the right solution'. Expressed alternatively:**

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Find relative probability of what we think the right answer is!

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1. Our ignorance is usually represented by a random variable X

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Conclusion: Not knowing 'the truth' we may introduce several competing hypotheses & calculate their relative probabilities!

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"Adso, if I had, I would teach theology in Paris"

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"Never", said William,
"but there they are quite confident of their errors".

Part II

About Fundamental Method of Parameter Optimisation of Applied Mathematics:

Inverse Problem Theory

- Consider an arbitrary, e.g., many-body theory with its Hamiltonian:

$$\boxed{\hat{H} = \hat{T} + \hat{V}_{int}(\ldots\{p\}); \quad \{p\} \to \text{optimal parameters}}$$

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- However, before any comparison theory-experiment, and even more generally: Before any calculation we must solve the Inverse Problem:

Determine Hamiltonian parameters using experimental data

- Given parameters $\{p\}$ $\rightarrow$ The theoretical modeling produces data:

$$\hat{H}(p) \rightarrow \{E_p, \psi(p)\} \leftrightarrow \boxed{\hat{\mathcal{O}}_H(p) = d^{th} \leftarrow \textit{Direct Problem}}$$

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- To find the optimal parameters we must invert the above relation:

$$\boxed{p^{opt} = \hat{\mathcal{O}}_H^{-1}(d^{exp}) \leftarrow \textit{Inverse Problem}}$$

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- Since $\mathcal{O}_H^{-1}$ remains unknown, instead of solving Inverse Problem
  $\rightarrow$ "In physics – one minimises χ^2 "

- If the Inverse Problem is ill-posed, equation $p^{opt} = \hat{\mathcal{O}}_H^{-1}(d^{exp})$ cannot be solved, there is no relation between experimental data and the Hamiltonian parameters in this model – no way to find p^{opt}

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No reason to employ χ^2 because no solution exists

- "Fortunately", since we have no way of constructing $\hat{\mathcal{O}}_H^{-1}$, we do not know whether our projects are ill-posed or not, we hope for the best and engage χ^2-minimisation – but there will be a price to pay!

- If the Inverse Problem is ill-posed, equation $p^{opt} = \hat{\mathcal{O}}_H^{-1}(d^{exp})$ cannot be solved, there is no relation between experimental data and the Hamiltonian parameters in this model – no way to find p^{opt}

- In other words: Correlation between parameters and data is lost!

$$\boxed{\text{No reason to employ } \chi^2 \text{ because no solution exists}}$$

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- **Finding the minimum will be just the beginning, not the end**

About the So-Called Chi-By-the-Eye "Method"

• After laborious theoretical constructions, we get terribly exhausted and forget that: *Professional parameter determination is a noble, mathematically sophisticated procedure based on statistical theories often more involved than the physical problems under our studies!*

Theory and Its Possible Statistical In-Significance

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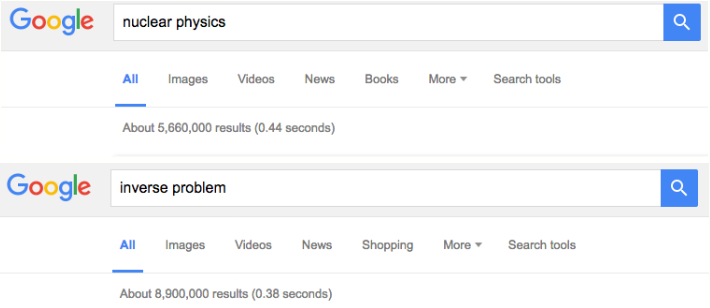

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• In their introduction to the book chapter *'Modelling of Data'*, the authors of *'Numerical Recipes*" (p. 651), observe with sarcasm:

"Unfortunately, many practitioners of parameter estimation never proceed beyond determining the numerical values of the parameter fit. They deem a fit acceptable if a graph of data and model ' l o o k s   g o o d '. This approach is known as chi-by-the-eye. Luckily, its practitioners get what they deserve" [what is meant is: "they" obtain a 'meaningless result']

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• **Meaningless result ← less politely → Equivalent to random numbers**

Part III

How to profit from χ^2-techniques

(Or: How to "χ^2 professionally")

Using χ^2 Instead of $\hat{\mathcal{O}}_H^{-1}$

- We know that in principle we should solve this $\boxed{p^{opt} = \hat{\mathcal{O}}_H^{-1}(d^{exp})}$

- On the other hand, we are forced to do this $\boxed{\min_p \chi^2(p^{opt}) = \,?}$

- One may show an existence of an algebraic linearised representation

$$\boxed{\frac{\partial \chi^2}{\partial p_i} = 0 \;\; \rightarrow \;\; (J^T J) \cdot p = J^T\, d^{exp} \;\; \leftrightarrow \;\; J^T J \overset{df}{=} \mathcal{A}}$$

- We thus obtain an algebraic analogue of $p^{opt} = \hat{\mathcal{O}}_H^{-1}(d^{exp})$

$$\boxed{\underbrace{\mathcal{A} \cdot \mathcal{P} = \mathcal{D}^{\exp}}_{\text{Direct Problem}} \;\rightarrow\; \underbrace{\mathcal{P} = \mathcal{A}^{-1} \cdot \mathcal{D}^{\exp}}_{\text{Inverse Problem}} \;\leftrightarrow\; \mathcal{D}^{\exp} \equiv J^T d^{exp}}$$

- We consider the linear equations: $\boxed{\mathcal{P} = \mathcal{A}^{-1} \cdot \mathcal{D} \leftrightarrow \mathcal{P} = \mathcal{C} \cdot \mathcal{D}}$

$$\text{Parameters} \rightarrow \begin{bmatrix} \mathcal{P}_1 \\ \mathcal{P}_2 \\ \cdots \\ \mathcal{P}_m \end{bmatrix} = \underbrace{\begin{bmatrix} \mathcal{C}_{11} & \mathcal{C}_{12} & \cdots & \mathcal{C}_{1d} \\ \mathcal{C}_{21} & \mathcal{C}_{22} & \cdots & \mathcal{C}_{2d} \\ \cdots & \cdots & \cdots & \cdots \\ \mathcal{C}_{m1} & \mathcal{C}_{m2} & \cdots & \mathcal{C}_{md} \end{bmatrix}}_{\text{m}\times\text{d rectangular matrix}} \begin{bmatrix} \mathcal{D}_1 \\ \mathcal{D}_2 \\ \cdots \\ \mathcal{D}_d \end{bmatrix} \leftarrow \text{Data}$$

Stability of Solutions of "χ^2 Inverse Problem"

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- If this happens $\rightarrow$ $\mathcal{C}$-matrix becomes singular [Ill-Posed Problem]

If we wish using χ^2 – parameter correlations must be removed

Part IV

Detection of Parametric Correlations and Their Removal

ILLUSTRATIONS

Parameter Correlations and Correlation Matrix [WS]

- Given random variables X and Y. Correlation matrix in this case:

$$\mathrm{corr}(X,Y)=\frac{\sum_i[(X_i-\bar{X})(Y_i-\bar{Y})]}{\sqrt{\sum_i(X_i-\bar{X})^2}\sqrt{\sum_i(Y_i-\bar{Y})^2}};\;\; \bar{X}\equiv\frac{1}{n}\sum_{i=1}^{n}X_i,\;\; \bar{Y}\equiv\frac{1}{n}\sum_{i=1}^{n}Y_i$$

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- Generally: $\{X, Y\} \to \{X_k\} = \{V_0^c, r_0^c, a_0^c, V_0^{so}, r_0^{so}\}$ we obtain:

Correlation matrix for the Woods-Saxon Hamiltonian parameters
as obtained from the Monte-Carlo simulation

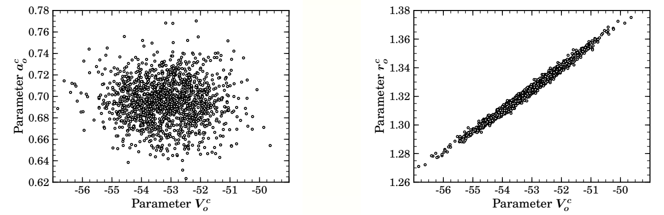
	V_0^c	r_0^c	a_0^c	V_0^{so}	r_0^{so}
V_0^c	1.000	0.994	-0.028	0.000	0.265
r_0^c	0.994	1.000	0.016	0.005	0.270
a_0^c	0.028	0.016	1.000	0.259	0.288
V_0^{so}	0.000	0.005	0.259	1.000	0.506
r_0^{so}	0.265	0.270	0.288	0.506	1.000

The non-diagonal matrix elements close to 1 signify strong matrix correlations

Verbal Description of Monte-Carlo Simulations

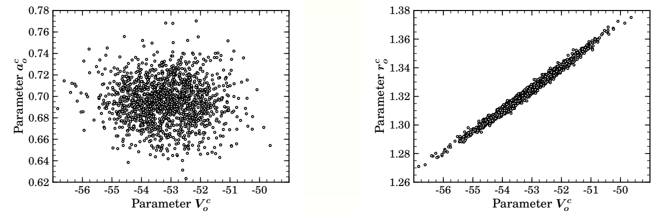
One can demonstrate that parametric correlations of this kind can conveniently be studied using Monte Carlo methods

- **Given space of data $\{d_1, d_2, \dots\ d_{\rm n}\}$ with uncertainty σ**
- **With random-number generator we define Gaussian 'noise' distribution around each d_i**
- **We fit the parameter sets great number of times, $\mathcal{N}$**
- **From m-tuplets of so obtained parameters, $\{p_1, p_2, \dots\ p_m\}$, we construct the tables and projection plots like the ones which follow**



Monte-Carlo fitting results for ^{208}Pb with the Woods-Saxon potential
Left:(a_0^c vs. V_0^c)-plane and Right: (r_0^c vs. V_0^c)-plane

Parameter-Correlations and Correlation Matrix [WS]



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Parametric Correlations for Skyrme Hamiltonian

To follow the illustrations it will be sufficient to know that our Skyrme Hamiltonian depends 6 adjustable constants:

$$C_0^{\rho},\, C_1^{\rho},\, C_o^{\rho\alpha},\, C_0^{\tau},\, C_1^{\tau},\, C_0^{\nabla J}$$

Parameter-Correlations in Skyrme-HF

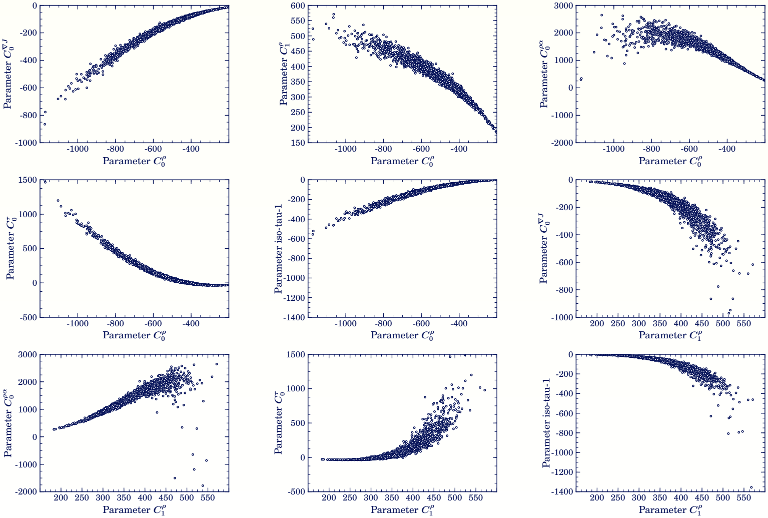

Illustration suggesting that majority of these parameters are strongly correlated excluding the prediction capacities of the model [B. Szpak, PhD thesis]

Part V

Uncertainty Probability Densities

ILLUSTRATIONS

- **Observe than in the presented example uncertainties increase with angular momentum**

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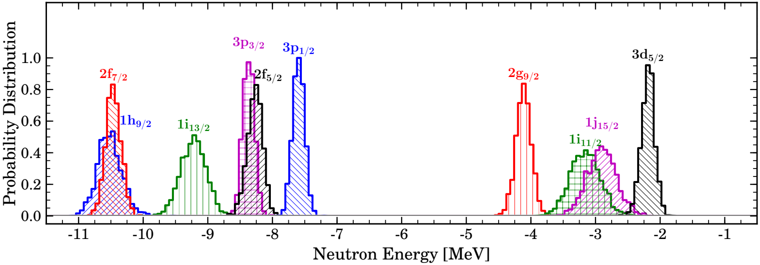
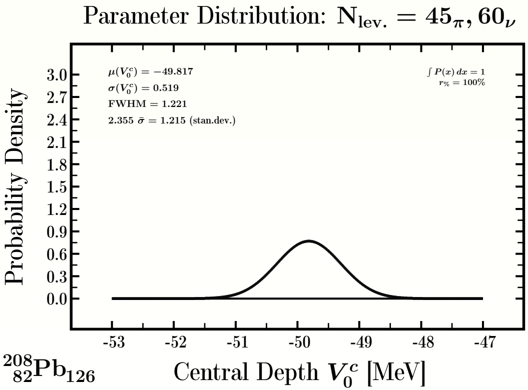


Single-neutron uncertainty probability distributions for ^{208}Pb with our ‘universal’ Woods-Saxon Hamiltonian

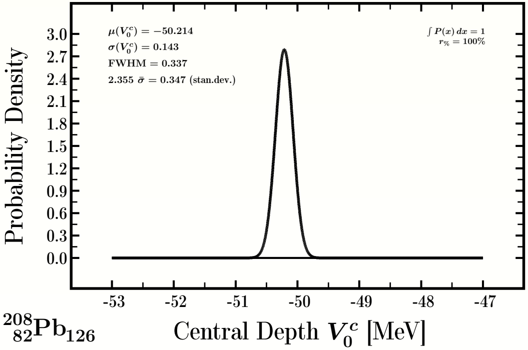
- **Parametric correlations present**



Probability of Uncertainty. Here: Central potential depth, V_0^c, for Woods-Saxon Universal

- **Parametric correlations removed**

Parameter Distribution: $\mathbf{N_{lev.} = 45_\pi, 60_\nu}$



$^{208}_{82}\mathrm{Pb}_{126}$

Probability of Uncertainty. Here: Central potential depth, V_0^c, for Woods-Saxon Universal

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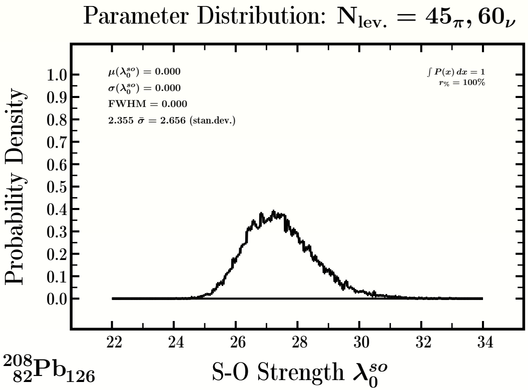
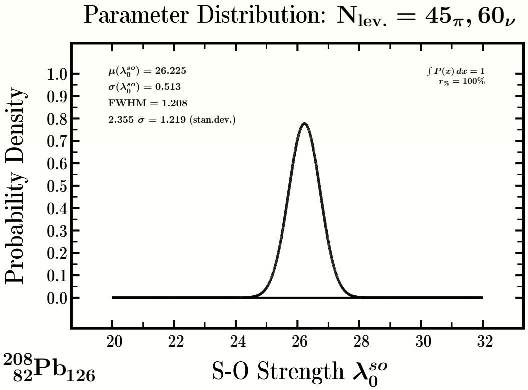


Probability of Uncertainty. Here: Central potential depth, λ_0^{so}, for Woods-Saxon Universal

- **Parametric correlations removed**



Probability of Uncertainty. Here: Central potential depth, λ_0^{so}, for Woods-Saxon Universal

Part V

Extraordinary Shell Effects*) in Light Nuclei

*) **Exotic toroidal and super-deformed configurations in light atomic nuclei: Predictions using a mean-field Hamiltonian without parametric correlations;**

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Extraordinary Shell Effect in Light Nuclei

- We have re-adjusted the new set of the Universal WS parameters
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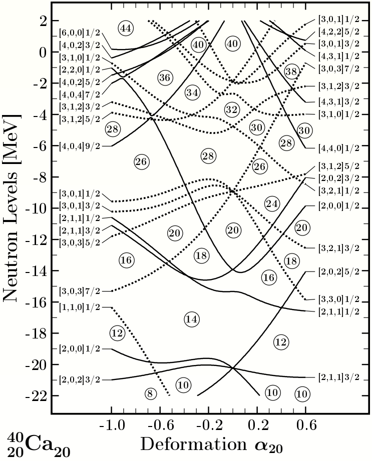
• Since parametric correlation are removed we stabilise predictions for exotic nuclei $\rightarrow$ we believe that other predictions are trustworthy

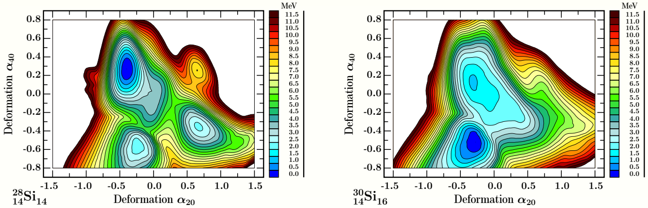
Extraordinarily Strong Shell Effect in Light Nuclei



- **Note that the shell-gaps for strongly oblate nuclei are significantly stronger than those for the spherical ones – contrasting with beliefs**

Prediction of Exotic Shapes and Structures in Light Nuclei

Super-Hexadecapole Shapes Never Seen



- Hexadecapole deformations α_{40} are stronger than large quadrupole α_{20} ones – to our knowledge the mechanism never seen in the literature

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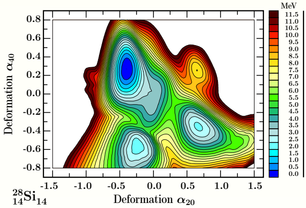

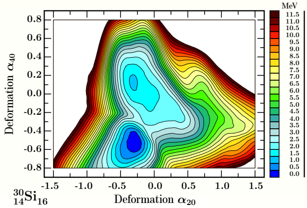

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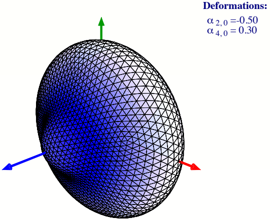
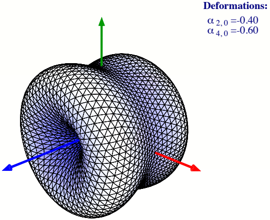
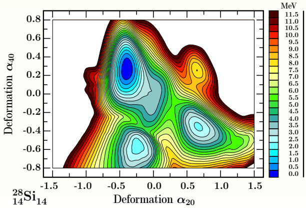
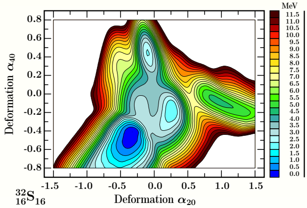




- The corresponding shapes: SUPER-OBLATE and TOROIDAL

Super-, Hyper-Deformed Shapes Never Seen





- Focus on very elongated shapes with $\alpha_{20} > 0$

$\rightarrow$ to our knowledge the effect never seen in the literature

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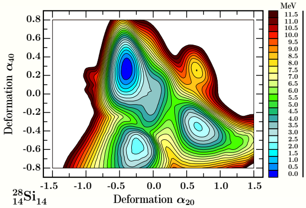

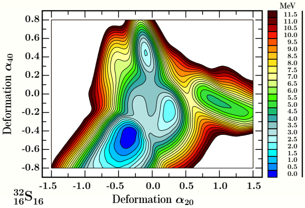

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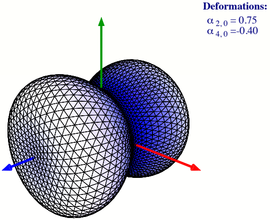

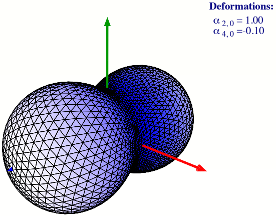

- Exotic SUPER-DEFORMED and HYPER-DEFORMED shapes

Part VI

From Unprecedented Extreme Shapes To Unprecedented Exotic Shapes*)

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

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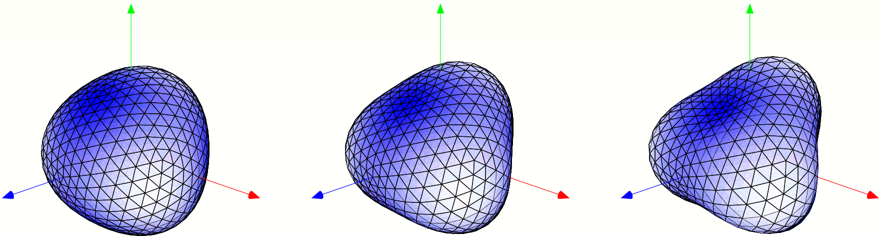
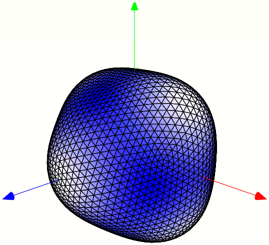
About Newly Discovered Tetrahedral and Octahedral Symmetries



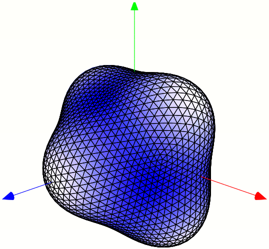
$\alpha_{32} \equiv t_3 = 0.1$ $\alpha_{32} \equiv t_3 = 0.2$ $\alpha_{32} \equiv t_3 = 0.3$

Examples: Nuclear TETRAHEDRAL symmetry shapes

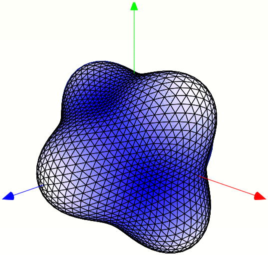
About Newly Discovered
Tetrahedral and Octahedral Symmetries



$o_4 = 0.1$



$o_4 = 0.2$

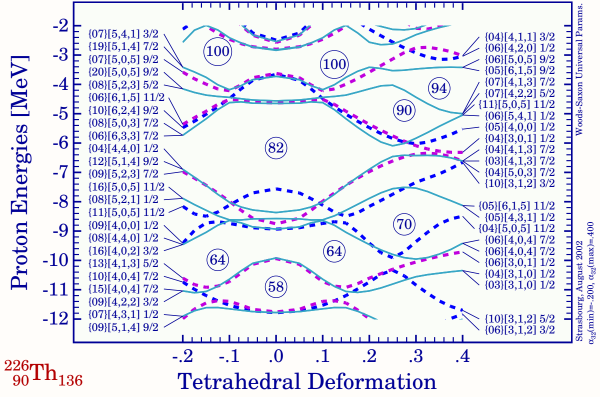


$o_4 = 0.3$

Examples: Nuclear OCTAHEDRAL symmetry shapes

Nuclear Tetrahedral Shapes - Proton Spectra

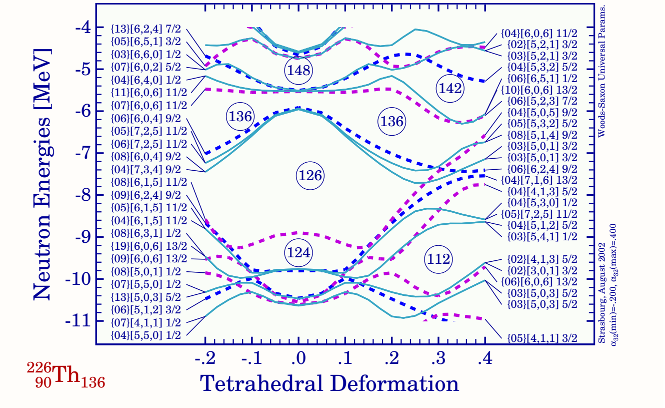
Double group T_d^D has two 2-dimensional - and one 4-dimensional irreducible representations: Three distinct families of nucleon levels



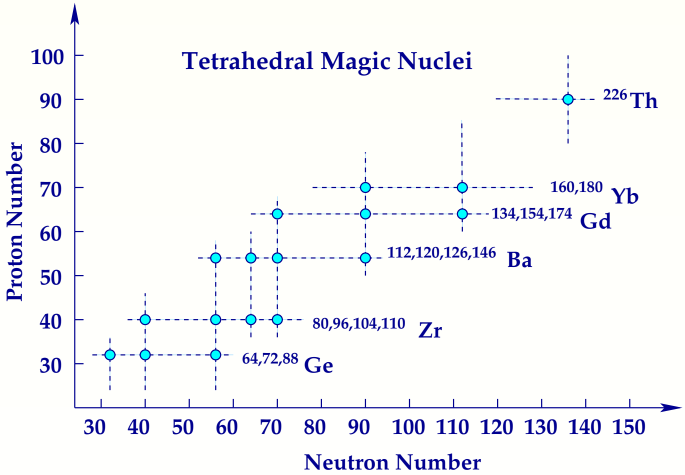
Full lines $\leftrightarrow$ 4-dimensional irreducible representations - marked with double Nilsson labels. Observe huge gaps at N=64, 70, 90-94, 100.

Nuclear Tetrahedral Shapes - Neutron Spectra

Double group T_d^D has two 2-dimensional - and one 4-dimensional irreducible representations: Three distinct families of nucleon levels

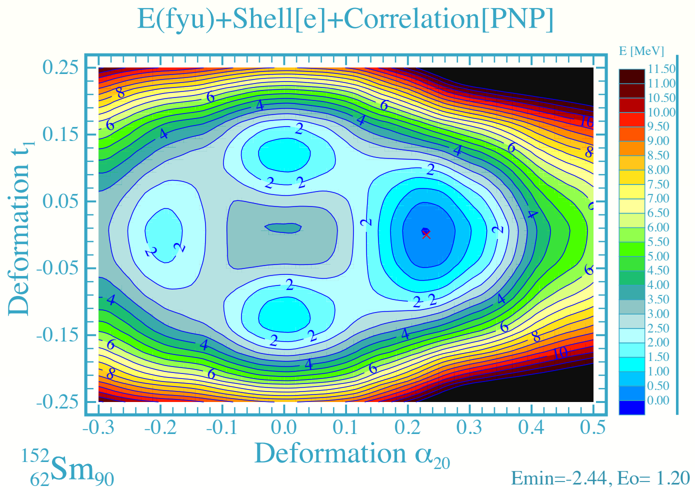


Full lines ↔ 4-dimensional irreducible representations - marked with double Nilsson labels. Observe huge gaps at N=112, 136.



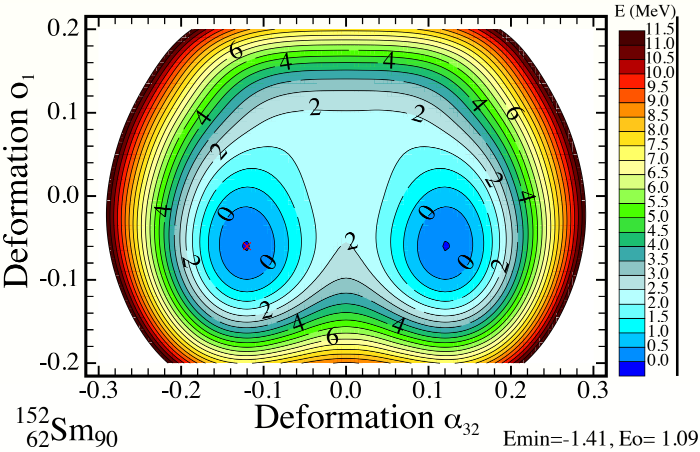
It is essential to recall that in the exact symmetry limit tetrahedral nuclei <u>emit neither E2 nor E1 transitions</u> $\rightarrow$ ISOMERS

The Following Discussion Is Focussed on ^{152}Sm



- **Symmetric minima at $\alpha_{20} = 0$ represent tetrahedral symmetry**

The Following Discussion Is Focussed on ^{152}Sm



- **Tetrahedral minima at $\alpha_{32} = \pm 0.13$ are accompanied by non-vanishing octahedral deformation $o_1 \approx -0.06$**

In what follows we take into account both tetrahedral and octahedral shape components simultaneously

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This decision is encouraged by the fact that the tetrahedral symmetry point group is a sub-group of the octahedral symmetry one

Quantum Rotors: Tetrahedral vs. Octahedral

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

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Quantum Rotors: Tetrahedral vs. Octahedral

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- One shows that the analogue structure in the octahedral symmetry

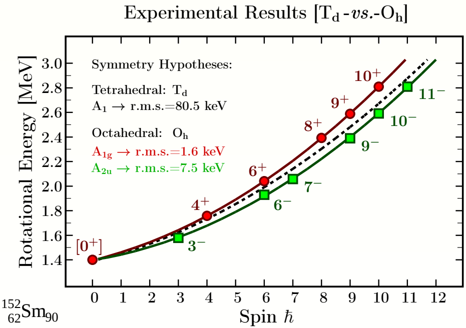
$$\underbrace{A_{1g}: \; 0^+, 4^+, 6^+, 8^+, 9^+, 10^+, \; \ldots, \quad I^\pi = I^+}_{\textbf{Forming a common parabola}}$$

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

As a result of the "group / sub-group relation"

we should expect 2 parabolic structures

- **These two sequences represent the coexistence between tetrahedral and octahedral symmetries. Curves represent the parabolic fit and are not meant to guide the eye. This is the first evidence based on the experimental data**



FROM: **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)

- **After publication of the first discovery in subatomic physics:**

Spectroscopic Criteria for Identification of Nuclear Tetrahedral and Octahedral Symmetries: Illustration On a Rare Earth Nucleus

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

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

The journal Frontiers in Physics invites a special edition with the working title: "Tetrahedral ad Octahedral Symmetries: Crypto-Symmetries in Nuclear Physics"

[Guest Editor J. D.]

- We invite texts addressing GENERALLY physics of exotic symmetries $\neq$ quadrupole

Part VII

Microscopic View of Collective Nuclear Rotation

• **Some authors chose comparing experimental and theoretical rotational bands in the form of energy to energy comparisons**

Possibly High Precision Level In the Description I

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- **A higher precision is offered by employing the first derivatives**

$$\boxed{I_y(I,K) \equiv \sqrt{I(I+1)-K^2}} \quad \leftrightarrow \quad \boxed{\omega_y(I) \to \frac{dE_I}{dI_y} \approx \frac{E_{I+1}-E_{I-1}}{I_y(I+1)-I_y(I-1)}}$$

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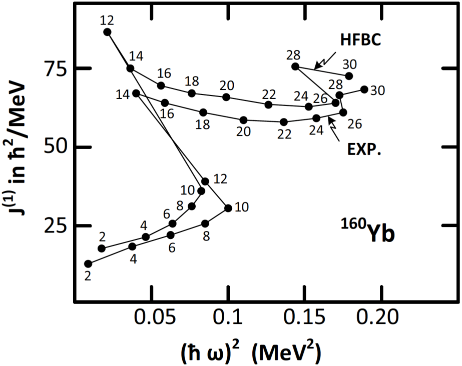
- **The notion of frequency $\omega_y(I)$ leads to kinematical moments**

$$\boxed{\mathcal{J}_y^{(1)}(I) \equiv \frac{I_y(I)}{\omega_y(I)}}$$

Possibly High Precision Level In the Description I

- We apply the Hartree-Fock-Bogolyubov self-consistent Cranking method and the Woods-Saxon 'Universal' mean field approximation



- Observe reproduction of a double back-bending (no parameter fit)

Possibly Highest Precision Level In the Description II

- **Higher precision of comparison is offered by 2^{nd} derivatives**

$$\boxed{J_y^{(2)} \equiv \left[\frac{d^{\,2} E_I}{dI_y^2}\right]^{-1} = \left[\frac{d\omega_y}{dI_y}\right]^{-1} = \frac{dI_y}{d\omega_y},}$$

- **Simplifying notation we find dynamical moments as follows**

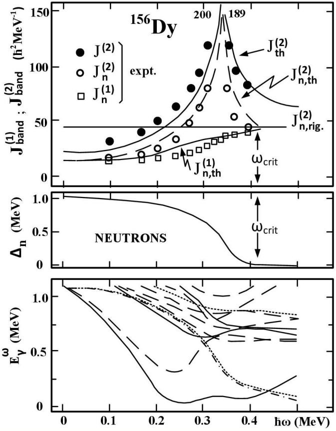
$$\boxed{J_y^{(2)} = J_y^{(1)} + \omega_y \frac{dJ_y^{(1)}}{d\omega_y} \;\leftrightarrow\; J^{(2)} = J^{(1)} + \omega \frac{dJ^{(1)}}{d\omega}}$$

- We apply the Hartree-Fock-Bogolyubov self-consistent Cranking method and the Woods-Saxon ‘Universal’ mean field approximation

- Dynamical $\mathcal{J}^{(2)}$ moments (HFBC) compared to experiment; observe manifestation of the pairing phase transition and the related $\mathcal{J}^{(2)}$-peak

- Neutron pairing gap-Δ_n calculated self-consistently. Here $\omega_{\rm crit}$ denotes cranking frequency for vanishing gap

- Neutron single quasiparticle levels



- Observe reproduction of the $\mathcal{J}^{(2)}$ peak-position (no parameter fit)

Why Important for Experiment-Theory Projects?

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• By placing an odd-nucleon on the high-j orbital (neighbouring odd-A nuclei) the 2qp alignments (back-bending) are blocked and by checking this – we double-check the exactitude of interpretations

Part VIII

K-Isomers and Yrast-Traps: Building Blocks of Understanding the Underlying Nucleonic Structure

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- **What are they?**

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K-Isomers and Yrast - Traps: Building Blocks of Understanding the Underlying Nucleonic Structure

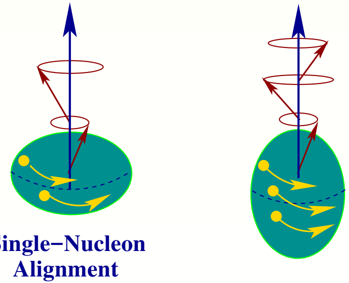
- What are they?
- Their role as the stepping stones in γ-spectrometry, in mass-spectrometry, in nuclear structure recognition . . .

Condition Sine-Quoi-Non: <u>Axial</u> Symmetry

• We use the mean-field approach; In the case of axial symmetry with respect to, say $\mathcal{O}_z$-axis, we have:

$$\boxed{[\hat{H}, \hat{\jmath}_z] = 0}$$

Projections of Angular Momenta Are Conserved in the Presence of Axial Symmetry



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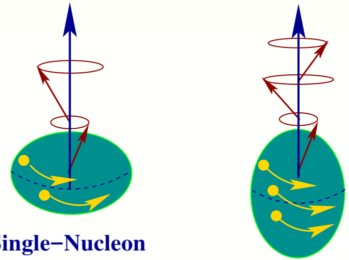

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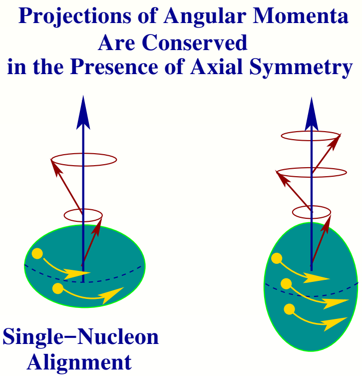
- Maximum alignment Ansatz

$$\boxed{I \approx M = \sum_\nu m_\nu}$$



Following A. Bohr: Tilted Fermi Surface Method

- Find the minimum of the sum $\boldsymbol{E} = \sum_\nu \boldsymbol{e}_\nu$ of single nucleon energies under the condition that the spin $\boldsymbol{M} = \sum_\nu \boldsymbol{m}_\nu$ has 'user' prescribed value

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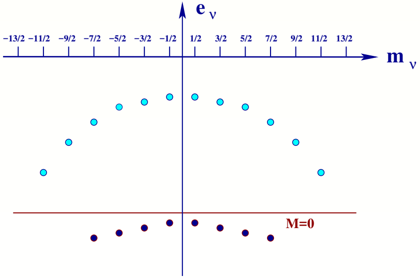

Here: just 'normal' i.e. un-tilted Fermi surface

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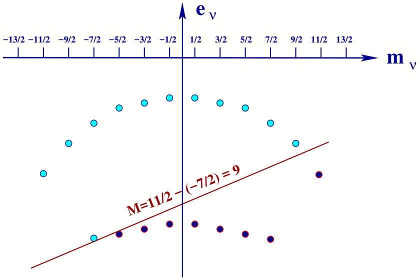

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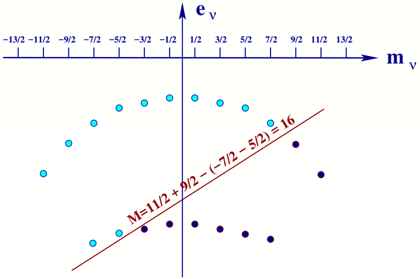


Here: The second titled solution

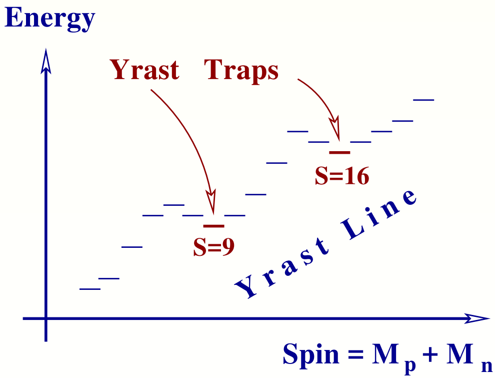
Next step:

Since the titled-Fermi surface solutions come in jumps
we fill in the missing spin values
constructing the particle-hole excitations
with respect to the Lagrange solutions
the latter guaranteed*) yrast!

*) Guaranteed – as the result of the Lagrange minimisation theorem

Particle-Hole Excitations Generate Yrast "Traps"

- **Because of all the jumps and irregularities the resulting *n*-particle *n*-hole excitations are irregular forming local minima (called "yrast traps")**

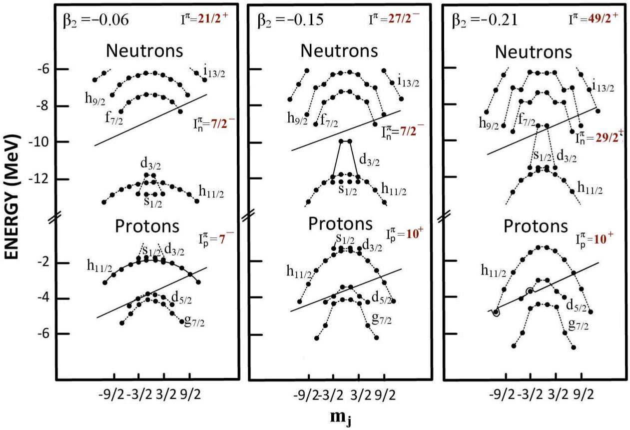


$$\boxed{E^* = \sum_p e_{p,m_p} - \sum_h e_{h,m_h}} \quad \text{and} \quad \boxed{I \approx M^* = \sum_p m_p - \sum_h m_h}$$

Next step:

REALISTIC CALCULATIONS
and
COMPARISON with EXPERIMENT

How Powerful Bohr's Idea Is → See Experiment I

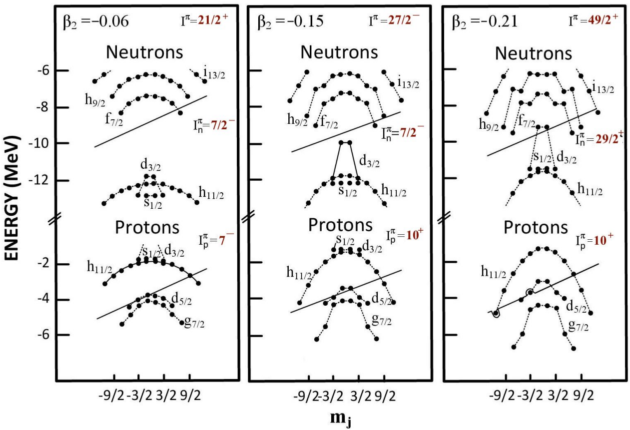


Experimentally known isomers [Theoretical I^π from the diagrams]

$I^\pi = 21/2^+ \leftrightarrow$ 4.50 *ns*

$I^\pi = 27/2^- \leftrightarrow$ 26.8 *ns*

$I^\pi = 49/2^+ \leftrightarrow$ 530 *ns*



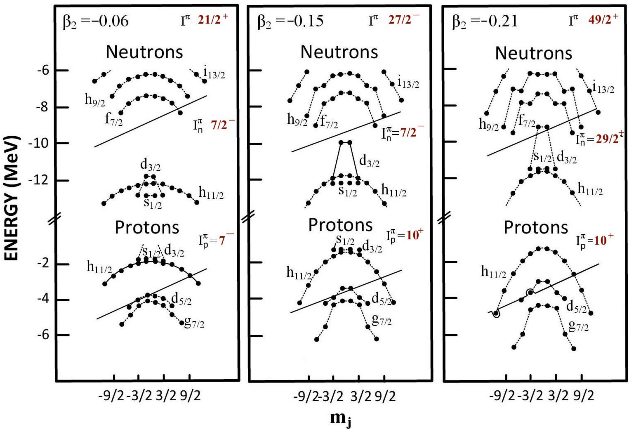
Experimentally known isomers [Theoretical I^π from the diagrams]

$G.s.: \; I^\pi = 7/2^- \leftrightarrow 38\, h$

$I^\pi = 9/2^- \leftrightarrow 0.35\, ps$

$I^\pi = 13/2^+ \leftrightarrow 21.4\, ns$

How Powerful Bohr's Idea Is → See Experiment III



Spins & parities of all experimentally known isomers can be deduced from the diagrams:

E.g. : $\boxed{I^\pi = 19/2^- \leftrightarrow 0.37\ ns}$ is given by $[\pi d^{-2}_{5/2}]_0 \times [h^2_{11/2}]^{\rm max}_6 \times \nu[f^1_{7/2}]^{\rm max}_{7/2}$

How Powerful the Approach Is $\longrightarrow$ See Experiment IV

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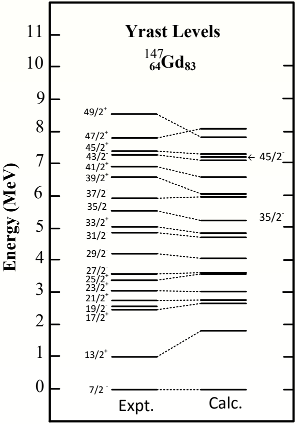

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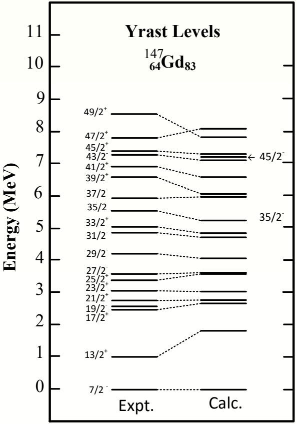

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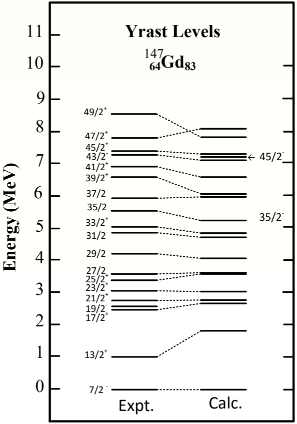

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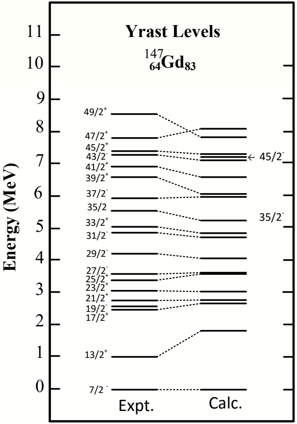
• It is natural to ask:

How many parameters have been fitted to obtain the result on the right?



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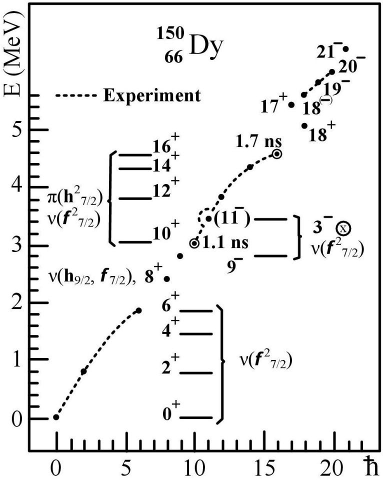
Configurations of 2 nucleons in a j-shell form the "inverted parabolic patterns":

$E_{j^2\to 0},\quad E_{j^2\to 2},\quad E_{j^2\to 4},\quad \ldots E_{j^2\to I_{max}},$

For instance : $f^2_{7/2} \to I = 0, 2, 4, 6$



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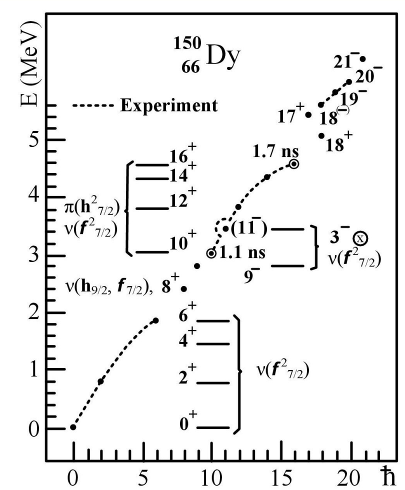

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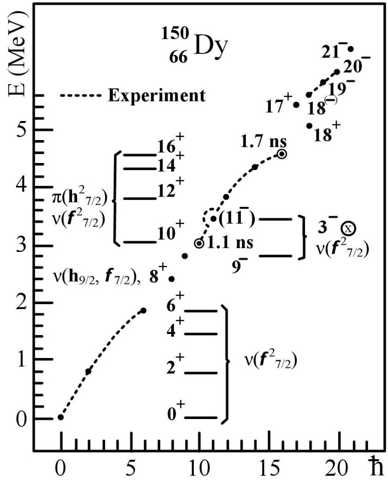
- We show 2 sequences of $f^2_{7/2}$-type, the first one built on the ground-state and yet another one, on the maximum-alignment $h^2_{9/2}$ excited configuration.

- The inverted parabola patterns are easily spotted in the decay spectra and can be used to identify these relatively simple configurations.



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NONE – no parameter adjusted to the presented data;
This is what is meant as Woods-Saxon Universal mean-field

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• The axial-symmetry nuclei may choose to rotate collectively

$$\boxed{(\vec{I} \perp \mathcal{O}_{\text{symmetry}}) \; - \; \text{bands}}$$

as alternative to

$$\boxed{(\vec{I} \parallel \mathcal{O}_{\text{symmetry}}) \; - \; \text{isomers}}$$

or both at the same shape at the same time (in competition).

Why? Which mechanisms cause this or that behaviour?

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– **Signals of spontaneous axial-symmetry breaking [K-mixing]**

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• By the way: No serious tests of the mean-field theory are possible without the cross-checking of the above information!