Realistic Phenomenological Nuclear Mean Field Theory: Physics Background for Experimentalists

Jerzy DUDEK

University of Strasbourg/IPHC/CNRS, France
and
The Henryk Niewodniczański Institute of Nuclear Physics
Polish Academy of Sciences, Kraków, Poland

Trento – Part 1

Theo4Exp EUROLABS Hands-on Workshop

About This Presentation I

In this presentation Phenomenological Mean Field Theory is associated with Woods-Saxon Hamiltonian

About This Presentation I

In this presentation Phenomenological Mean Field Theory is associated with Woods-Saxon Hamiltonian

It turns out that Woods-Saxon Hamiltonian has very special features which remain principally unknown to many colleauges

About This Presentation I

In this presentation Phenomenological Mean Field Theory is associated with Woods-Saxon Hamiltonian

It turns out that Woods-Saxon Hamiltonian has very special features which remain principally unknown to many colleauges

It is strongly advised downloading these slides to learn about our Mean-Field Hamiltonian before learning to use the computer codes

Attention:

This presentation is NOT about clicking on the screen

Attention:

This presentation is NOT about clicking on the screen

It is about explaining Physics Problems solved for you by complex computer codes which were prepared for you by us

Attention:

This presentation is NOT about clicking on the screen

It is about explaining Physics Problems solved for you by complex computer codes which were prepared for you by us

We discuss often unknown aspects of models, very important when applying them and give warnings about oversimplified or incorrect information found in the literature

COLLABORATORS

Irene Dedes

IFJ, Polish Academy of Sciences, Cracow, Poland

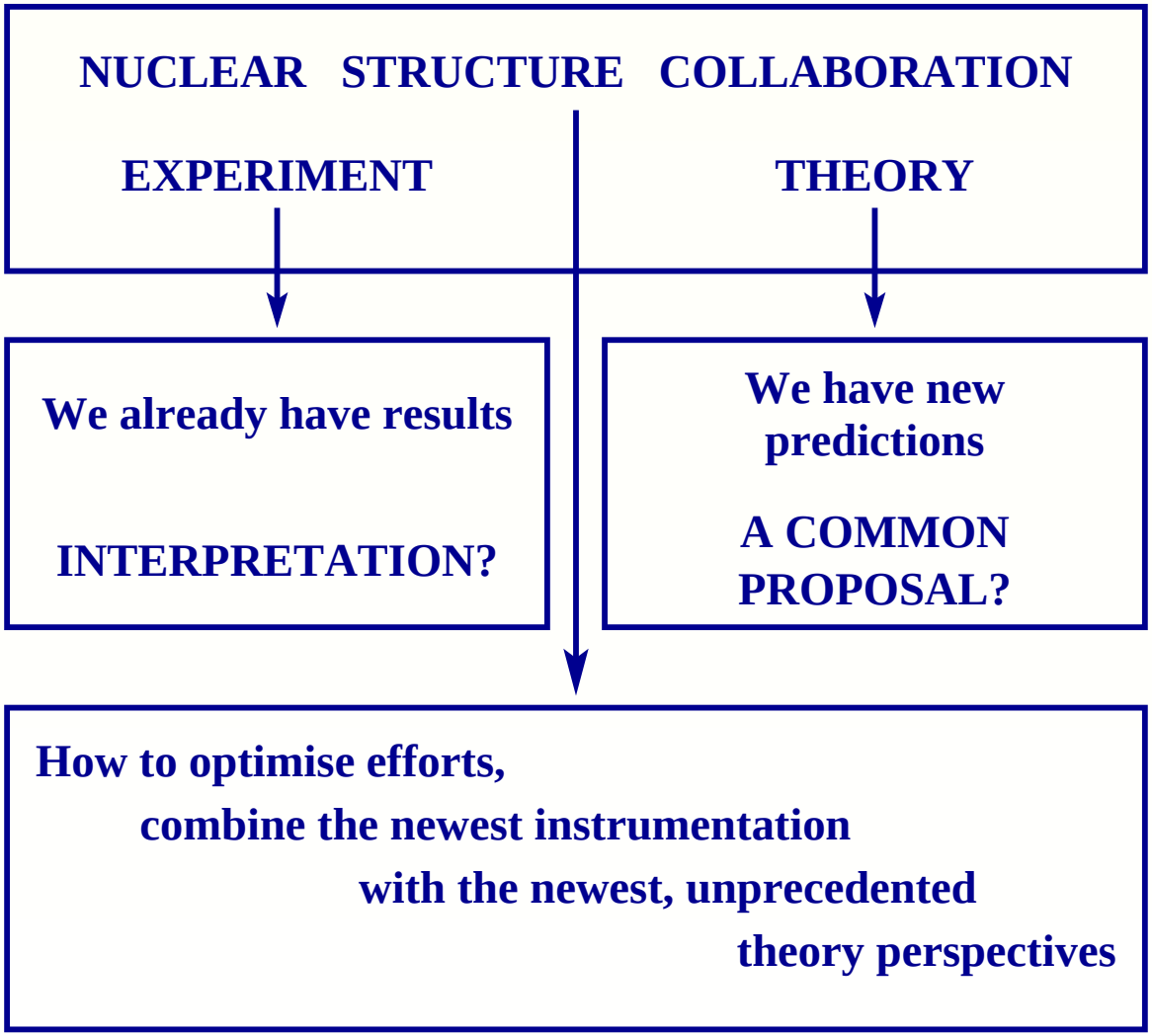
Andrzej Baran

UMCS, Lublin, Poland

Adam Maj, Kasia Mazurek, Michał Ciemała

IFJ, Polish Academy of Sciences, Cracow, Poland

About This Presentation II



About This Presentation III

More precisely $\rightarrow\rightarrow$

It is about nuclear structure projects

which could become

of common experiment & theory interests

Examples of Possible Research Subjects: Part 1

1. Isomers

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

Examples of Possible Research Subjects: Part 1

1. Isomers

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

2. Nuclear Masses

New/Improved measurements of nuclear masses

Examples of Possible Research Subjects: Part 1

1. **Isomers**

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

2. **Nuclear Masses**

New/Improved measurements of nuclear masses

3. **Rotational band properties**

Bands based on isomers,
Quasiparticle band structures,
Band crossings and interactions,
Shape evolution with spin,
So-called paring phase transitions, etc.;

Examples of Possible Research Subjects: Part 2

4. Exotic symmetries and shapes

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

Examples of Possible Research Subjects: Part 2

4. Exotic symmetries and shapes

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

5. Fission and exotic fission modes

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

Examples of Possible Research Subjects: Part 2

4. Exotic symmetries and shapes

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

5. Fission and exotic fission modes

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

6. Specific nuclear excitations modes

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

This Talk is NOT about Clicking: Here Exceptions

Choice of LINKS to click:

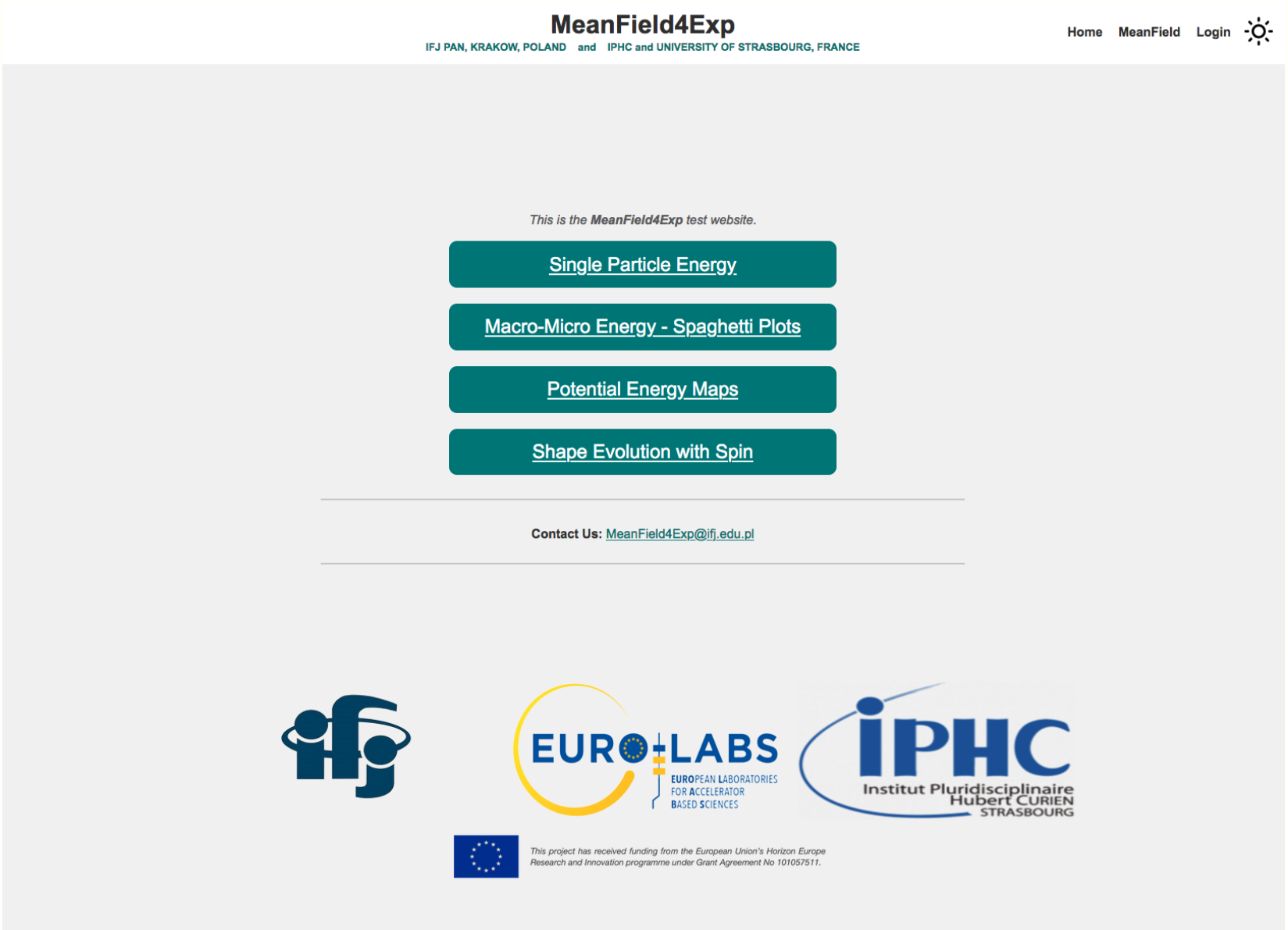
In Cracow

https://meanfield4exp.ifj.edu.pl

In Sevilla

https://institucional.us.es/theo4exp/

An Option of the Entrance Screen: 4 Choices



Example: Single Particle Drawings

Proton Number: 32

Neutron Number: 40

Woods-Saxon Parameters: Universal Woods-Saxon Parameters

Choose the Deformation: a32 Step: 0.025; a22 Value: 0

Choose the Type of Labels

- Cartesian $[n_x, n_y, n_z]$
- Nilsson $[N, n_z, \Lambda]\ \Omega$
- Spherical $[N, \ell, j]\ j_z$

Deformation axis: Min: -0.3 Max: 0.3 Step: 0.1

Proton energy: Min: -10 Max: 4 Step: 2

Neutron energy: Min: -16 Max: -2 Step: 2

Generate

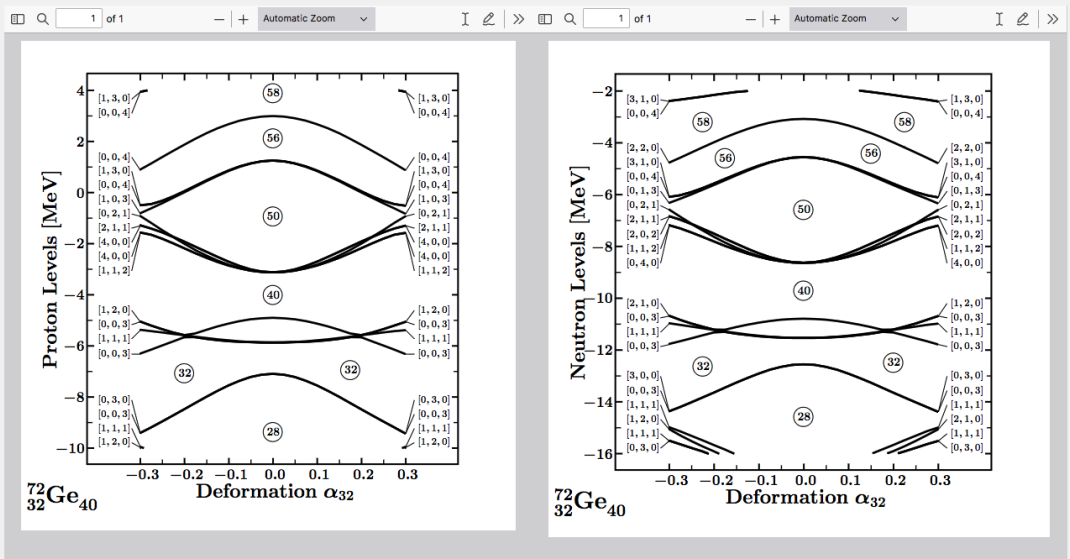
This web page allows you to calculate the single particle energies for a given nucleus using Realistic Phenomenological Mean-Field Theory with the universal Woods-Saxon Hamiltonian. The generated plot will show the single particle energies for protons and neutrons as a function of the selected deformation, providing insight into the shell structure versus nuclear shape.

Instructions

To generate a single particle energy plot:

1. Enter the proton and neutron numbers of the nucleus of interest. Only even-even nuclei are supported.
2. Select the Woods-Saxon parameter set to use in the calculations from the dropdown menu.
3. Choose the nuclear deformation parameter (e.g. quadrupole, octupole, hexadecapole) to explore from the "Deformation" dropdown menu.
4. Select the labeling scheme for the single particle energies:
   - **Cartesian:** $[n_x, n_y, n_z]$
   - **Nilsson:** $[N, n_z, \Lambda]\ \Omega$
   - **Spherical:** $[N, \ell, j]\ j_z$
5. Specify the minimum, maximum, and step values for the deformation axes. This controls the range deformations plotted.
6. Once you have entered the required information, click the "Generate" button to submit the run.

For more details, please follow this link: Woods-Saxon Mean-Field Calculations.



Another Option: Total Energy Drawings

Proton Number: 32

Neutron Number: 40

Δ Z: 6 Δ N: 6

Woods-Saxon Parameters: Universal Woods-Saxon Parameters

Choose the Type of Energy: Total energy = E(FYU) + Shell[e] + Correlation[

Choose the Deformation: a32 Step: 0.025

a20 Value: 0

Deformation axis: Min: -0.3 Max: 0.3 Step: 0.1

Isotopes energy: Min: -4 Max: 12 Step: 2

Isotones energy: Min: -4 Max: 12 Step: 2

Generate

This form allows you to generate spaghetti plots of the macro-micro energy for a chain of isotopes and isotones using

Realistic Phenomenological Nuclear Mean-Field Theory Calculations
with the
Universal Woods-Saxon Hamiltonian.

Instructions for Formatting the Plot

1. **Specification of the Nucleus and Parametrisation**

   Choose a central nucleus by entering the proton and neutron numbers.

   Select the range of nuclei by adjusting Δ Z and Δ N.

   "Woods-Saxon Parameters" allows you to select a parameter set for the Woods-Saxon Hamiltonian from the dropdown menu.

2. **Energy Specifications**

   Choose the variant of the total energy formula according to which

   $$E_{tot} = E_{Macro} + E_{shell} + E_{pairing}$$

   The macroscopic energy, E_{Macro}, appears in two variants, the so-called Yukawa-folded [E(FYU)] and the Lublin-Strasbourg Drop [E(LSD)] liquid drop models. The standard Strutinsky shell-correction energy is denoted E_{shell}, whereas the pairing term, E_{pair}, can be chosen in the form of the so-called pairing correlation energy with a simple (BCS) approximation or a more advanced Particle Number Projection (PNP) approximation.

   Those interested can find the original references clicking "Reference List"..

3. **Description of Nuclear Deformation**

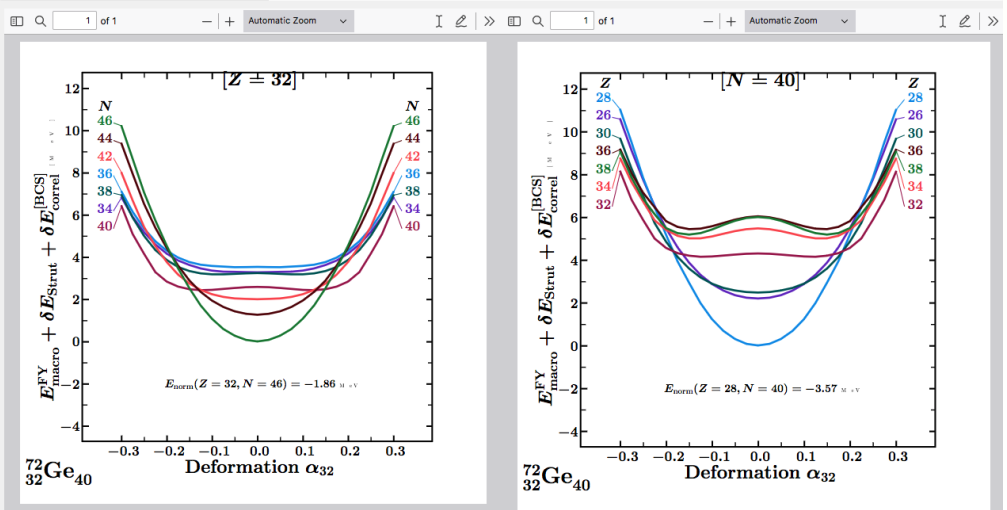
   "Choose the Deformation" Allows you to select the nuclear deformation from the dropdown menu.

   Deformation axis, Isotope energy, and Isotone energy allow you to adjust the x and y axes.

4. **Execution**

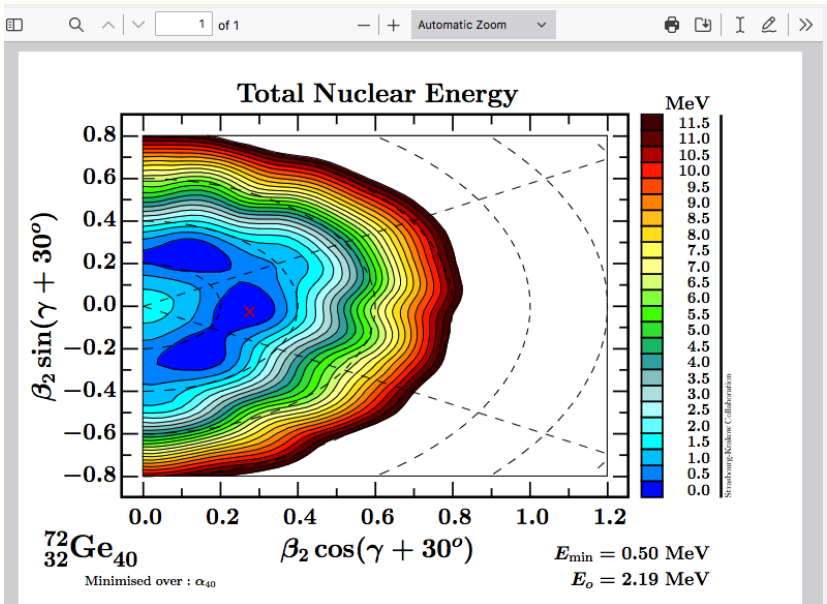
   Once all input data is specified, click "Generate" to submit the run.

   For more details, please follow the link: Woods-Saxon Mean-Field Calculations.



Another Option: Total Energy Map Drawings

- **Left: Potential energy contour plot. Right: Table of minima**



Strasbourg-Krakow Collaboration

Nucleus $^{72}_{32}Ge_{40}$

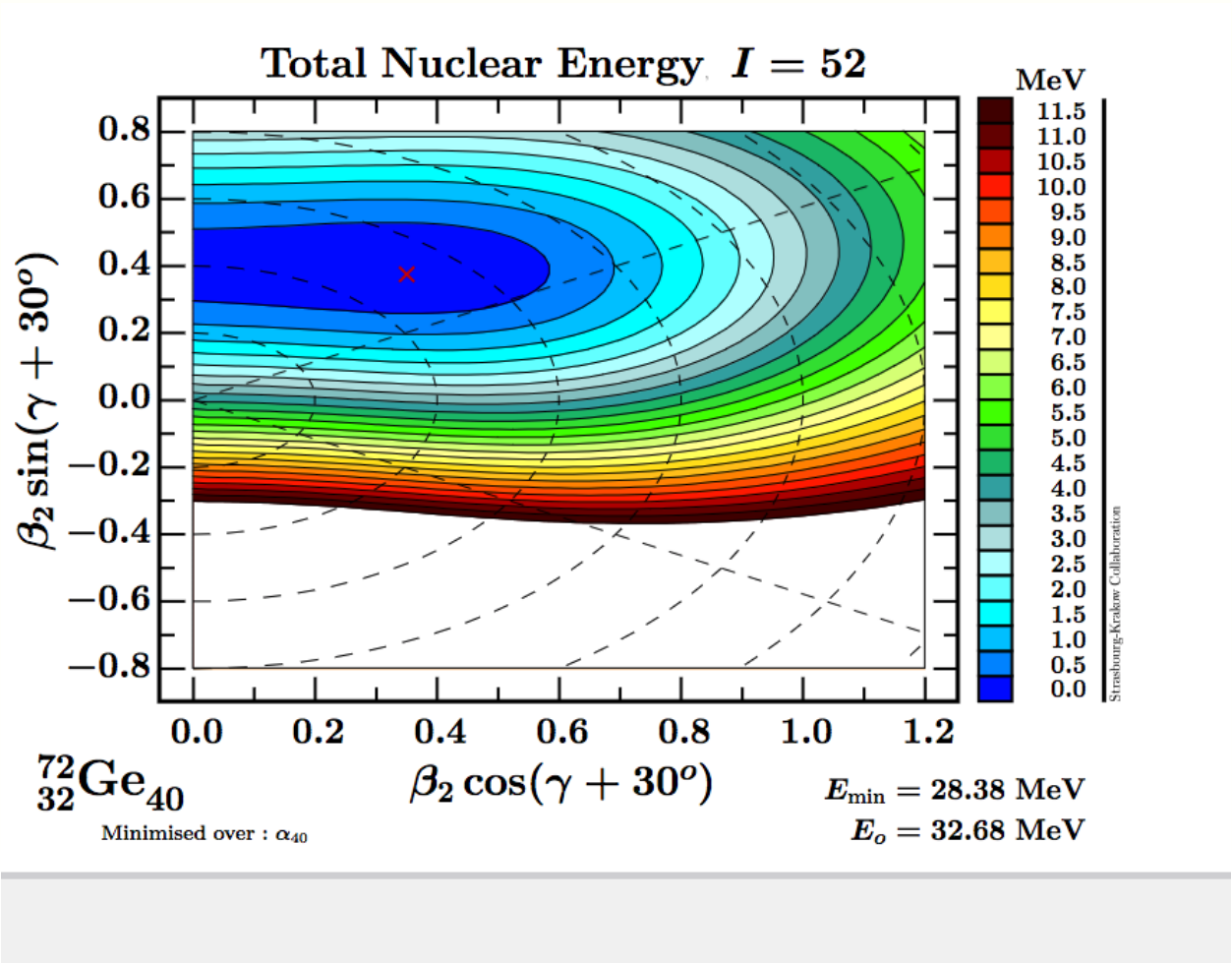
- **Total Energy:** E(FYU) + Shell[e] + Correlation[BCS]
- **Minimum Energy:** $E_{\min} = 0.50$ MeV
- **Spherical-point Energy:** $E_o = 2.19$ MeV

Energy [MeV]	$\beta_2 \cos(\gamma + 30^o)$	$\beta_2 \sin(\gamma + 30^o)$	α_{40}	β	$\gamma(^o)$
0.0000	0.275	-0.025	-0.025	0.276	-35
0.0015	0.125	0.250	-0.025	0.280	33
0.0718	0.150	-0.225	0.000	0.270	-86

Table 1: Map Energy minima for $Z = 32$, $N = 40$; Com-OxCaCANiZrSnGdPb. Dark-red rows mean minimum at the edge of the rectangle

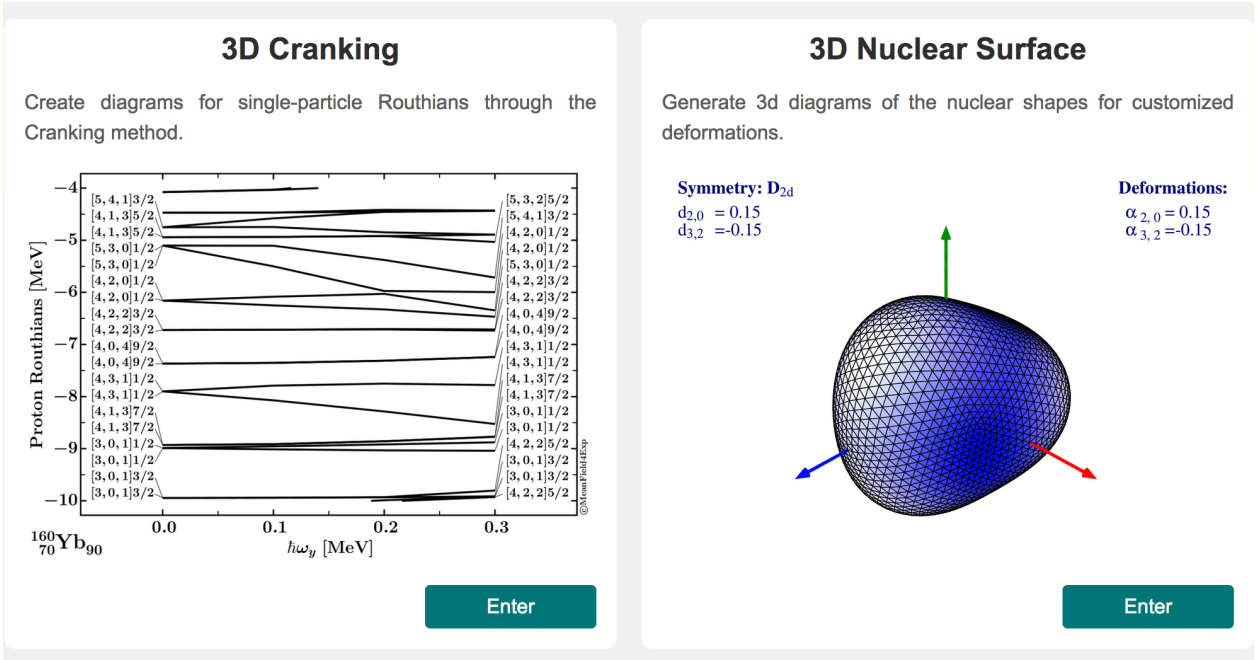
Another Example: Total Routhian at Spin=56$\hbar$

- **Energy minimised: Here over β_4 only. The final results will contain higher order minimisations: β_4, β_6 and β_8**



Another Example: 3D Cranking and Nuclear Shapes

- **Single particle Routhians as functions of rotational frequency; Alternatively plotting of a user selected nuclear shape/surface**



Next: New Options Being Considered for You

Provisorily List:

01. *Shape coexistence and evolution with spin and temperature;*
02. *Pairing and its evolution with spin and temperature;*
03. *Axial symmetry and related isomers: K-isomers, yrast traps;*
04. *Many-particle many hole excited configurations – degeneracies;*
05. *Electromagnetic transitions;*
06. *Cranking, 3D cranking and chirality;*
07. *Nuclear point group symmetries;*
08. *Band crossings, Band termination;*
09. *Jacobi and Poincare shape transitions;*
10. *Giant-Dipole Resonances – spin & temperature dependence;*
11. *Configuration controlled shape evolution;*
12. *Mass parameters, mass tensor, collective motion;*

Section 1

Physical Background of Nuclear Mean-Field:

Beginning with Nucleon-Nucleon Two-Body Interactions As the General Nuclear Physics Framework

Fundamental Structure of Nuclear Interactions [1]

Let $\hat{x} \stackrel{df.}{=} \{\hat{\vec{r}}, \hat{\vec{p}}, \hat{\vec{s}}, \hat{\vec{t}}\}$. Nuclear interactions contain following terms

$$\widehat{V}(\hat{x}_1, \hat{x}_2) \equiv \widehat{V}_C(\hat{x}_1, \hat{x}_2) + \widehat{V}_T(\hat{x}_1, \hat{x}_2) + \widehat{V}_{LS}(\hat{x}_1, \hat{x}_2) + \widehat{V}_{LL^2}(\hat{x}_1, \hat{x}_2)$$

where: C-central, T-tensor, LS-spin-orbit and LL^2-quadratic LS

Central Interaction ($r_{12} \equiv |\vec{r}_1 - \vec{r}_2|$)

$$\begin{aligned}\widehat{V}_C(\hat{x}_1, \hat{x}_2) = V_0(r_{12}) &+ V_s(r_{12})\,[\vec{s}^{(1)} \cdot \vec{s}^{(2)}] \\ &+ V_t(r_{12})\,[\vec{t}^{(1)} \cdot \vec{t}^{(2)}] \\ &+ V_{s-t}(r_{12})\,[\vec{s}^{(1)} \cdot \vec{s}^{(2)}]\,[\vec{t}^{(1)} \cdot \vec{t}^{(2)}]\end{aligned}$$

Invariant under rotations, translations, inversion and time-reversal

Fundamental Structure of Nuclear Interactions [2]

Let $\hat{x} \stackrel{df.}{=} \{\hat{\vec{r}}, \hat{\vec{p}}, \hat{\vec{s}}, \hat{\vec{t}}\}$. Nuclear interactions contain following terms

$$\widehat{V}(\hat{x}_1, \hat{x}_2) \equiv \widehat{V}_C(\hat{x}_1, \hat{x}_2) + \widehat{V}_T(\hat{x}_1, \hat{x}_2) + \widehat{V}_{LS}(\hat{x}_1, \hat{x}_2) + \widehat{V}_{LL^2}(\hat{x}_1, \hat{x}_2)$$

where: C-central, T-tensor, LS-spin-orbit and LL^2-quadratic LS

Tensor Interaction [Non-Central]

$$\vec{S}^{(12)} \stackrel{df.}{=} \frac{3\,(\vec{s}_1 \cdot \vec{r}_{12})(\vec{s}_2 \cdot \vec{r}_{12}) - (\vec{s}_1 \cdot \vec{s}_2)\, r_{12}^2}{r_{12}^2} \quad \textit{and} \quad r_{12} \stackrel{df.}{=} |\vec{r}_1 - \vec{r}_2|$$

$$\widehat{V}_T(\hat{x}_1, \hat{x}_2) = [V_{t_0}(r_{12}) + V_{t_1}(r_{12})\, \vec{t}_1 \cdot \vec{t}_2]\, \vec{S}^{(12)}$$

Invariant under rotations, translations, inversion and time-reversal

Fundamental Structure of Nuclear Interactions [3]

Let $\hat{x} \stackrel{df.}{=} \{\hat{\vec{r}}, \hat{\vec{p}}, \hat{\vec{s}}, \hat{\vec{t}}\}$. Nuclear interactions contain following terms

$$\widehat{V}(\hat{x}_1, \hat{x}_2) \equiv \widehat{V}_C(\hat{x}_1, \hat{x}_2) + \widehat{V}_T(\hat{x}_1, \hat{x}_2) + \widehat{V}_{LS}(\hat{x}_1, \hat{x}_2) + \widehat{V}_{LL^2}(\hat{x}_1, \hat{x}_2)$$

where: C-central, T-tensor, LS-spin-orbit and LL^2-quadratic LS

Spin-Orbit Interaction [Non-Local]

$$\vec{L} \stackrel{df.}{=} \frac{1}{2}(\vec{r}_1 - \vec{r}_2) \wedge (\vec{p}_1 - \vec{p}_2), \quad r_{12} \stackrel{df.}{=} |\vec{r}_1 - \vec{r}_2| \quad \textit{and} \quad \vec{S} \stackrel{df.}{=} \vec{s}_1 + \vec{s}_2$$

$$\widehat{V}_{LS}(\hat{x}_1, \hat{x}_2) = V_{LS}(r_{12})\, \vec{L} \cdot \vec{S}$$

Invariant under rotations, translations, inversion and time-reversal

Fundamental Structure of Nuclear Interactions [4]

Let $\hat{x} \stackrel{df.}{=} \{\hat{\vec{r}}, \hat{\vec{p}}, \hat{\vec{s}}, \hat{\vec{t}}\}$. Nuclear interactions contain following terms

$$\widehat{V}(\hat{x}_1, \hat{x}_2) \equiv \widehat{V}_C(\hat{x}_1, \hat{x}_2) + \widehat{V}_T(\hat{x}_1, \hat{x}_2) + \widehat{V}_{LS}(\hat{x}_1, \hat{x}_2) + \widehat{V}_{LL^2}(\hat{x}_1, \hat{x}_2)$$

where: C-central, T-tensor, LS-spin-orbit and LL^2-quadratic LS

Quadratic Spin-Orbit Interaction [Non-Local]

$$\vec{L} \stackrel{df.}{=} \frac{1}{2}(\vec{r}_1 - \vec{r}_2) \wedge (\vec{p}_1 - \vec{p}_2) \quad \text{and} \quad r_{12} \stackrel{df.}{=} |\vec{r}_1 - \vec{r}_2|$$

$$\widehat{V}_{LL}(\hat{x}_1, \hat{x}_2) = V_{LL}(r_{12})\{(\vec{s}_1 \cdot \vec{s}_2)\,\vec{L}^2 - \tfrac{1}{2}[(\vec{s}_1 \cdot \vec{L})(\vec{s}_2 \cdot \vec{L}) + (\vec{s}_2 \cdot \vec{L})(\vec{s}_1 \cdot \vec{L})]\}$$

Invariant under rotations, translations, inversion and time-reversal

Trying to Solve Implied Problem of the Motion?

- **Consider the motion of a system of $N = 100$ nucleons**

Trying to Solve Implied Problem of the Motion?

- **Consider the motion of a system of $N = 100$ nucleons**
- **What is expected complexity of involved description?**

Trying to Solve Implied Problem of the Motion?

- **Consider the motion of a system of $N = 100$ nucleons**
- **What is expected complexity of involved description?**

$$\hat{H}(\underbrace{\hat{x}_1, \hat{x}_2, \ \ldots \ \hat{x}_N}_{100\times 12=1200 \text{ operators}})\Psi = E\,\Psi$$

Trying to Solve Implied Problem of the Motion?

- **Consider the motion of a system of $N = 100$ nucleons**
- **What is expected complexity of involved description?**

$$\hat{H}(\underbrace{\hat{x}_1, \hat{x}_2, \ \ldots \ \hat{x}_N}_{100\times 12=1200 \text{ operators}})\Psi = E\,\Psi$$

Conclusions:

- **Effective solution of this problem is out of question here...**

Trying to Solve Implied Problem of the Motion?

- **Consider the motion of a system of $N = 100$ nucleons**
- **What is expected complexity of involved description?**

$$\hat{H}(\underbrace{\hat{x}_1, \hat{x}_2, \ \ldots \ \hat{x}_N}_{100\times 12=1200 \text{ operators}})\Psi = E\,\Psi$$

Conclusions:

- **Effective solution of this problem is out of question here...**
- **We know no methods of solving the Schrödinger equation of this complexity thus need to search for approximate solutions**

Trying to Solve Implied Problem of the Motion?

- **Consider the motion of a system of $N = 100$ nucleons**
- **What is expected complexity of involved description?**

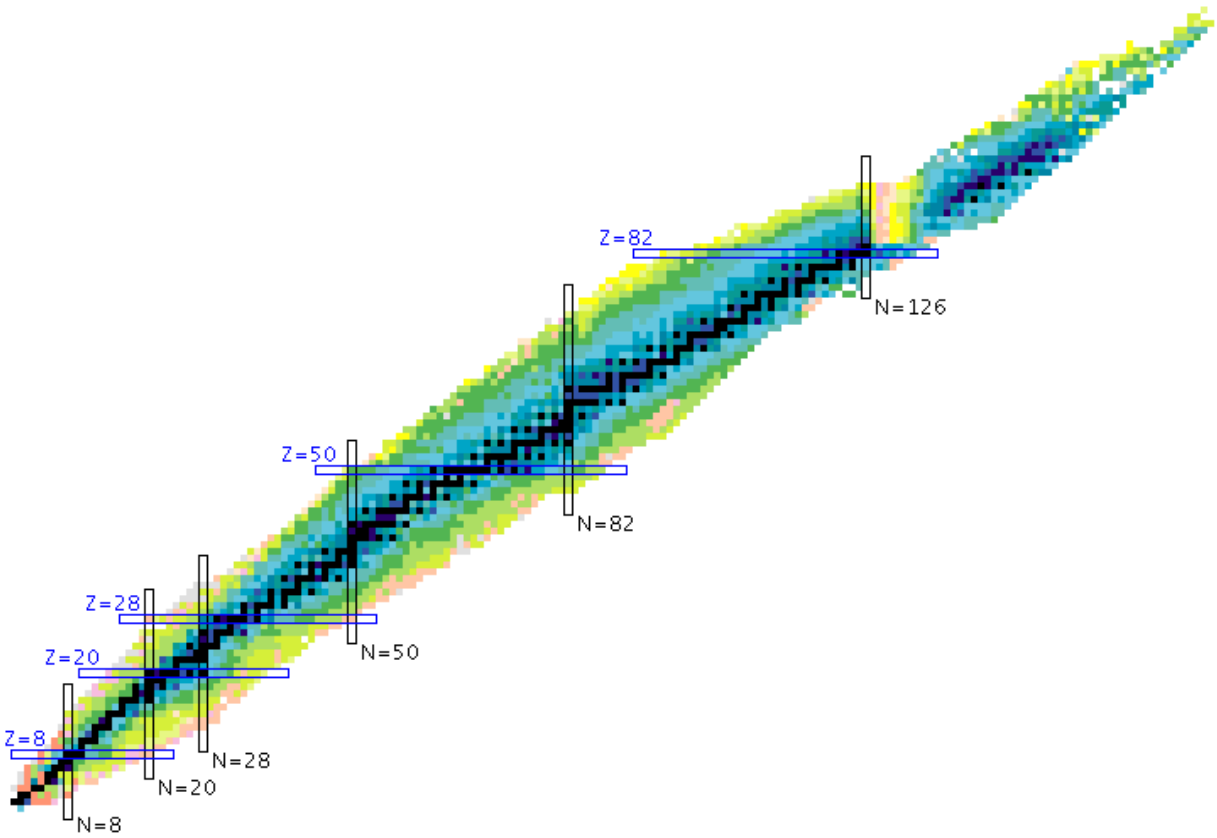
$$\hat{H}(\underbrace{\hat{x}_1, \hat{x}_2, \ \ldots \ \hat{x}_N}_{100\times 12=1200 \text{ operators}})\Psi = E\,\Psi$$

Conclusions:

- **Effective solution of this problem is out of question here...**
- **We know no methods of solving the Schrödinger equation of this complexity thus need to search for approximate solutions**
- **To look for simplifications we will consult experiment: Shapes**

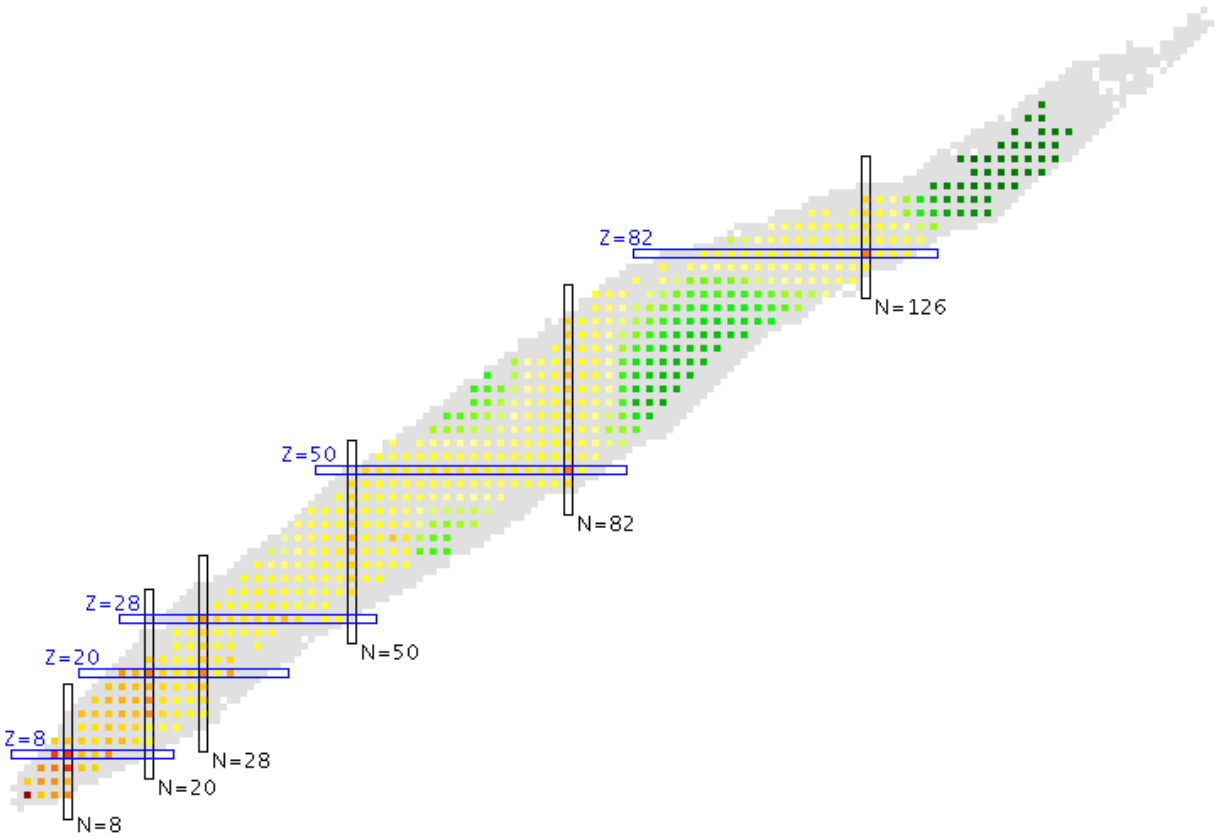
From now on: We wish to start collecting experimental information to be able to construct theory approximations

There Were Nearly 3000 Systems Seen in Laboratory...



- *Among nearly 3000 systems known experimentally, we find only about two hundreds stable – marked as black rectangles*

In Majority of Them Spherical Symmetry is Broken



- *However among nearly 3000 systems known experimentally, over 80% are measured - or predicted - to be non spherical*

We Need To Face: Spontaneous Symmetry Breaking

How come that the interactions invariant under rotation and inversion

thus spherically symmetric,

We Need To Face: Spontaneous Symmetry Breaking

How come that the interactions invariant under rotation and inversion

thus spherically symmetric,

acting among tightly packed nucleons in a nucleus

We Need To Face: Spontaneous Symmetry Breaking

How come that the interactions invariant under rotation and inversion

thus spherically symmetric,

acting among tightly packed nucleons in a nucleus

end up producing "the well known" nuclei

often with strongly deformed shapes?

We Need To Face: Spontaneous Symmetry Breaking

How come that the interactions invariant under rotation and inversion

thus spherically symmetric,

acting among tightly packed nucleons in a nucleus

end up producing "the well known" nuclei

often with strongly deformed shapes?

This phenomenon is called: Spontaneous Symmetry Breaking

Symmetry: Exact, Approximate, Spontaneously Broken

From preceding discussion we must assume that the N-N interaction

$$\widehat{V}(\hat{x}_1, \hat{x}_2) \equiv \widehat{V}_C(\hat{x}_1, \hat{x}_2) + \widehat{V}_T(\hat{x}_1, \hat{x}_2) + \widehat{V}_{LS}(\hat{x}_1, \hat{x}_2) + \widehat{V}_{LL^2}(\hat{x}_1, \hat{x}_2)$$

is invariant under rotations, translations, inversion and time-reversal

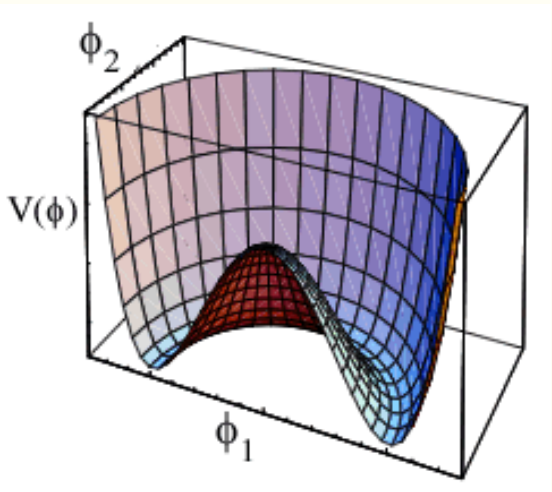
Symmetry: Exact, Approximate, Spontaneously Broken

From preceding discussion we assume that the N-N interaction

$$\widehat{V}(\hat{x}_1, \hat{x}_2) \equiv \widehat{V}_C(\hat{x}_1, \hat{x}_2) + \widehat{V}_T(\hat{x}_1, \hat{x}_2) + \widehat{V}_{LS}(\hat{x}_1, \hat{x}_2) + \widehat{V}_{L^2}(\hat{x}_1, \hat{x}_2)$$

is invariant under rotations, translations, inversion and time-reversal

Broken Symmetry?



The Nuclear Mean Field Theory ...

... is empirically very successful, based on

$$\widehat{V}_{mf}(\hat{x}) = \int \psi^*(x')\widehat{V}(\hat{x}, \hat{x}')\psi(x')\, dx'$$

Thus: Some or all of the above symmetries will be broken by mean-field Hamiltonian

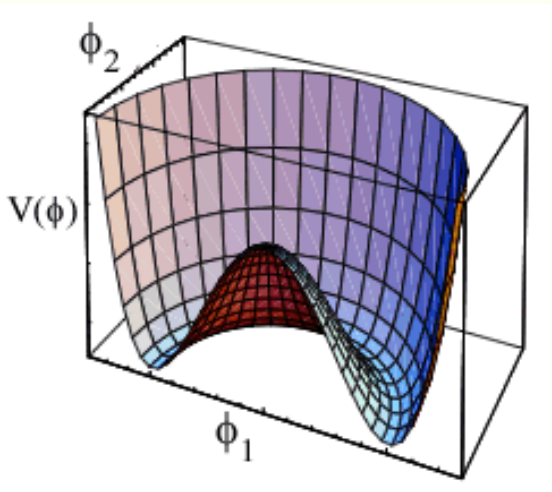
Symmetry: Exact, Approximate, Spontaneously Broken

From preceding discussion we assume that the N-N interaction

$$\widehat{V}(\hat{x}_1, \hat{x}_2) \equiv \widehat{V}_C(\hat{x}_1, \hat{x}_2) + \widehat{V}_T(\hat{x}_1, \hat{x}_2) + \widehat{V}_{LS}(\hat{x}_1, \hat{x}_2) + \widehat{V}_{LL^2}(\hat{x}_1, \hat{x}_2)$$

is invariant under rotations, translations, inversion and time-reversal

Broken Symmetry?



The Nuclear Mean Field Theory ...

... is empirically very successful, based on

$$\widehat{V}_{mf}(\hat{x}) = \int \psi^*(x')\widehat{V}(\hat{x}, \hat{x}')\psi(x')\, dx'$$

Thus: Some or all of the above symmetries will be broken by mean-field Hamiltonian

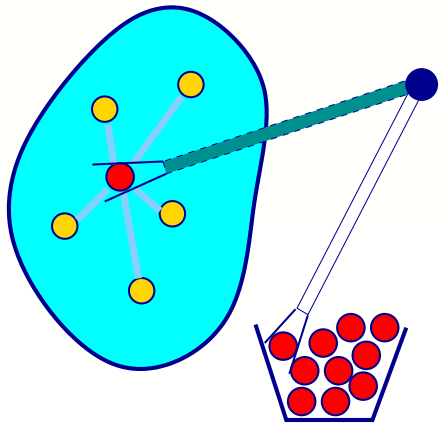
- **We will need to learn how to find $\widehat{V}_{mf}(\hat{x})$ because integral definition is not profitable since solutions $\psi(x)$ are not known**

To learn about possible approximate theory we will systematically examine the stability of the nuclear systems via experiment

- Removing the particles we learn about interactions with the others
- A mean-field interaction can be seen as an algorithm probing the two-body interactions through a generalised weighted average $\leftrightarrow \widehat{V}$

$$\widehat{V}(\hat{x}) = \frac{1}{N-1} \sum_{j=1}^{(N-1)} \int dx_j \, \psi^*(x_j) \, \widehat{V}(\hat{x}, \hat{x}_j) \, \psi(x_j)$$

An N–Body System



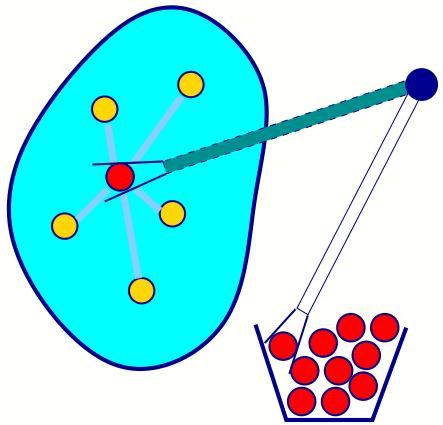
Schematic: Probing 2-body interactions with an 'external' test-particle

- Removing the particles we learn about interactions with the others
- A mean-field interaction can be seen as an algorithm probing the two-body interactions through a generalised weighted average $\leftrightarrow \widehat{V}$

$$\widehat{V}(\hat{x}) = \frac{1}{N-1} \sum_{j=1}^{(N-1)} \int dx_j \, \psi^*(x_j) \, \widehat{V}(\hat{x}, \hat{x}_j) \, \psi(x_j)$$

- Observe that summation above implies an averaging over all (N-1) remaining particles

An N–Body System

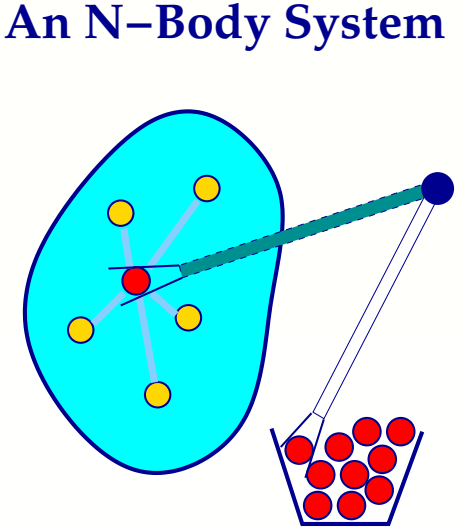


Schematic: Probing 2-body interactions with an 'external' test-particle

- Removing the particles we learn about interactions with the others
- A mean-field interaction can be seen as an algorithm probing the two-body interactions through a generalised weighted average $\leftrightarrow \widehat{V}$

$$\widehat{V}(\hat{x}) = \frac{1}{N-1} \sum_{j=1}^{(N-1)} \int dx_j \, \psi^*(x_j) \, \widehat{V}(\hat{x}, \hat{x}_j) \, \psi(x_j)$$

- Observe that summation above implies an averaging over all (N-1) remaining particles
- Observe also that the resulting mean-field potential $\widehat{V} = \widehat{V}(\hat{x})$ is a one-body operator

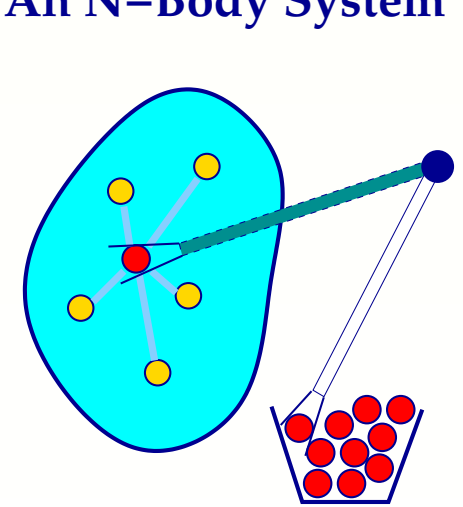


Schematic: Probing 2-body interactions with an 'external' test-particle

- Removing the particles we learn about interactions with the others
- A mean-field interaction can be seen as an algorithm probing the two-body interactions through a generalised weighted average $\leftrightarrow \widehat{V}$

$$\widehat{V}(\hat{x}) = \frac{1}{N-1} \sum_{j=1}^{(N-1)} \int dx_j \, \psi^*(x_j) \, \widehat{V}(\hat{x}, \hat{x}_j) \, \psi(x_j)$$

- Observe that summation above implies an averaging over all (N-1) remaining particles
- Observe also that the resulting mean-field potential $\widehat{V} = \widehat{V}(\hat{x})$ is a one-body operator
- Right: An artist view of the binding energy experiment as the average interaction tests



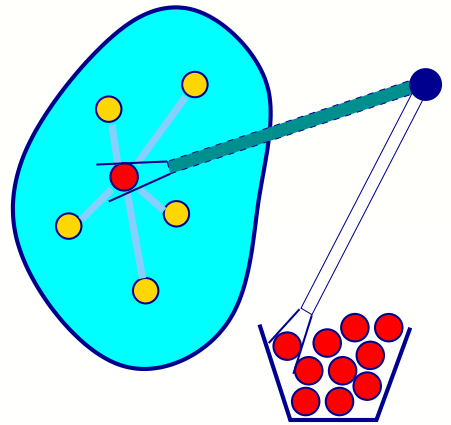
Schematic: Probing 2-body interactions with an 'external' test-particle

From Separation Energies To the Many-Body Mean-Field Concept

- Removing the particles we learn about interactions with the others
- A mean-field interaction can be seen as an algorithm probing the two-body interactions through a generalised weighted average $\leftrightarrow \widehat{V}$

$$\widehat{V}(\hat{x}) = \frac{1}{N-1} \sum_{j=1}^{(N-1)} \int dx_j \, \psi^*(x_j) \, \widehat{V}(\hat{x}, \hat{x}_j) \, \psi(x_j)$$

- Observe that summation above implies an averaging over all (N-1) remaining particles
- Observe also that the resulting mean-field potential $\widehat{V} = \widehat{V}(\hat{x})$ is a one-body operator
- Right: An artist view of the binding energy experiment as the average interaction tests
- The mean field potential binding non-interacting nucleons $\longrightarrow$ is a simple container



Schematic: Probing 2-body interactions with an 'external' test-particle

But when measuring
the nucleon separation energies from nuclei,
Maria Göppert Meyer*) and Hans Jensen
encountered a number of puzzles,
already over 50 years back.

*) **Born on June 28, 1906, Katowice, Poland**

But when measuring the nucleon separation energies from nuclei, Maria Göppert Meyer*) and Hans Jensen encountered a number of puzzles, already over 50 years back.

Certain separation energies were significantly larger than the other.

*) **Born on June 28, 1906, Katowice, Poland**

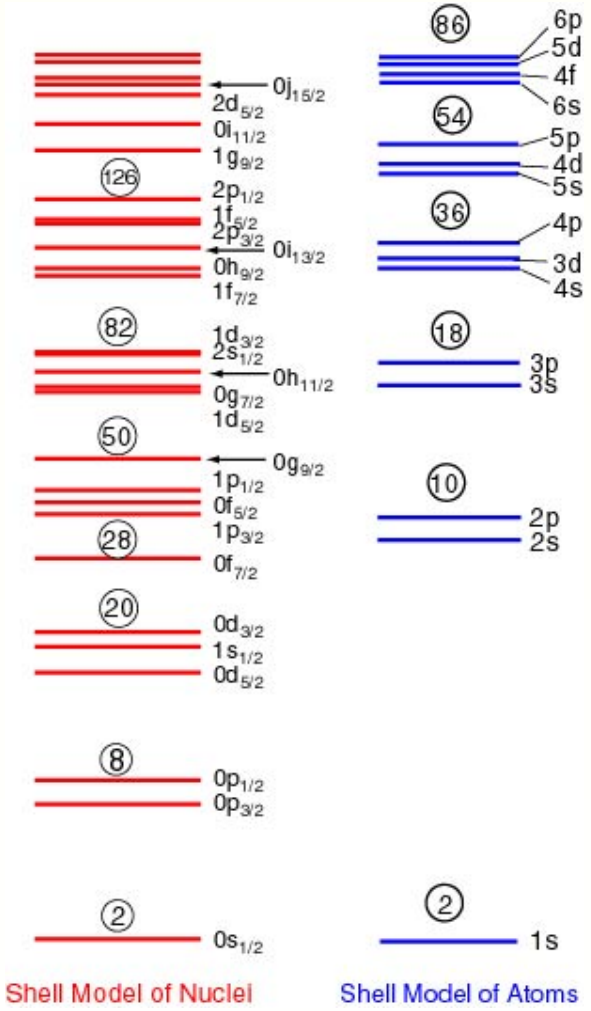
But when measuring the nucleon separation energies from nuclei, Maria Göppert Meyer*) and Hans Jensen encountered a number of puzzles, already over 50 years back.

Certain separation energies were significantly larger than the other.

Not knowing the reasons they called the corresponding nucleon numbers m a g i c.

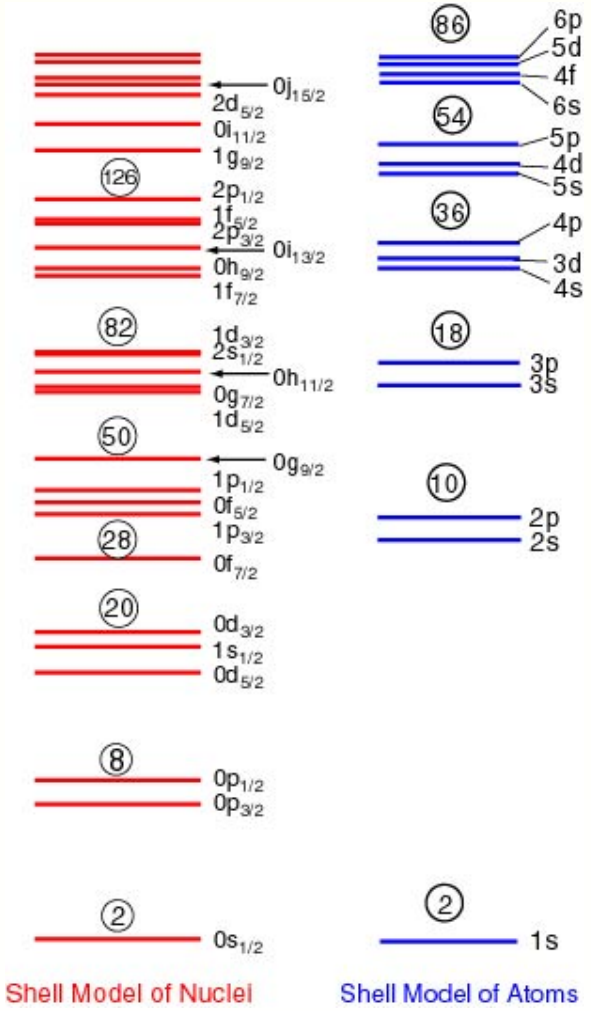
*) **Born on June 28, 1906, Katowice, Poland**

- **Observe characteristic differences between the nucleonic and electronic separation spectra**



- Observe characteristic differences between the nucleonic and electronic separation spectra

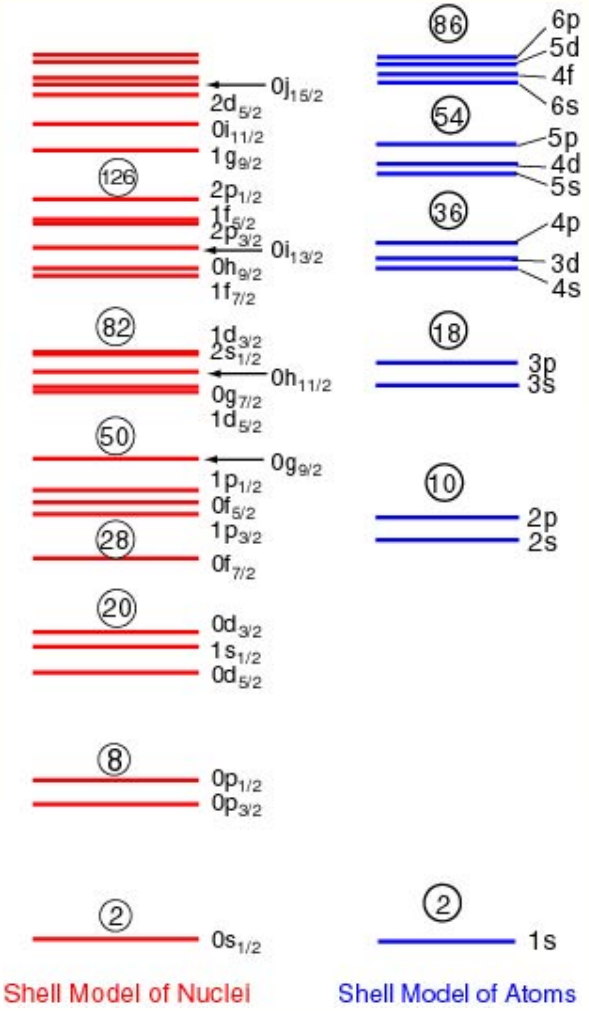
- The 1963 Nobel Prize for the study of the nuclear effect to M. Göppert-Mayer, J. Jensen and E. Wigner ↔ See: "Shell Model of Nuclei"



- Observe characteristic differences between the nucleonic and electronic separation spectra

- The 1963 Nobel Prize for the study of the nuclear effect to M. Göppert-Mayer, J. Jensen and E. Wigner ↔ See: "Shell Model of Nuclei"

- In atomic nuclei the highest-j orbital in an N-shell is ejected to the (N-1st)–shell below it

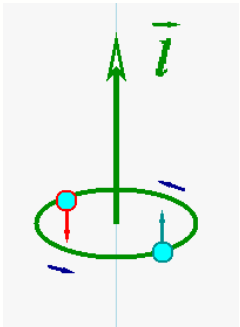


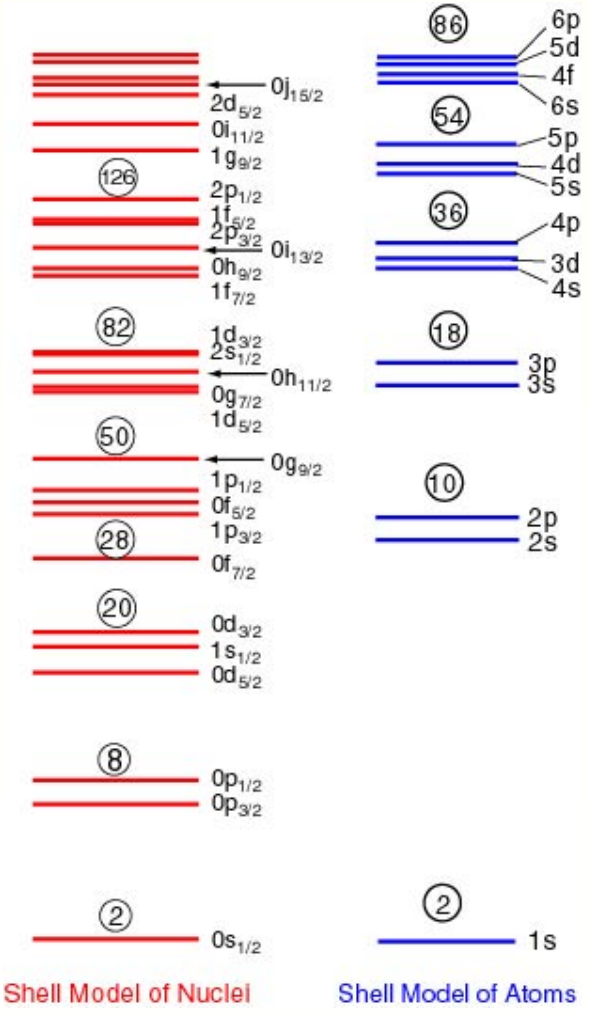
- Observe characteristic differences between the nucleonic and electronic separation spectra

- The 1963 Nobel Prize for the study of the nuclear effect to M. Göppert-Mayer, J. Jensen and E. Wigner ↔ See: "Shell Model of Nuclei"

- In atomic nuclei the highest-j orbital in an N-shell is ejected to the (N-1st)–shell below it

- The big gaps at $Z/N = 20, 28, 50, 82, 126$ are confirmed by spin-orbit mean-field coupling





We just learned about the strongest nucleon binding properties which the mean field potential should generate.

We just learned about the strongest nucleon binding properties which the mean field potential should generate.

But so far we do not know the spatial form / structure of the potential itself.

We just learned about the strongest nucleon binding properties which the mean field potential should generate.

But so far we do not know the spatial form / structure of the potential itself.

We intend to derive the Woods-Saxon potentials of interest for us using well known relativistic meson-exchange theory (see Annex)

We just learned about the strongest nucleon binding properties which the mean field potential should generate.

But so far we do not know the spatial form / structure of the potential itself.

We intend to derive the Woods-Saxon potentials of interest for us using well known relativistic meson-exchange theory (see Annex)

However, it will be convenient to begin by presenting the well known explicit forms of these potentials right away as an introduction

Spherical Nuclear Mean-Field: Woods-Saxon Form

Simple geometrical features are often described employing Woods-Saxon Mean Field Hamiltonian:

$$\hat{H}^{\rm ws} = \underbrace{\hat{t}}_{kinetic} + \underbrace{\hat{V}^{\rm ws}_{\rm cent}}_{central} + \underbrace{\hat{V}^{\rm ws}_{\ell\cdot s}}_{spin-orbit}$$

- **Central potential** in the simplest, spherical-symmetry case:

$$V^{ws}_{\rm cent}(r; V_o, r_o, a_o) \stackrel{df}{=} \frac{V_o}{1+\exp\left[(r-R_o)/a\right]}; \quad R_o = r_o A^{1/3}$$

- **Corresponding potential parameters:**

V_o - central potential depth parameter
r_o - central potential radius parameter
a_o - central potential diffuseness parameter

Spherical Nuclear Mean-Field: Woods-Saxon Form

- **Switching to spin-orbit, simplest spherical-symmetry case:**

$$V^{ws}_{\ell\cdot s}(r;\lambda_{\ell\cdot s},r_{\ell\cdot s},a_{\ell\cdot s}) \stackrel{df}{=} \frac{d\mathcal{V}^{ws}_{\ell\cdot s}}{dr}\,\hat{\vec{\ell}}\cdot\hat{\vec{s}}$$

where by definition

$$\mathcal{V}^{ws}_{\ell\cdot s}(r;\lambda_{\ell\cdot s},r_{\ell\cdot s},a_{\ell\cdot s}) \stackrel{df}{=} \frac{V_{\ell\cdot s}}{1+\exp\left[(r-R_{\ell\cdot s})/a_{\ell\cdot s}\right]};\ R_{\ell\cdot s}=r_{\ell\cdot s}A^{1/3}$$

- **Corresponding parameters:**

$\lambda_{\ell\cdot s}$ - **spin-orbit potential depth parameter**
$r_{\ell\cdot s}$ - **spin-orbit potential radius parameter**
$a_{\ell\cdot s}$ - **spin-orbit potential diffuseness parameter**

... and this is how it acts $\rightarrow\rightarrow\rightarrow$

Unique Features of the WS Parameterisation

As one student put it:

1) Single nucleon energies depend on parameters in an extremely simple, and yet an "intuitive & pedagogical" manner (see 6 pedagogical illustrations below).

Unique Features of the WS Parameterisation

As one student put it:

1) Single nucleon energies depend on parameters in an extremely simple, and yet an "intuitive & pedagogical" manner (see 6 pedagogical illustrations below).

2) He added: One could almost predict such a dependence before running calculations.

Unique Features of the WS Parameterisation

As one student put it:

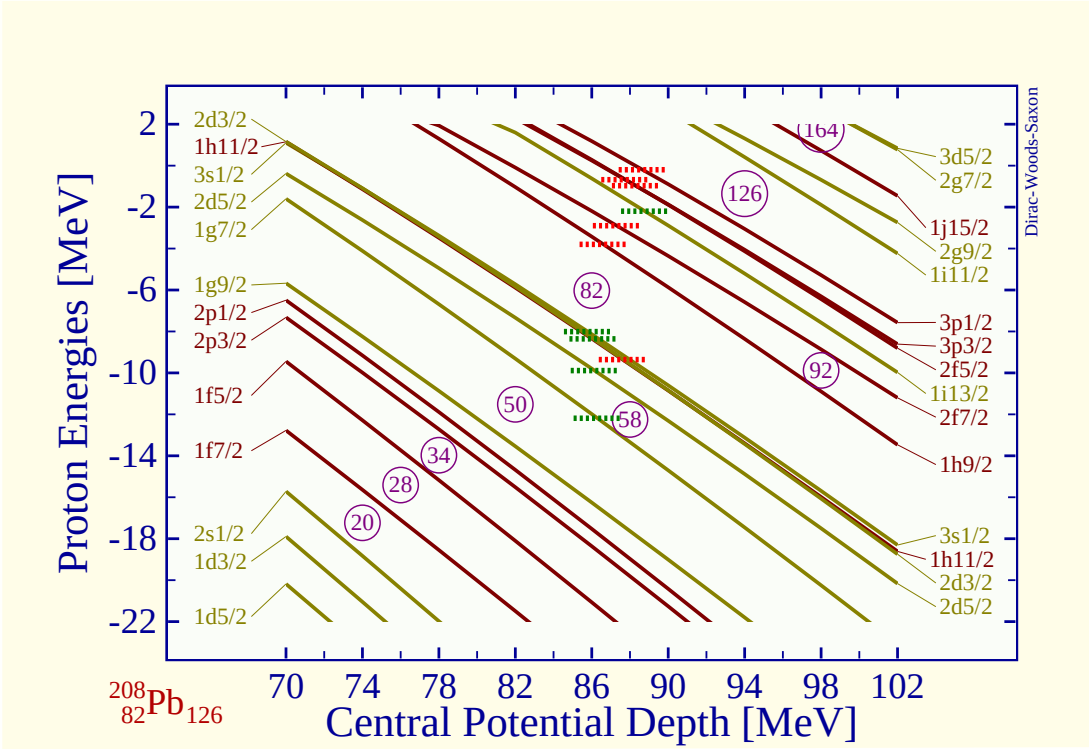
1) Single nucleon energies depend on parameters in an extremely simple, and yet an "intuitive & pedagogical" manner (see 6 pedagogical illustrations below).

2) He added: One could almost predict such a dependence before running calculations.

3) But we believe that it will be much more instructive to show calculation results systematically.

Nucleon Energies: Central Potential Impact

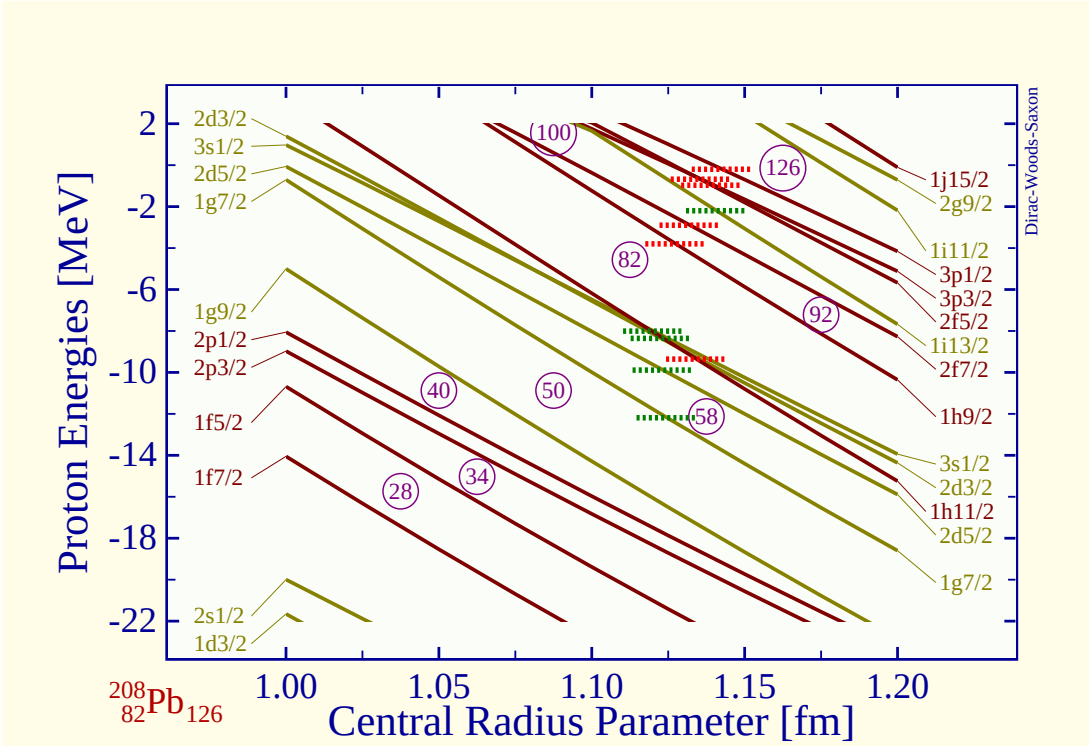
• The nuclear mean-field Woods-Saxon potentials have a very important feature - *each of its parameters dominates a certain mechanism.*



Mechanism No. 1: The potential depth parameter is primarily responsible for the nucleonic binding energies. Observe nearly linear dependence and an ideal description of the experimental levels: ^{208}Pb.

Nucleon Energies: Central Potential Impact

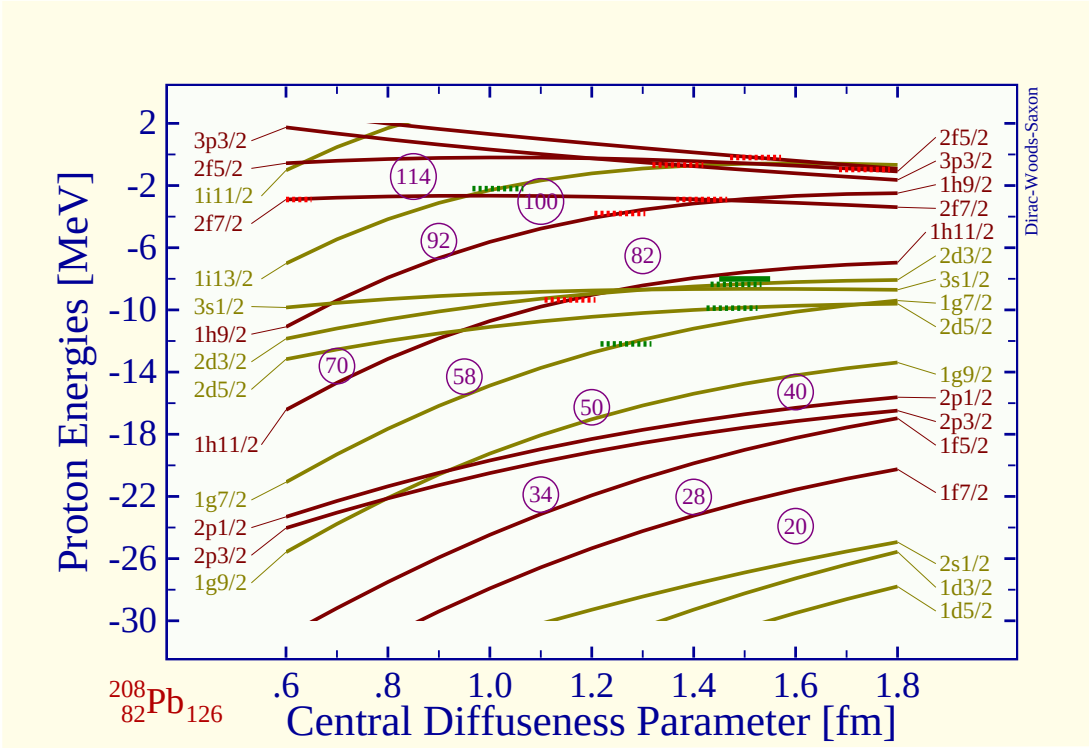
• The nucleonic binding energies vary nearly linearly also as functions of the central radius (even though some levels may cross "gently").



Mechanism No. 2: The central-radius parameter is co-responsible for the nucleonic binding energies but impacts importantly the r.m.s. radii. Note the correspondence with experiment. Here: For ^{208}Pb.

Nucleon Energies: Central Potential Impact

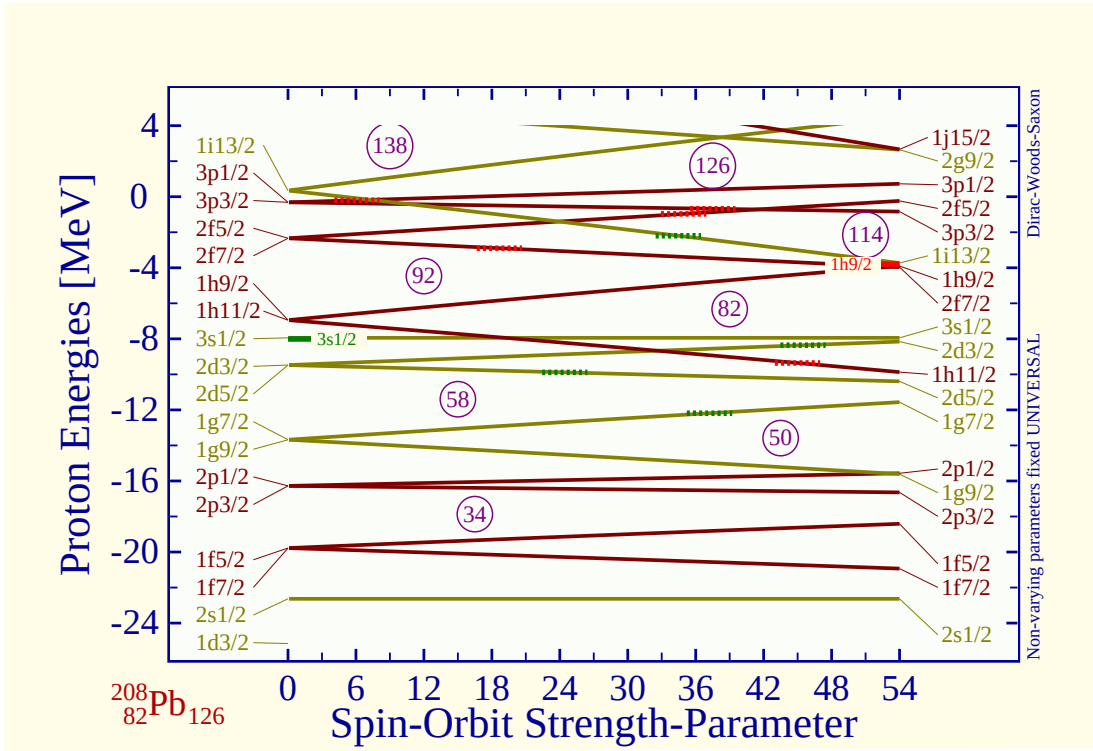
• The central diffuseness parameter is the only one that clearly distinguishes among the eigen-energies with various quantum numbers.



Mechanism No. 3: Observe the existence of families of nearly parallel lines, which are characterised by the common ℓ quantum number.

Nucleon Energies: Spin-Orbit Potential Impact

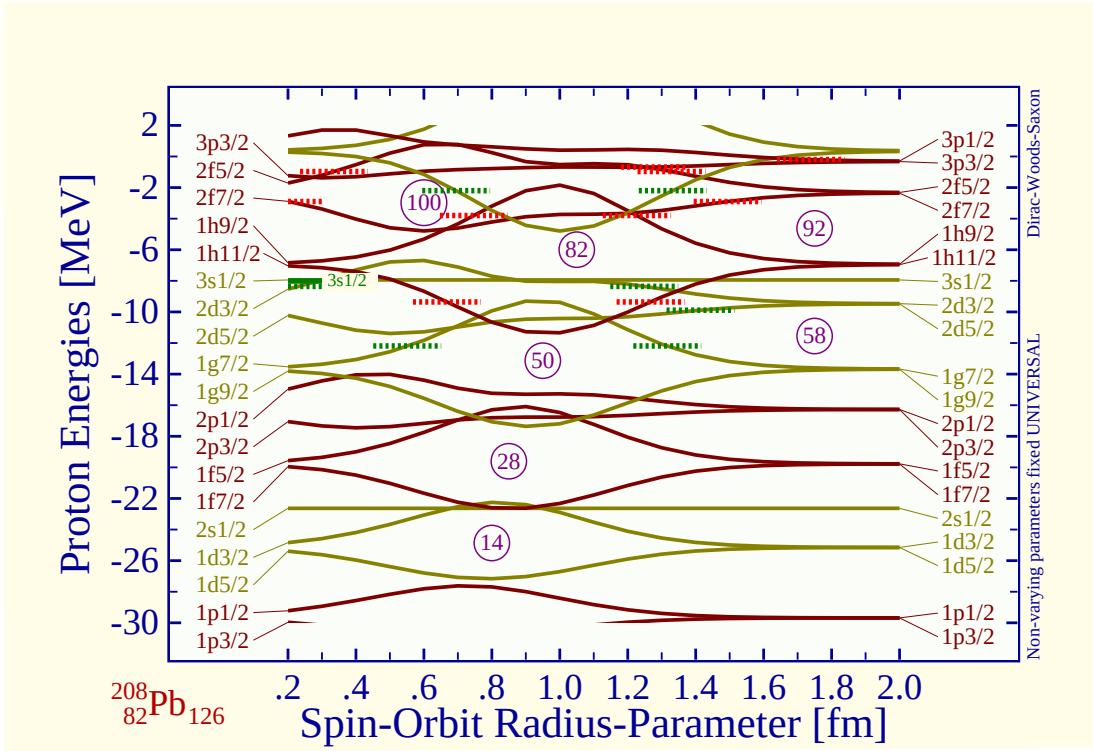
- Single nucleon levels as functions of the *s-o strength parameter*



Mechanism No. 4: Note that the separation between the spin-orbit partners is linear in λ and ℓ $\rightarrow$ We can plot this diagram knowing ℓ and the start positions at $\lambda = 0$.

Nucleon Energies: Spin-Orbit Potential Impact

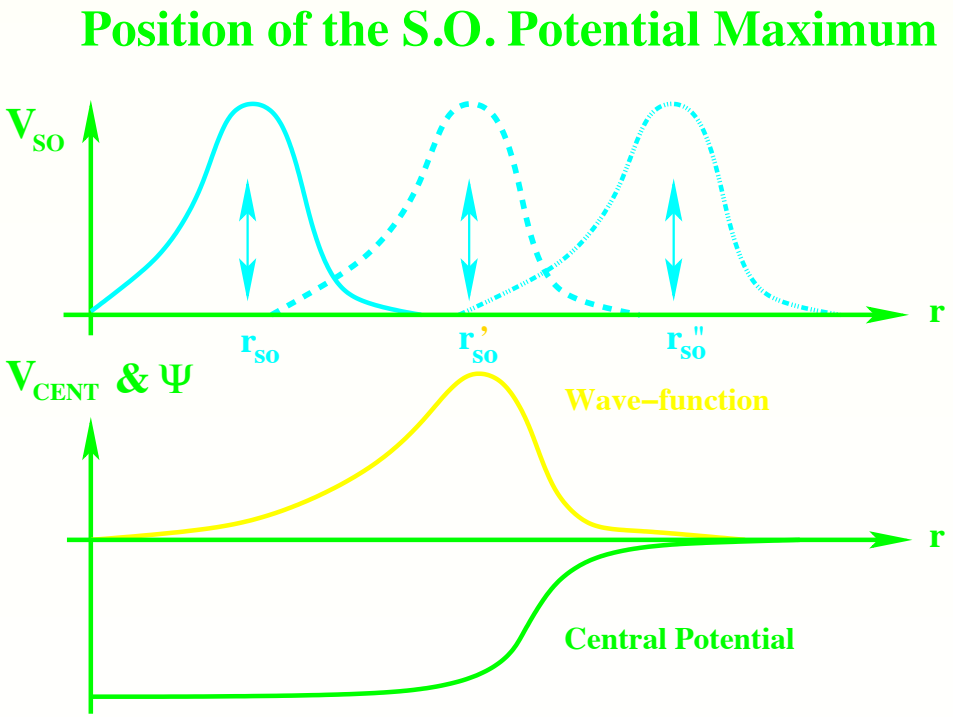
- Observe an increase of the spin-orbit splitting first, then a decrease and characteristic 'bubble structures' for all the $\ell \neq 0$ energy levels



Mechanism No. 5: A spin-orbit effect giving rise to two solutions: a 'standard' one for $r_{so} \sim 1.2$ fm and a 'compact' one at $r_{so} \sim 0.6$ fm

Nucleon Energies: Spin-Orbit Potential Impact

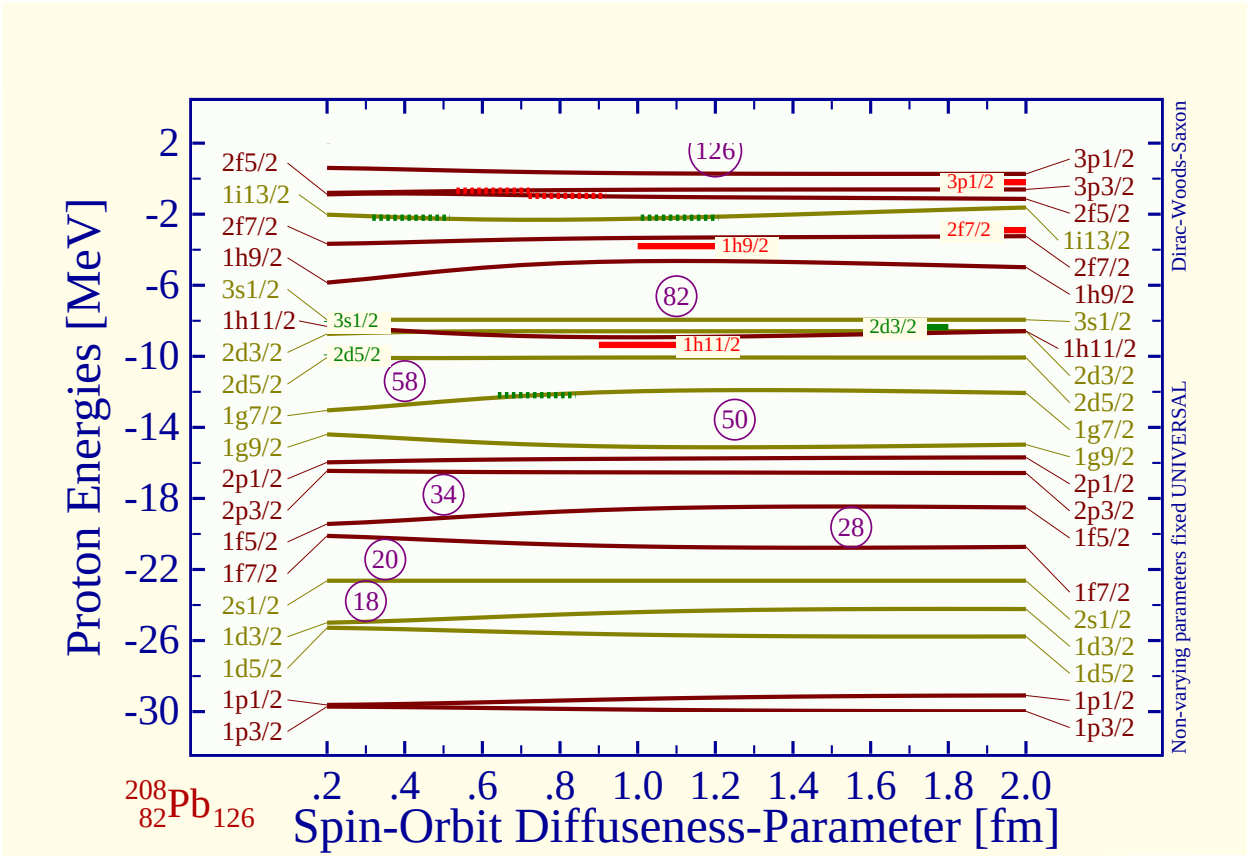
- Consider fixed central potential and let vary only one spin-orbit parameter *viz.* $r_{\ell s}$ so that $r_{\ell s} < r'_{\ell s}$, next $r'_{\ell s} < r''_{\ell s}$, etc. We have:



The maxima of the blue curves result from the derivative in the s-o potential; The yellow curve simulates typical wave functions as generated by the central potential: a Gaussian $\times$ polynomial

Nucleon Energies: Spin-Orbit Potential Impact

- Single nucleon levels as functions of *s-o diffuseness parameter*



Mechanism No. 6: Observe a regular gentle increase of the spin-orbit splitting with a_{so}, which is followed by a stretch of independence

From Simple Plots to Universal Woods-Saxon?

Another student noticed:

1) Wait a moment: Here we are in the process of discovering a new, seemingly fundamental feature....

She added:

*) **The person chooses to remain incognito**

From Simple Plots to Universal Woods-Saxon?

Another student noticed:

1) Wait a moment: Here we are in the process of discovering a new, seemingly fundamental feature....

She added:

2) If the levels manifest so many similarities and partnerships in behaviour, then the repetitive shell structures will be obtained with the same, unique "universal" parameter set...

*) The person chooses to remain incognito

From Simple Plots to Universal Woods-Saxon?

Another student noticed:

1) Wait a moment: Here we are in the process of discovering a new, seemingly fundamental feature....

She added:

2) If the levels manifest so many similarities and partnerships in behaviour, then the repetitive shell structures will be obtained with the same, unique "universal" parameter set...

3) Your Hamiltonian will be functioning within a mode published already earlier as "Woods-Saxon Universal"

*) The person chooses to remain incognito

From Simple Plots to Universal Woods-Saxon?

Another student noticed:

1) Wait a moment: Here we are in the process of discovering a new, seemingly fundamental feature....

She added:

2) If the levels manifest so many similarities and partnerships in behaviour, then the repetitive shell structures will be obtained with the same, unique "universal" parameter set...

3) Your Hamiltonian will be functioning within a mode published already earlier as "Woods-Saxon Universal"

4) She invested a few more weeks and transformed her suggestions into mathematical arguments*)

*) The person chooses to remain incognito

From Simple Plots to Universal Woods-Saxon?

Another student noticed:

1) Wait a moment: Here we are in the process of discovering a new, seemingly fundamental feature....

She added:

2) If the levels manifest so many similarities and partnerships in behaviour, then the repetitive shell structures will be obtained with the same, unique "universal" parameter set...

3) Your Hamiltonian will be functioning within a mode published already earlier as "Woods-Saxon Universal"

4) She invested a few more weeks and transformed her suggestions into mathematical arguments*)

5) We will show that excellent comparisons with experiment are obtained for all treated nuclei with 7 to 9 universal WS parameters (universal $\leftrightarrow$ common for Mass Table)

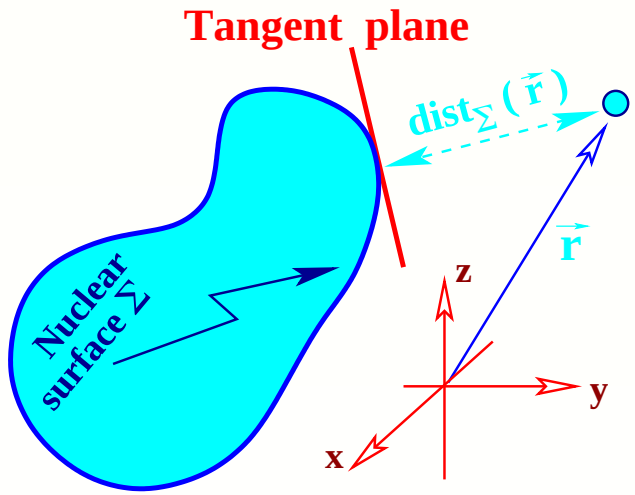
*) The person chooses to remain incognito

- **Nuclear surface Σ is parametrised in terms of spherical harmonics**

$$R(\vartheta,\varphi) = c(\{\alpha_{\lambda\mu}\})\,[r_o * A^{1/3}]\,\{1 + \sum\sum \alpha_{\lambda\mu}\, Y_{\lambda,\mu}(\vartheta,\varphi)\}$$

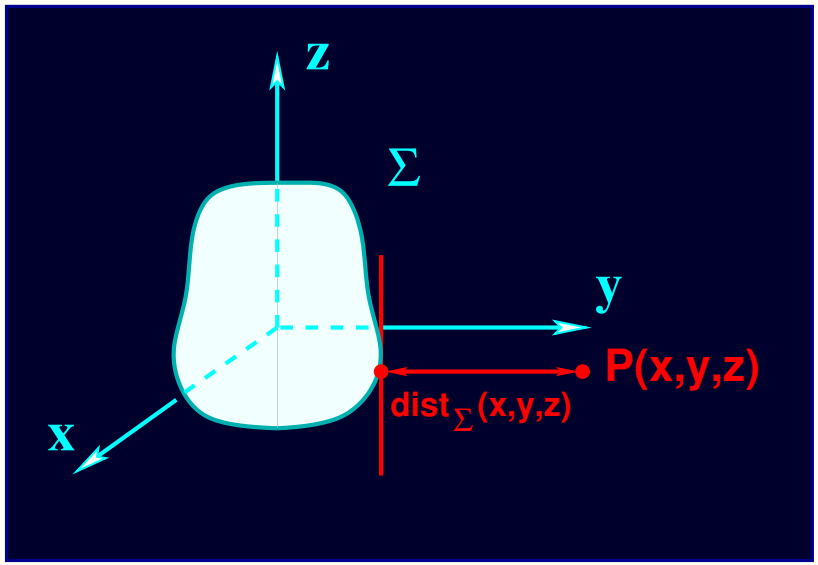
Geometrical interpretation of the distance function and the related deformed Woods-Saxon potential:

$$V_{WS}(\vec{r};\, r_o, a, V_o) = \frac{V_o}{1 + \exp[\,\mathrm{dist}_{\Sigma(r_o)}(\vec{r})/a\,]}$$



Distance function $\mathrm{dist}_\Sigma(\vec{r})$

Given surface Σ



Constructing distance function

Deformed Woods-Saxon potential generates surfaces and nucleonic densities of similar shapes:

$$\hat{V}^{\rm WS}_{\rm defor.}(\vec{r}) \equiv \frac{V_0}{1+\exp\{{\rm dist}_\Sigma(\vec{r})/a\}}$$

$$\hat{V}^{\rm WS}_{\rm spher.}(\vec{r}) \equiv \frac{V^c}{1+\exp[(r-R^c)/a^c]}$$

$$\boldsymbol{Def.=0 \leftrightarrow dist_\Sigma = r - R^c}$$

• Nucleons inside a nucleus can be seen as "nearly touching each other" - being pulled by nuclear short-range interactions: it follows that the density falls exponentially to 0 outside of nuclear surface Σ

Section 2

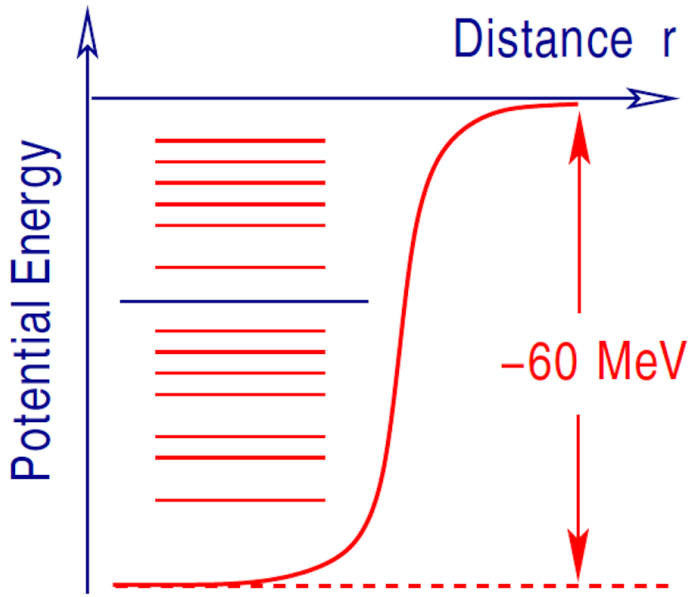
Mean-Field Theory as an Approximation of Non-Interacting Nucleons Residing on Single-Particle Levels

- We need now experimental data to find parameters of the model

$$\hat{H}^{\rm ws} = \hat{t} + \hat{V}^{\rm ws}_{\rm cent} + \hat{V}^{\rm ws}_{\ell\cdot s}$$

We will need to figure out which experiments can help us to find single particle levels schematically represented in the figure on the right $\rightarrow$ adjustment of parameters

$$V_{WS}(\vec{r};\, r_o, a, V_o) = \frac{V_o}{1 + exp[(r - R^c)/a^c]}$$



Even a theorist can produce an experimental single-nucleon energy on his/her computer...

Theory, Experiment, Experimental Data Bases

Even a theorist can produce an experimental single-nucleon energy on his/her computer...

ILLUSTRATIVE EXAMPLES FOLLOW →

Example from Ref.[1]: Neutron States in ^{91}Zr

- We consider the reaction $^{90}Zr\,(\vec{d},p)\,^{91}Zr$, with polarised d-beam

[1] **Nuclear Hamiltonians: the question of their spectral predictive power and the associated inverse problem; J. Dudek and collaborators, J. Phys. G: Nucl. Part. Phys. 37 (2010) 064031**

Example from Ref.[1]: Neutron States in ^{91}Zr

- We consider the reaction $^{90}Zr\,(\vec{d},p)\,^{91}Zr$, with polarised d-beam
- We observe peaks in the proton spectrum corresponding to each $|jm\rangle$ state populated in ^{91}Zr

---

[1] Nuclear Hamiltonians: the question of their spectral predictive power and the associated inverse problem; J. Dudek and collaborators, J. Phys. G: Nucl. Part. Phys. 37 (2010) 064031

Example from Ref.[1]: Neutron States in ^{91}Zr

- We consider the reaction $^{90}Zr\,(\vec{d},p)\,^{91}Zr$, with polarised d-beam
- We observe peaks in the proton spectrum corresponding to each $|jm\rangle$ state populated in ^{91}Zr
- Angular distributions from the measured proton spectrum allow to deduce the associated proton orbital momenta ℓ - and through conservation - possible orbital momenta of the odd neutron in ^{91}Zr

---

[1] Nuclear Hamiltonians: the question of their spectral predictive power and the associated inverse problem; J. Dudek and collaborators, J. Phys. G: Nucl. Part. Phys. 37 (2010) 064031

Example from Ref.[1]: Neutron States in ^{91}Zr

- We consider the reaction $^{90}Zr\,(\vec{d},p)\,^{91}Zr$, with polarised d-beam
- We observe peaks in the proton spectrum corresponding to each $|jm\rangle$ state populated in ^{91}Zr
- Angular distributions from the measured proton spectrum allow to deduce the associated proton orbital momenta ℓ - and through conservation - possible orbital momenta of the odd neutron in ^{91}Zr
- From polarisation of the deuterons we deduce the orientation of intrinsic spins $\vec{s}$ with respect to orbital momentum $\vec{\ell} \rightarrow$ we deduce j

---

[1] Nuclear Hamiltonians: the question of their spectral predictive power and the associated inverse problem; J. Dudek and collaborators, J. Phys. G: Nucl. Part. Phys. 37 (2010) 064031

Example from Ref.[1]: Neutron States in ^{91}Zr

- We consider the reaction $^{90}Zr\,(\vec{d},p)\,^{91}Zr$, with polarised d-beam
- We observe peaks in the proton spectrum corresponding to each $|jm\rangle$ state populated in ^{91}Zr
- Angular distributions from the measured proton spectrum allow to deduce the associated proton orbital momenta ℓ - and through conservation - possible orbital momenta of the odd neutron in ^{91}Zr
- From polarisation of the deuterons we deduce the orientation of intrinsic spins $\vec{s}$ with respect to orbital momentum $\vec{\ell} \rightarrow$ we deduce j

- **<u>To summarise:</u> Such experiments provide: $\ell \leftrightarrow$ parity, j and, with an extra effort, the spectroscopic factors**

---

[1] Nuclear Hamiltonians: the question of their spectral predictive power and the associated inverse problem; J. Dudek and collaborators, J. Phys. G: Nucl. Part. Phys. 37 (2010) 064031

Selection of Nuclei and Testing Model-Hamiltonians

Selection of Nuclei and Testing Model-Hamiltonians

• We will be interested in extracting today's single-nucleon energies in the so-called well-known doubly-magic spherical-nuclei:

$$^{16}\mathrm{O},\ ^{40}\mathrm{Ca},\ ^{48}\mathrm{Ca},\ ^{56}\mathrm{Ni},\ ^{90}\mathrm{Zr},\ ^{132}\mathrm{Sn}\ \text{and}\ ^{208}\mathrm{Pb}$$

Selection of Nuclei and Testing Model-Hamiltonians

• We will be interested in extracting today's single-nucleon energies in the so-called well-known doubly-magic spherical-nuclei:

$$^{16}\mathrm{O},\ ^{40}\mathrm{Ca},\ ^{48}\mathrm{Ca},\ ^{56}\mathrm{Ni},\ ^{90}\mathrm{Zr},\ ^{132}\mathrm{Sn}\ \text{and}\ ^{208}\mathrm{Pb}$$

• We wish to find mean-field Hamiltonian $\mathrm{H_{mf}}$ which reproduces the single-particle energies exactly (Exact "Reference Hamiltonian")

Selection of Nuclei and Testing Model-Hamiltonians

• We will be interested in extracting today's single-nucleon energies in the so-called well-known doubly-magic spherical-nuclei:

$$^{16}\mathrm{O},\ ^{40}\mathrm{Ca},\ ^{48}\mathrm{Ca},\ ^{56}\mathrm{Ni},\ ^{90}\mathrm{Zr},\ ^{132}\mathrm{Sn}\ \text{and}\ ^{208}\mathrm{Pb}$$

• We wish to find mean-field Hamiltonian $\mathrm{H_{mf}}$ which reproduces the single-particle energies exactly (Exact "Reference Hamiltonian")

• The only simple Hamiltonian that we know of, which reproduces the single-particle spectra exactly, is the Woods-Saxon Hamiltonian

$$\boxed{H^{ws}_{mf} = T + V^{ws}_{cent} + V^{ws}_{so}}$$

Selection of Nuclei and Testing Model-Hamiltonians

• We will be interested in extracting today's single-nucleon energies in the so-called well-known doubly-magic spherical-nuclei:

$$^{16}\mathrm{O},\ ^{40}\mathrm{Ca},\ ^{48}\mathrm{Ca},\ ^{56}\mathrm{Ni},\ ^{90}\mathrm{Zr},\ ^{132}\mathrm{Sn}\ \text{and}\ ^{208}\mathrm{Pb}$$

• We wish to find mean-field Hamiltonian $\mathrm{H_{mf}}$ which reproduces the single-particle energies exactly (Exact "Reference Hamiltonian")

• The only simple Hamiltonian that we know of, which reproduces the single-particle spectra exactly, is the Woods-Saxon Hamiltonian

$$\boxed{H^{ws}_{mf} = T + V^{ws}_{cent} + V^{ws}_{so}}$$

• **The simple Woods-Saxon mean-field has certain advantages: Clearly defined roles of the size, depth and surface-diffuseness**

We return to the interpretation of this kind of correspondence between experiment and modelling slightly later

Realistic Phenomenological Nuclear Mean Field Theory: Physics Background for Experimentalists

Jerzy DUDEK

University of Strasbourg/IPHC/CNRS, France
and
The Henryk Niewodniczański Institute of Nuclear Physics
Polish Academy of Sciences, Kraków, Poland

Trento – Part 2

Theo4Exp EUROLABS Hands-on Workshop

TRENTO: Part II

Stochastic Methods for Prediction Capacities of Our Mean Field Modelling

Recall:

Experimental results are known within error bars:

$$\boxed{E = E_0 \pm \delta e}$$

Consequently the adjusted modelling parameters satisfy:

$$\boxed{P = P_0 \pm \delta p}$$

Therefore modelling results $\rightarrow$ have uncertainty margins:

$$\boxed{F = F_0 \pm \delta f}$$

Recall:

Experimental results are known within error bars:

$$\boxed{E = E_0 \pm \delta e}$$

Consequently the adjusted modelling parameters satisfy:

$$\boxed{P = P_0 \pm \delta p}$$

Therefore modelling results $\rightarrow$ have uncertainty margins:

$$\boxed{F = F_0 \pm \delta f}$$

They carry an extremely important information about predicting capacity (usually ignored) - Now: Central Point

Predictive Power of Theories: Stochastic Approach

The present research project is formulated within

Stochastic Theory of Predictive Power[*)]

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

Predictive Power of Theories: Stochastic Approach

The present research project is formulated within

Stochastic Theory of Predictive Power*)

- Given theory $\mathcal{T}$, of a quantum phenomenon $\mathcal{P}$, employing observables

$$\hat{\mathcal{F}}_1, \hat{\mathcal{F}}_2, \ldots \hat{\mathcal{F}}_p$$

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

Predictive Power of Theories: Stochastic Approach

The present research project is formulated within

Stochastic Theory of Predictive Power[*)]

- Given theory $\mathcal{T}$, of a quantum phenomenon $\mathcal{P}$, employing observables
$$\hat{\mathcal{F}}_1, \hat{\mathcal{F}}_2, \ldots \hat{\mathcal{F}}_p$$
- Observables will be characterised not only by related eigenvalues i.e. $\{f_j\}$
$$\left[\hat{\mathcal{F}}_1 \to \{f_1\}, \quad \hat{\mathcal{F}}_2 \to \{f_2\}, \quad \ldots \ \hat{\mathcal{F}}_p \to \{f_p\}\right]$$

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

Predictive Power of Theories: Stochastic Approach

The present research project is formulated within

Stochastic Theory of Predictive Power*)

- Given theory $\mathcal{T}$, of a quantum phenomenon $\mathcal{P}$, employing observables

$$\hat{\mathcal{F}}_1, \hat{\mathcal{F}}_2, \ldots \hat{\mathcal{F}}_p$$

- Observables will be characterised not only by related eigenvalues i.e. $\{f_j\}$

$$\left[\hat{\mathcal{F}}_1 \to \{f_1\}, \quad \hat{\mathcal{F}}_2 \to \{f_2\}, \quad \ldots \ \hat{\mathcal{F}}_p \to \{f_p\}\right]$$

but also by distributions of probability of their validity - or applicability

$$\mathcal{P}_1 = \mathcal{P}_1(f_1), \ \ \mathcal{P}_2 = \mathcal{P}_2(f_2), \ \ldots \ \mathcal{P}_p = \mathcal{P}_1(f_p)$$

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

Predictive Power of Theories: Stochastic Approach

The present research project is formulated within

Stochastic Theory of Predictive Power*)

- Given theory $\mathcal{T}$, of a quantum phenomenon $\mathcal{P}$, employing observables

$$\hat{\mathcal{F}}_1, \hat{\mathcal{F}}_2, \ldots \hat{\mathcal{F}}_p$$

- Observables will be characterised not only by related eigenvalues i.e. $\{f_j\}$

$$\left[\hat{\mathcal{F}}_1 \to \{f_1\}, \quad \hat{\mathcal{F}}_2 \to \{f_2\}, \quad \ldots \ \hat{\mathcal{F}}_p \to \{f_p\}\right]$$

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 **all the uncertainties known-, or possible to estimate today**

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

Section I

Probabilities of Uncertainties of Theory-Modelling

Section I

Probabilities of Uncertainties of Theory-Modelling

$$\mathcal{P}_1 = \mathcal{P}_1(f_1), \;\; \mathcal{P}_2 = \mathcal{P}_2(f_2), \;\; \ldots \;\; \mathcal{P}_p = \mathcal{P}_1(f_p)$$

Begin With Theory Uncertainties: Concepts

Begin With Theory Uncertainties: Concepts

- What we usually wish to find is the so-called scientific 'full truth'

$$\hat{H}^{true}\,\psi_n = e_n\,\psi_n \quad - \quad \textit{where we wish to know:} \quad \hat{H} = \hat{H}_{\rm true}$$

Begin With Theory Uncertainties: Concepts

- What we usually wish to find is the so-called scientific 'full truth'

$$\hat{H}^{true}\,\psi_n = e_n\,\psi_n \quad - \quad \textit{where we wish to know:} \quad \hat{H} = \hat{H}_{\rm true}$$

- The way physicists do their research can be schematised like this:

$$\hat{H} = \underbrace{\hat{H}_1}_{\text{of 1949}} + \underbrace{\hat{H}_2}_{\text{of 1964}} + \underbrace{\hat{H}_3}_{\text{of 2012}} + \cdots + \underbrace{\hat{H}_n}_{\text{of 2055}} + \cdots \rightarrow \underbrace{\hat{H}_{\rm true}}_{\text{say:}\infty}$$

In other words: The human physical theories are usually incomplete

Begin With Theory Uncertainties: Concepts

- What we usually wish to find is the so-called scientific 'full truth'

$$\hat{H}^{true}\,\psi_n = e_n\,\psi_n \quad - \quad \textit{where we wish to know:} \quad \hat{H} = \hat{H}_{\rm true}$$

- The way physicists do their research can be schematised like this:

$$\hat{H} = \underbrace{\hat{H}_1}_{\text{of 1949}} + \underbrace{\hat{H}_2}_{\text{of 1964}} + \underbrace{\hat{H}_3}_{\text{of 2012}} + \cdots + \underbrace{\hat{H}_n}_{\text{of 2055}} + \cdots \rightarrow \underbrace{\hat{H}_{\rm true}}_{\text{say:}\infty}$$

In other words: The human physical theories are usually incomplete

- Our Hamiltonians can be written as follows: $\hat{H} = \hat{H}_{\rm true} - \delta\hat{H}_{\rm ign.}$

- **Conclusion:** The "exact truth" remains unknown to us because of $\delta\hat{H}_{\rm ign.}$ $\leftrightarrow$ ignorance hopefully decreasing in time

How to Diminish the Negative Impact of Not Knowing for Sure?

How to Diminish the Negative Impact of Not Knowing for Sure?

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

How to Diminish the Negative Impact of Not Knowing for Sure?

- There exist well known effective means of limiting the negative impact of ignorance originating from incompleteness of information
- Solution: In the case of doubt we 'just parametrise our ignorance'

How to Diminish the Negative Impact of Not Knowing for Sure?

• There exist well known effective means of limiting the negative impact of ignorance originating from incompleteness of information

• Solution: In the case of doubt we 'just parametrise our ignorance'

• In other words: We need to estimate which answer will be more,- and which less-likely 'the right solution'. Expressed alternatively:

How to Diminish the Negative Impact of Not Knowing for Sure?

• There exist well known effective means of limiting the negative impact of ignorance originating from incompleteness of information

• Solution: In the case of doubt we 'just parametrise our ignorance'

• In other words: We need to estimate which answer will be more,- and which less-likely 'the right solution'. Expressed alternatively:

Find *the relative probabilities* of what we think the right answers are

• There exist well known effective means of limiting the negative impact of ignorance originating from incompleteness of information

• Solution: In the case of doubt we 'just parametrise our ignorance'

• In other words: We need to estimate which answer will be more,- and which less-likely 'the right solution'. Expressed alternatively:

Find *the relative probabilities* of what we think the right answers are

In Applied Mathematics:

1. Represent un unsure information by a random variable $\rightarrow$ X

• There exist well known effective means of limiting the negative impact of ignorance originating from incompleteness of information

• Solution: In the case of doubt we 'just parametrise our ignorance'

• In other words: We need to estimate which answer will be more,- and which less-likely 'the right solution'. Expressed alternatively:

Find *the relative probabilities* of what we think the right answers are

In Applied Mathematics:

1. Represent un unsure information by a random variable $\rightarrow X$

2. Mathematically, variable X is represented by a probability distribution $P_X = P_X(x) - x$ called 'realisation' of variable X

• There exist well known effective means of limiting the negative impact of ignorance originating from incompleteness of information

• Solution: In the case of doubt we 'just parametrise our ignorance'

• In other words: We need to estimate which answer will be more,- and which less-likely 'the right solution'. Expressed alternatively:

Find *the relative probabilities* of what we think the right answers are

In Applied Mathematics:

1. Represent un unsure information by a random variable $\rightarrow X$

2. Mathematically, variable X is represented by a probability distribution $P_X = P_X(x) - x$ called 'realisation' of variable X

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

Section II

Combining Theoretical Uncertainties and Experimental Errors

[Probability Convolution Theorem]

Stochastic Nature of Theoretical Predictions

- Theories are incomplete while experiments accompanied by errors:

$$\text{Theo.} \rightarrow \boxed{e_n = e_n^{true}(p) + \delta e_n^{unc}} \;\; \& \;\; \boxed{\varepsilon_n = \varepsilon_n^{true} + \delta\varepsilon_n^{err}} \leftarrow \text{Exp.}$$

e_n and ε_n are random variables $\rightarrow$ distributions $P_n^{th.}(e_n)$ and $P_n^{exp}(\varepsilon_n)$

Stochastic Nature of Theoretical Predictions

- Theories are incomplete while experiments accompanied by errors:

$$\text{Theo.} \rightarrow \boxed{e_n = e_n^{true}(p) + \delta e_n^{unc}} \;\; \& \;\; \boxed{\varepsilon_n = \varepsilon_n^{true} + \delta\varepsilon_n^{err}} \leftarrow \text{Exp.}$$

e_n and ε_n are random variables $\rightarrow$ distributions $P_n^{th.}(e_n)$ and $P_n^{exp}(\varepsilon_n)$

- Errors propagate to the theory predictions through parameter fits

$$\chi^2(p) \sim \sum w_n \Big[\underbrace{\left(\varepsilon_n^{true} + \delta\varepsilon_n^{err}\right)}_{\textbf{Experiment}} - \underbrace{\left(e_n^{true} + \delta e_n^{unc}\right)}_{\textbf{Theory}} \Big]^2 \rightarrow \frac{\partial\chi^2}{\partial p} = 0$$

thus the optimal parameter values $p \equiv \{p_1, p_2, \ldots\ p_f\}$ are random variables and consequently characterised by probability distributions

Stochastic Nature of Theoretical Predictions

- Theories are incomplete while experiments accompanied by errors:

$$\text{Theo.} \rightarrow \boxed{e_n = e_n^{true}(p) + \delta e_n^{unc}} \;\; \& \;\; \boxed{\varepsilon_n = \varepsilon_n^{true} + \delta\varepsilon_n^{err}} \leftarrow \text{Exp.}$$

e_n and ε_n are random variables $\rightarrow$ distributions $P_n^{th.}(e_n)$ and $P_n^{exp}(\varepsilon_n)$

- Errors propagate to the theory predictions through parameter fits

$$\chi^2(p) \sim \sum w_n \Big[\underbrace{\left(\varepsilon_n^{true} + \delta\varepsilon_n^{err}\right)}_{\textbf{Experiment}} - \underbrace{\left(e_n^{true} + \delta e_n^{unc}\right)}_{\textbf{Theory}} \Big]^2 \rightarrow \frac{\partial\chi^2}{\partial p} = 0$$

thus the optimal parameter values $p \equiv \{p_1, p_2, \ldots\ p_f\}$ are random variables and consequently characterised by probability distributions

$$\boxed{\textit{Convolution} : P(p) = \{P^{th}(e) * P^{exp}(\varepsilon)\} \equiv \int_{-\infty}^{+\infty} P^{th}(e) P^{exp}(\varepsilon - e)\, de}$$

Stochastic Nature of Theoretical Predictions

- Theories are incomplete while experiments accompanied by errors:

$$\text{Theo.} \rightarrow \boxed{e_n = e_n^{true}(p) + \delta e_n^{unc}} \;\; \& \;\; \boxed{\varepsilon_n = \varepsilon_n^{true} + \delta\varepsilon_n^{err}} \leftarrow \text{Exp.}$$

e_n and ε_n are random variables $\rightarrow$ distributions $P_n^{th.}(e_n)$ and $P_n^{exp}(\varepsilon_n)$

- Errors propagate to the theory predictions through parameter fits

$$\chi^2(p) \sim \sum w_n \Big[\underbrace{\left(\varepsilon_n^{true} + \delta\varepsilon_n^{err}\right)}_{\textbf{Experiment}} - \underbrace{\left(e_n^{true} + \delta e_n^{unc}\right)}_{\textbf{Theory}} \Big]^2 \rightarrow \frac{\partial \chi^2}{\partial p} = 0$$

thus the optimal parameter values $p \equiv \{p_1, p_2, \ldots\ p_f\}$ are random variables and consequently characterised by probability distributions

$$\boxed{\textit{Convolution} : P(p) = \{P^{th}(e) * P^{exp}(\varepsilon)\} \equiv \int_{-\infty}^{+\infty} P^{th}(e) P^{exp}(\varepsilon - e)\, de}$$

- Thus sum of two random variables, e and ϵ, with probability densities P^{th} and P^{exp}, is a random variable, p, with the probability density $\rightarrow P(p)$

Stochastic Nature of Theoretical Predictions

- Theories are incomplete whereas experiments plagued with errors:

$$\text{Theo.} \rightarrow \boxed{e_n = e_n^{true}(p) + \delta e_n^{error}} \;\&\; \boxed{\varepsilon_n = \varepsilon_n^{true} + \delta\varepsilon_n^{err}} \leftarrow \text{Exp.}$$

e_n and ε_n are random variables $\rightarrow$ distributions $P_n^{th.}(e_n)$ and $P_n^{exp}(\varepsilon_n)$

- Errors propagate to the theory predictions through parameter fits

$$\chi^2(p) \sim \sum w_n \Big[\underbrace{\left(\varepsilon_n^{true} + \delta\varepsilon_n^{err}\right)}_{\textbf{Experiment}} - \underbrace{\left(e_n^{true} + \delta e_n^{err}\right)}_{\textbf{Theory}} \Big]^2 \rightarrow \frac{\partial\chi^2}{\partial p} = 0$$

thus the optimal parameter values $p \equiv \{p_1, p_2, \ldots\ p_f\}$ are random variables and consequently characterised by probability distributions

$$\boxed{\textit{Convolution} : P(p) = \{P^{th}(e) * P^{exp}(\varepsilon)\} \equiv \int_{-\infty}^{+\infty} P^{th}(e) P^{exp}(\varepsilon - e)\, de}$$

- Surprising Conclusion? Parameters of theories are not fixed numbers! They are random variables – characterised by their probability distributions

Learn Prediciting & Testing Predictive Power

• We examine the predictive power capacities of the nuclear mean-field theory and its fundamental degrees of freedom: nucleon levels

Learn Prediciting & Testing Predictive Power

- We examine the predictive power capacities of the nuclear mean-field theory and its fundamental degrees of freedom: nucleon levels
- A simple beginning: We focus on 'doubly magic' spherical nuclei:

$^{16}_{8}O_{8}$, $^{40}_{20}Ca_{20}$, $^{48}_{20}Ca_{28}$, $^{56}_{28}Ni_{28}$, $^{90}_{40}Zr_{50}$, $^{132}_{50}Sn_{82}$, $^{146}_{64}Gd_{82}$, $^{208}_{82}Pb_{126}$

Learn Prediciting & Testing Predictive Power

• We examine the predictive power capacities of the nuclear mean-field theory and its fundamental degrees of freedom: nucleon levels

• A simple beginning: We focus on 'doubly magic' spherical nuclei:

$^{16}_{8}O_{8}$, $^{40}_{20}Ca_{20}$, $^{48}_{20}Ca_{28}$, $^{56}_{28}Ni_{28}$, $^{90}_{40}Zr_{50}$, $^{132}_{50}Sn_{82}$, $^{146}_{64}Gd_{82}$, $^{208}_{82}Pb_{126}$

• Since certain experimental levels in these nuclei are known, we can test the theory predictions – thus the Hamiltonian and its parameters

Learn Prediciting & Testing Predictive Power

• We examine the predictive power capacities of the nuclear mean-field theory and its fundamental degrees of freedom: nucleon levels

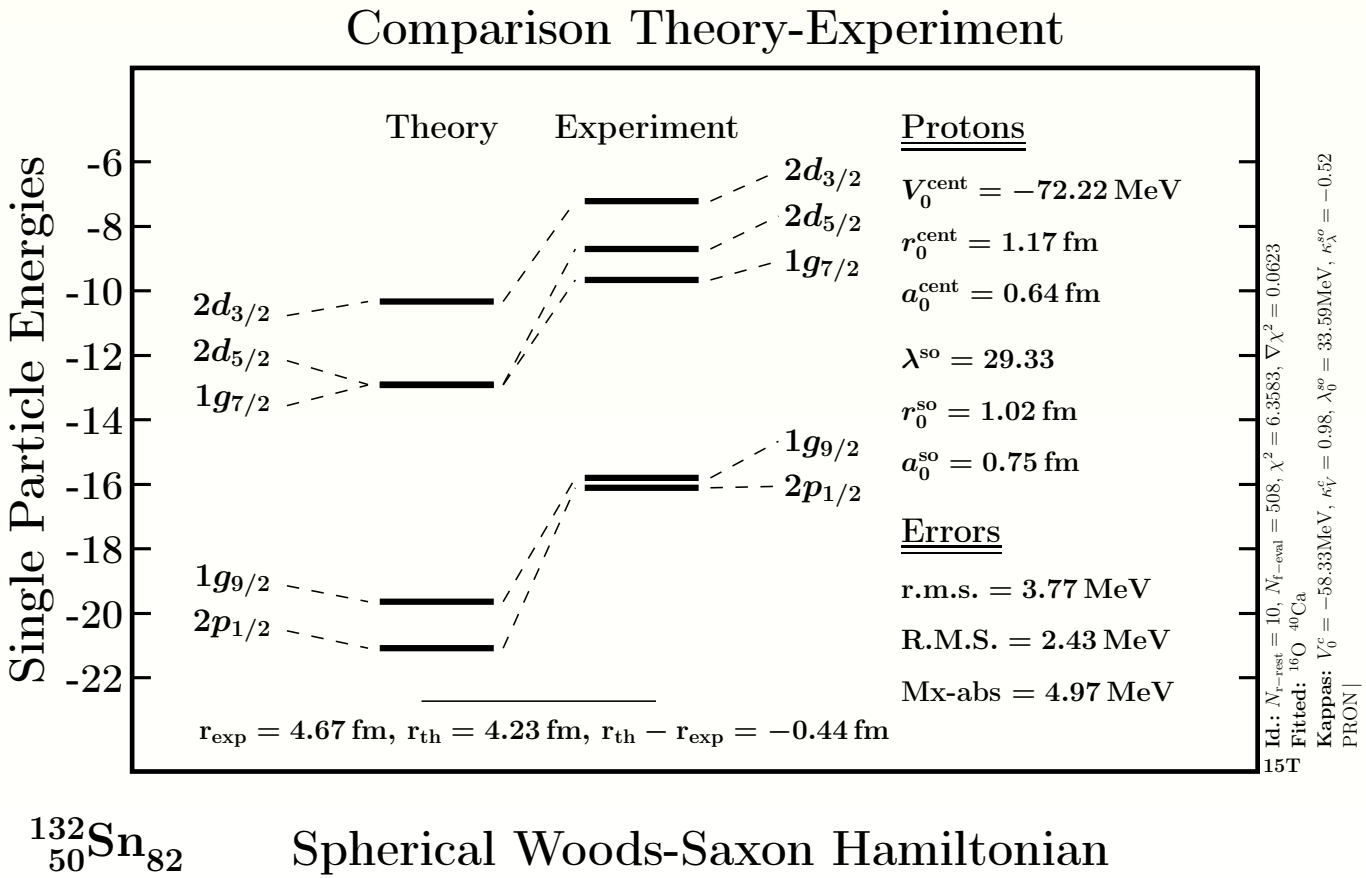
• A simple beginning: We focus on 'doubly magic' spherical nuclei:

$^{16}_{8}O_{8}$, $^{40}_{20}Ca_{20}$, $^{48}_{20}Ca_{28}$, $^{56}_{28}Ni_{28}$, $^{90}_{40}Zr_{50}$, $^{132}_{50}Sn_{82}$, $^{146}_{64}Gd_{82}$, $^{208}_{82}Pb_{126}$

• Since certain experimental levels in these nuclei are known, we can test the theory predictions – thus the Hamiltonian and its parameters

• Since we have a sample composed of 8 nuclei we can use sub-samples (=new samples) to test the predictions for remaining cases

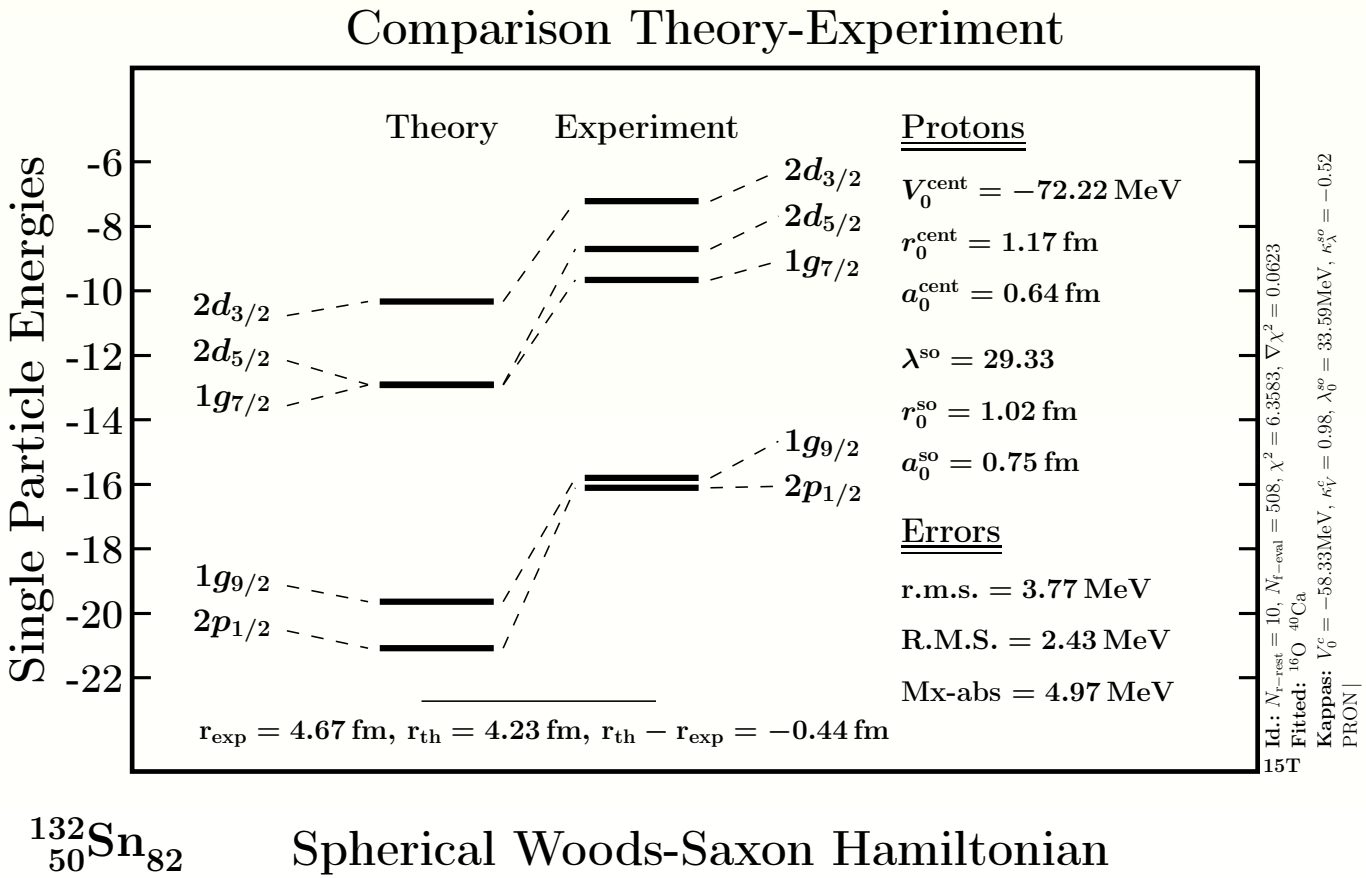
Sampling and Predicting: ^{132}Sn from ^{16}O and ^{40}Ca



$^{132}_{50}$Sn$_{82}$ Spherical Woods-Saxon Hamiltonian

- Proton single particle levels predicted via adjusting the parameters in ^{16}O and ^{40}Ca; observe a huge r.m.s. deviation of 3.7 MeV - poor prediction?

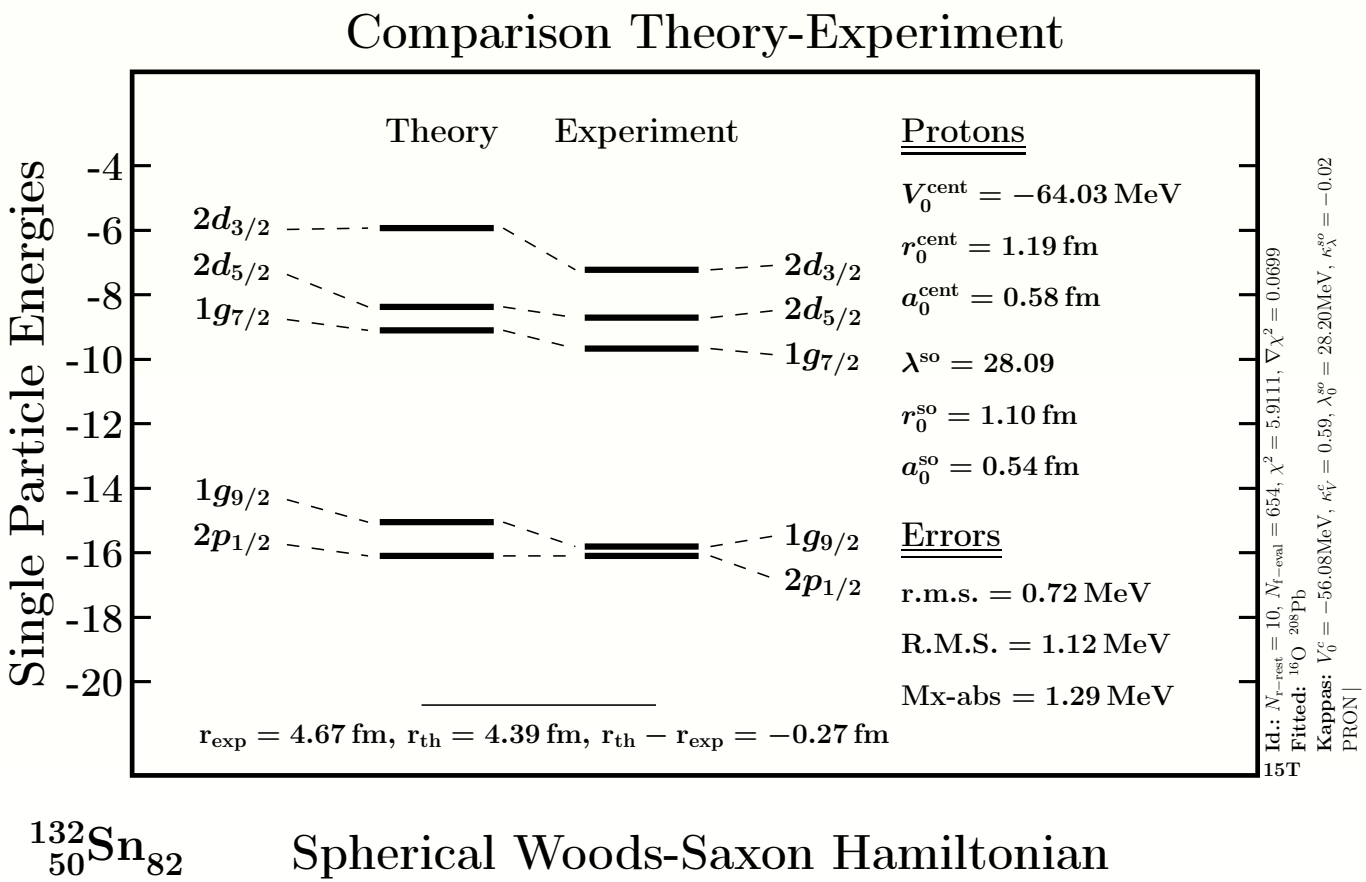
Sampling and Predicting: ^{132}Sn from ^{16}O and ^{40}Ca



$^{132}_{50}$Sn$_{82}$ Spherical Woods-Saxon Hamiltonian

• Proton single particle levels predicted via adjusting the parameters in ^{16}O and ^{40}Ca; observe a huge r.m.s. deviation of 3.7 MeV - poor prediction?
And yet - similarities are clear, main problem being 'only' a constant shift

Sampling and Predicting: ^{132}Sn from ^{16}O and ^{208}Pb



• Similar but adjusting the parameters in ^{16}O and ^{208}Pb; observe an improvement of the r.m.s. deviation by a factor of ≈ 5 ["better prediction"]

Section III

Towards more precision:

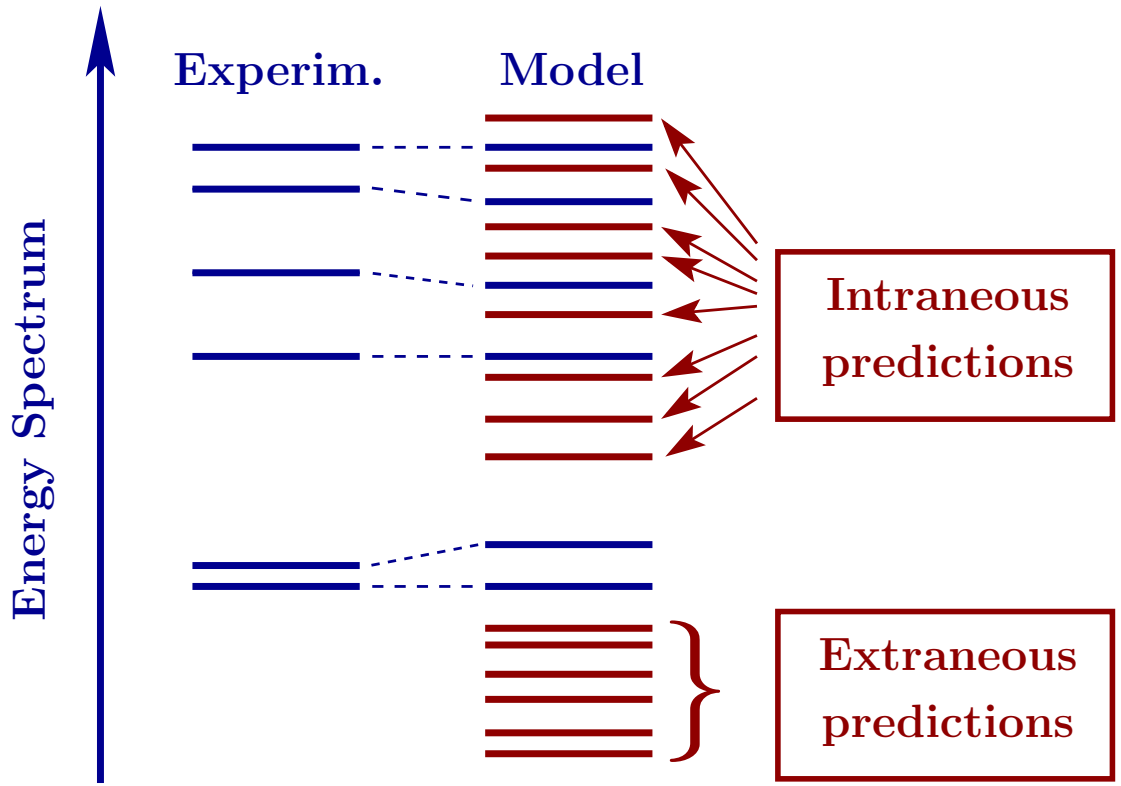
Section III

Towards more precision:

Intraneous vs. Extraneous Predictions

Intraneous Predictions – An Example

- Adjust Hamiltonian parameters using the data of a nucleus (Z, N)
- Energies intermixed with the experimental data are referred to as intraneous predictions

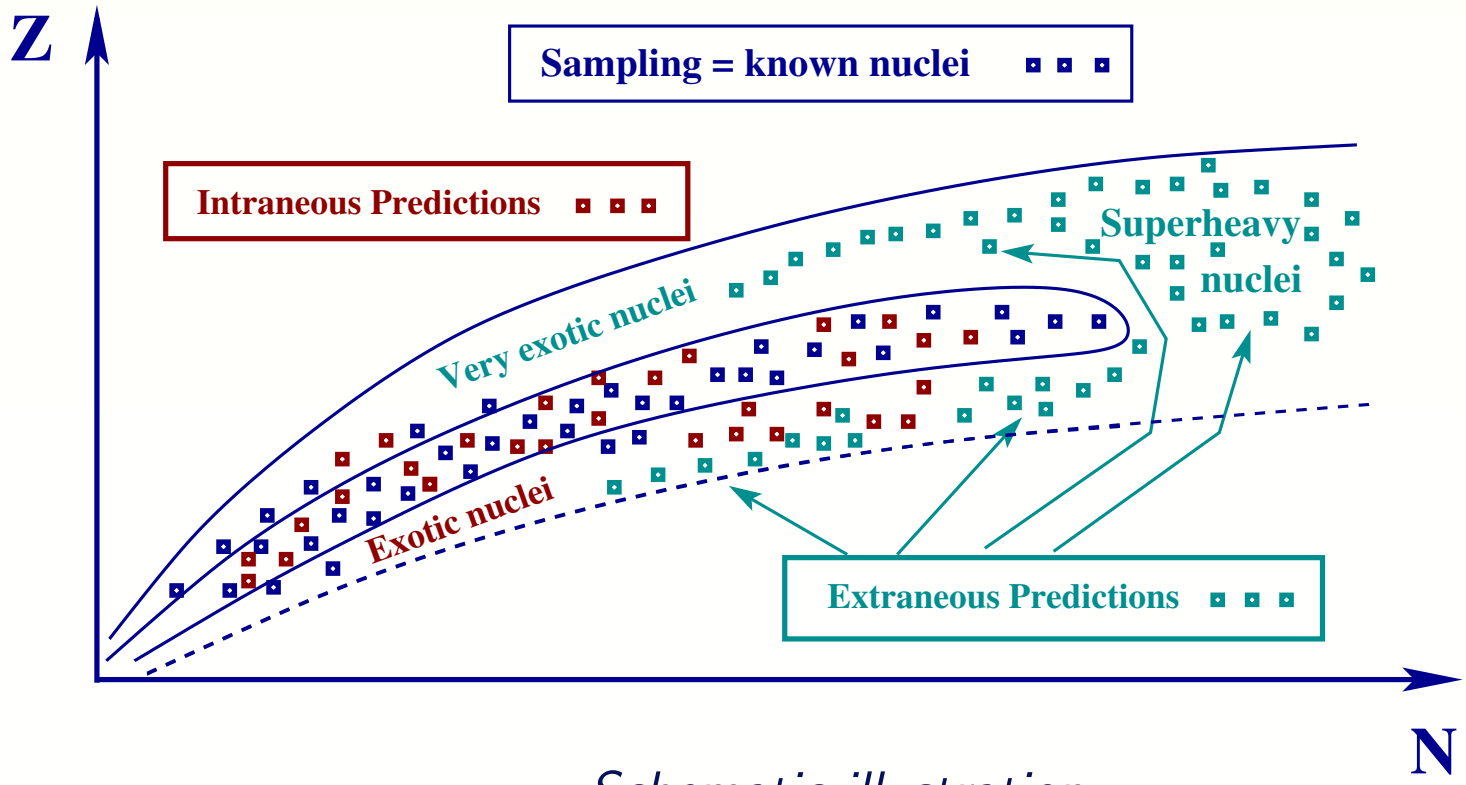


- This is just an example of intraneous predictions: There are more

Intraneous and Extraneous Predictions

• More generally - predictions related to nuclei 'in-between' the known ones ('interpolation') are referred to as intraneous prediction

• By the same token, predictions related to the nuclei far away from the known ones ('extrapolation') - are called extraneous predictions



Schematic illustration

We learn about Working Tools

1) Sampling
2) Intranous Prediction Zones
3) Extranous Prediction Zones

Section IV

Our Nuclear Mean-Field Realisation will be optimised employing

Inverse Problem Theory of Applied Mathematics

Direct and Inverse Problems in Quantum Theories

Direct and Inverse Problems in Quantum Theories

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

$$\hat{H} = \hat{T} + \hat{V}_{int}(...\{p\}); \quad \{p\} \rightarrow \text{Optimal parameters}$$

Direct and Inverse Problems in Quantum Theories

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

$$\hat{H} = \hat{T} + \hat{V}_{int}(...\{p\}); \quad \{p\} \rightarrow \text{Optimal parameters}$$

- If we know the parameters, we are able to solve the Direct Problem:

$$\hat{H}\,\varphi_j(..., \{p\}) = e_j^{th}(..., \{p\})\,\varphi_j(..., \{p\}) \;\leftrightarrow\; (\varphi_j, e_j)$$

Direct and Inverse Problems in Quantum Theories

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

$$\hat{H} = \hat{T} + \hat{V}_{int}(...\{p\}); \quad \{p\} \rightarrow \text{Optimal parameters}$$

- If we know the parameters, we are able to solve the Direct Problem:

$$\hat{H}\,\varphi_j(...,\{p\}) = e_j^{th}(...,\{p\})\,\varphi_j(...,\{p\}) \;\leftrightarrow\; (\varphi_j, e_j)$$

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

To determine the optimal parameters of the Hamiltonian

Inverse Problem in Quantum Theories vs. χ^2-Test

- Given parameters $\{p\} \rightarrow$ The Schrödinger equation produces data:

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

Inverse Problem in Quantum Theories vs. χ^2-Test

- Given parameters $\{p\} \rightarrow$ The Schrödinger equation produces data:

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

- To find the optimal parameters we must <u>invert</u> the above relation:

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

Inverse Problem in Quantum Theories vs. χ^2-Test

- Given parameters $\{p\} \rightarrow$ The Schrödinger equation produces data:

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

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

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

- In many-body theories the existence of operator $\hat{\mathcal{O}}_{\mathbf{H}}^{-1}$ is doubtful, in fact no mathematical methods of such a construction are known

Inverse Problem in Quantum Theories vs. χ^2-Test

- Given parameters $\{p\} \rightarrow$ The Schrödinger equation produces data:

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

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

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

- In many-body theories the existence of operator $\hat{\mathcal{O}}_{\mathbf{H}}^{-1}$ is doubtful, in fact no mathematical methods of such a construction are known

- **If $\hat{\mathcal{O}}_{\mathbf{H}}$ has no inverse we say that inverse problem is ill-posed**

Inverse Problem in Quantum Theories vs. χ^2-Test

- Given parameters $\{p\} \rightarrow$ The Schrödinger equation produces data:

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

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

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

- In many-body theories the existence of operator $\hat{\mathcal{O}}_{\mathbf{H}}^{-1}$ is doubtful, in fact no mathematical methods of such a construction are known

- **If $\hat{\mathcal{O}}_{\mathbf{H}}$ has no inverse we say that inverse problem is ill-posed**

- In physics this issue remains unsolved: Instead of finding optimal parameters by solving the Inverse Problem $\rightarrow\rightarrow$ "one minimises χ^2"

The Central Point of These Lectures

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

$$\begin{bmatrix} \mathcal{P}_1 \\ \mathcal{P}_2 \\ \cdots \\ \mathcal{P}_m \end{bmatrix} = \underbrace{\begin{bmatrix} \mathcal{A}_{11} & \mathcal{A}_{12} & \cdots & \mathcal{A}_{1d} \\ \mathcal{A}_{21} & \mathcal{A}_{22} & \cdots & \mathcal{A}_{2d} \\ \cdots & \cdots & \cdots & \cdots \\ \mathcal{A}_{m1} & \mathcal{A}_{m2} & \cdots & \mathcal{A}_{md} \end{bmatrix}^{-1}}_{\mathcal{A}^{-1}\text{: m}\times\text{d rectangular matrix}} \begin{bmatrix} \mathcal{D}_1 \\ \mathcal{D}_2 \\ \cdots \\ \mathcal{D}_d \end{bmatrix}$$

The Central Point of These Lectures

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

$$\begin{bmatrix} \mathcal{P}_1 \\ \mathcal{P}_2 \\ \cdots \\ \mathcal{P}_m \end{bmatrix} = \underbrace{\begin{bmatrix} \mathcal{A}_{11} & \mathcal{A}_{12} & \cdots & \mathcal{A}_{1d} \\ \mathcal{A}_{21} & \mathcal{A}_{22} & \cdots & \mathcal{A}_{2d} \\ \cdots & \cdots & \cdots & \cdots \\ \mathcal{A}_{m1} & \mathcal{A}_{m2} & \cdots & \mathcal{A}_{md} \end{bmatrix}^{-1}}_{\mathcal{A}^{-1}\text{: m}\times\text{d rectangular matrix}} \begin{bmatrix} \mathcal{D}_1 \\ \mathcal{D}_2 \\ \cdots \\ \mathcal{D}_d \end{bmatrix}$$

- $[\mathcal{A}_{ik}]$ depend on: 1) Hamiltonian, and 2) Selection of data points

The Central Point of These Lectures

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

$$\begin{bmatrix} \mathcal{P}_1 \\ \mathcal{P}_2 \\ \cdots \\ \mathcal{P}_m \end{bmatrix} = \underbrace{\begin{bmatrix} \mathcal{A}_{11} & \mathcal{A}_{12} & \cdots & \mathcal{A}_{1d} \\ \mathcal{A}_{21} & \mathcal{A}_{22} & \cdots & \mathcal{A}_{2d} \\ \cdots & \cdots & \cdots & \cdots \\ \mathcal{A}_{m1} & \mathcal{A}_{m2} & \cdots & \mathcal{A}_{md} \end{bmatrix}^{-1}}_{\mathcal{A}^{-1}\text{: m}\times\text{d rectangular matrix}} \begin{bmatrix} \mathcal{D}_1 \\ \mathcal{D}_2 \\ \cdots \\ \mathcal{D}_d \end{bmatrix}$$

- $[\mathcal{A}_{ik}]$ depend on: 1) Hamiltonian, and 2) Selection of data points

- If one of the parameters is a function of another, say, $p_k = f(p_{k'})$ then one may show, that two columns of $\mathcal{A}$ are linearly dependent

The Central Point of These Lectures

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

$$\begin{bmatrix} \mathcal{P}_1 \\ \mathcal{P}_2 \\ \cdots \\ \mathcal{P}_m \end{bmatrix} = \underbrace{\begin{bmatrix} \mathcal{A}_{11} & \mathcal{A}_{12} & \cdots & \mathcal{A}_{1d} \\ \mathcal{A}_{21} & \mathcal{A}_{22} & \cdots & \mathcal{A}_{2d} \\ \cdots & \cdots & \cdots & \cdots \\ \mathcal{A}_{m1} & \mathcal{A}_{m2} & \cdots & \mathcal{A}_{md} \end{bmatrix}^{-1}}_{\mathcal{A}^{-1}\text{: m}\times\text{d rectangular matrix}} \begin{bmatrix} \mathcal{D}_1 \\ \mathcal{D}_2 \\ \cdots \\ \mathcal{D}_d \end{bmatrix}$$

- $[\mathcal{A}_{ik}]$ depend on: 1) Hamiltonian, and 2) Selection of data points

- If one of the parameters is a function of another, say, $p_k = f(p_{k'})$ then one may show, that two columns of $\mathcal{A}$ are linearly dependent

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

Ill-Posed: Correlation between parameters and the data is lost!

The Central Point of These Lectures

Since the last observations form the central discussion issue of the whole series of lectures let us repeat them

The Central Point of These Lectures

Since the last observations form the central discussion issue of the whole series of lectures let us repeat them

If one of the parameters is a function of another one, say,
$$p_k = f(p_{k'}) \leftrightarrow \text{ parametric correlation}$$
one may show, that two columns of $\mathcal{A}$ are linearly dependent

The Central Point of These Lectures

Since the last observations form the central discussion issue of the whole series of lectures let us repeat them

If one of the parameters is a function of another one, say,
$p_k = f(p_{k'}) \leftrightarrow$ **parametric correlation**
one may show, that two columns of $\mathcal{A}$ are linearly dependent

If this happens $\rightarrow$ $\mathcal{A}$ in $\mathcal{P} = \mathcal{A}^{-1} \cdot \mathcal{D}$ becomes singular:
The model does NOT constrain parameters
χ^2-test has no solutions $\leftrightarrow$ Ill-Posed Inverse Problem

Correlation between parameters and the data is lost!

Running χ^2-codes gives equivalent of random numbers

Don't Try Solving the Ill-Posed Inverse Problem

Here we face replacing solutions by a non-sense [largely unknown, or deliberately ignored, or both]:

Don't Try Solving the Ill-Posed Inverse Problem

Here we face replacing solutions by a non-sense [largely unknown, or deliberately ignored, or both]:

- The inverse problem has no solution since modelling does not constrain parameters [changing data does not change parameters]

Don't Try Solving the Ill-Posed Inverse Problem

Here we face replacing solutions by a non-sense [largely unknown, or deliberately ignored, or both]:

- The inverse problem has no solution since modelling does not constrain parameters [changing data does not change parameters]
  - **... and yet some physicists keep χ^2-minimising!!**

Don't Try Solving the Ill-Posed Inverse Problem

Here we face replacing solutions by a non-sense [largely unknown, or deliberately ignored, or both]:

- The inverse problem has no solution since modelling does not constrain parameters [changing data does not change parameters]
  - **... and yet some physicists keep χ^2-minimising!!**
  - Unfortunately, the χ^2 usually "works perfectly well" $\longrightarrow$

Don't Try Solving the Ill-Posed Inverse Problem

Here we face replacing solutions by a non-sense [largely unknown, or deliberately ignored, or both]:

- The inverse problem has no solution since modelling does not constrain parameters [changing data does not change parameters]
- **... and yet some physicists keep χ^2-minimising!!**
- Unfortunately, the χ^2 usually "works perfectly well" $\longrightarrow$
- Some curves are generated, they may even go through experimental data... ["good r.m.s."]

Don't Try Solving the Ill-Posed Inverse Problem

Here we face replacing solutions by a non-sense [largely unknown, or deliberately ignored, or both]:

- The inverse problem has no solution since modelling does not constrain parameters [changing data does not change parameters]
- **... and yet some physicists keep χ^2-minimising!!**
- Unfortunately, the χ^2 usually "works perfectly well" $\longrightarrow$
- Some curves are generated, they may even go through experimental data... ["good r.m.s."]
- **... but these results have neither mathematical nor not much of the physical significance...**

Don't Try Solving the Ill-Posed Inverse Problem

Here we face replacing solutions by a non-sense [largely unknown, or deliberately ignored, or both]:

- The inverse problem has no solution since modelling does not constrain parameters [changing data does not change parameters]
- **... and yet some physicists keep χ^2-minimising!!**
- Unfortunately, the χ^2 usually "works perfectly well" $\longrightarrow$
- Some curves are generated, they may even go through experimental data... ["good r.m.s."]
- **... but these results have neither mathematical nor not much of the physical significance... ... and even less of prediction capacities!**

The 'Enemy' No. 1 of the Mean-Field Users:

Parametric Correlations
within the Inverse Problem:

a. How to determine their presence?

b. How to eliminate their consequences
which are disastrous for predictive power?

Reminder from Probability Calculus

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

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

Reminder from Probability Calculus

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

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

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

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

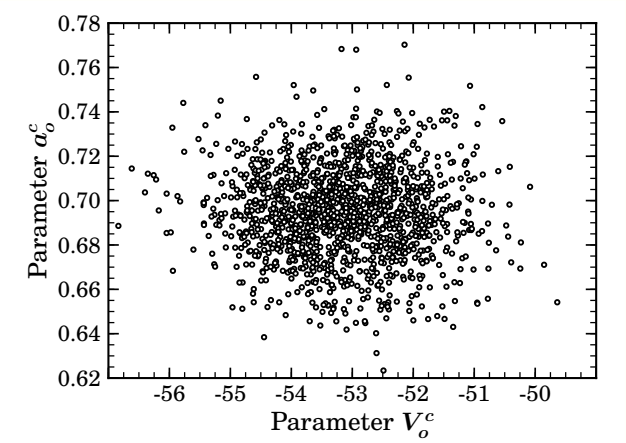
	V_0^c	r_0^c	a_0^c	V_0^{so}	r_0^{so}
V_0^c	1.000	0.994	-0.028	0.000	0.265
r_0^c	0.994	1.000	0.016	0.005	0.270
a_0^c	0.028	0.016	1.000	0.259	0.288
V_0^{so}	0.000	0.005	0.259	1.000	0.506
r_0^{so}	0.265	0.270	0.288	0.506	1.000

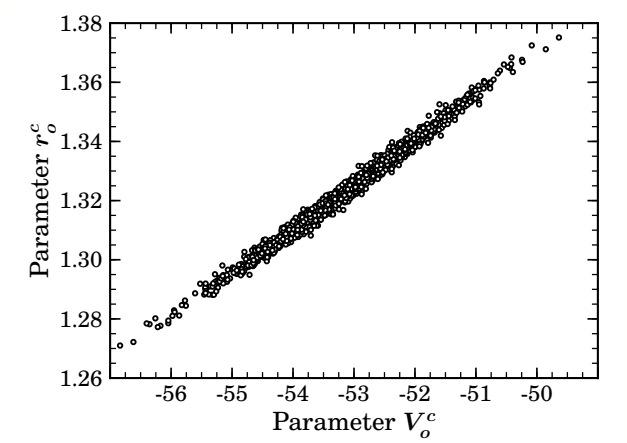
The non-diagonal matrix elements close to 1 signify strong matrix correlations

One can demonstrate that parametric correlations can easily be studied using Monte Carlo methods as follows:

- **Given space of data $\{d_1, d_2, \ldots\ d_n\}$ 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, $\{p_1, p_2, \ldots\ p_m\}$, we construct the tables and projection plots like the two which follow**

Parameter-Correlations and Correlation Matrix [W-S]

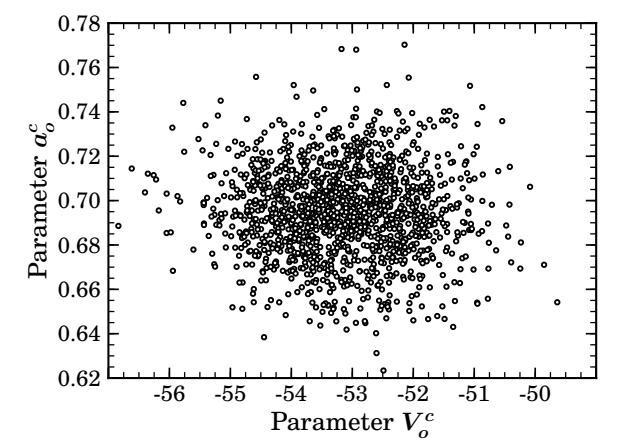


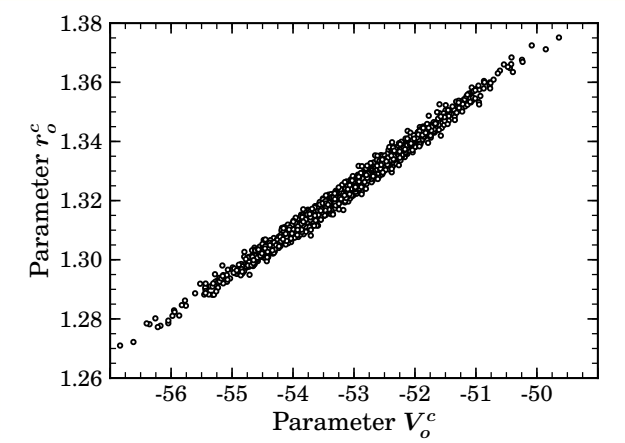


Monte-Carlo fitting results for ^{208}Pb with the Woods-Saxon potential

Left:(a_0^c vs. V_0^c) $\leftrightarrow$ no correlations; Right: (r_0^c vs. V_0^c)$\leftrightarrow$ strong correlations

Parameter-Correlations and Correlation Matrix [W-S]





Monte-Carlo fitting results for ^{208}Pb with the Woods-Saxon potential
Left:(a_0^c vs. V_0^c) $\leftrightarrow$ no correlations; Right: (r_0^c vs. V_0^c)$\leftrightarrow$ strong correlations

Correlation matrix for the Woods-Saxon Hamiltonian parameters

	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

Section V

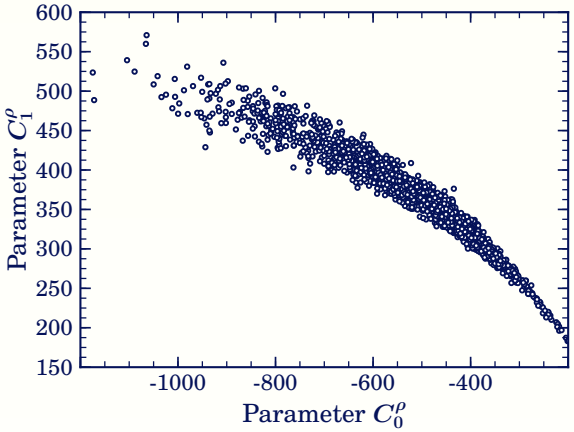
Instructive Comparisons with Skyrme Hartree-Fock Hamiltonian

Sampling and Parametric Correlations

To follow the discussion it will be sufficient to know that the Skyrme Hamiltonian depends on the adjustable constants:

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

Parameter-Correlations and Correlation Matrix [H-F]



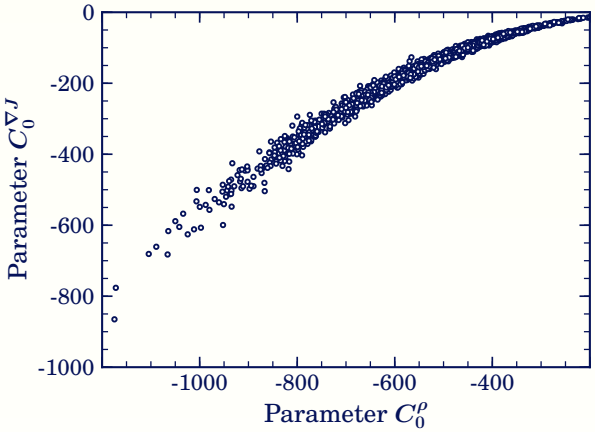
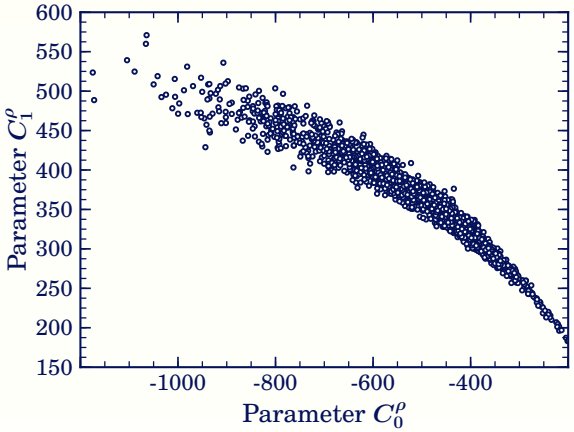


Illustration analogous to the preceding one; here Skyrme Hartree-Fock showing clear parameter correlations [B. Szpak, PhD tesis]

Parameter-Correlations and Correlation Matrix [H-F]



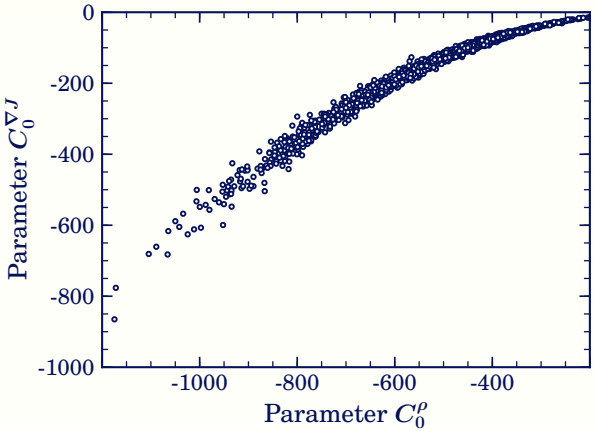
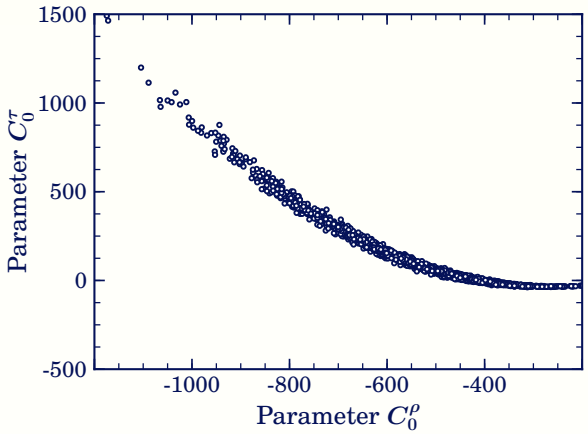


Illustration analogous to the preceding one; here Skyrme Hartree-Fock showing clear parameter correlations [B. Szpak, PhD tesis]

Correlation matrix for the Skyrme-Hartree-Fock Hamiltonian parameters

	C_0^ρ	C_1^ρ	$C_0^{\rho\alpha}$	C_0^τ	C_1^τ	$C_0^{\nabla J}$
C_0^ρ	1.000	-0.948	-0.506	-0.902	0.952	0.965
C_1^ρ	-0.948	1.000	0.682	0.745	-0.838	-0.854
$C_0^{\rho\alpha}$	-0.506	0.682	1.000	0.102	-0.243	-0.290
C_0^τ	-0.902	0.745	0.102	1.000	-0.985	-0.977
C_1^τ	0.952	-0.838	-0.243	-0.985	1.000	0.993
$C_0^{\nabla J}$	0.965	-0.854	-0.290	-0.977	0.993	1.000

Parameter-Correlations and Correlation Matrix [H-F]



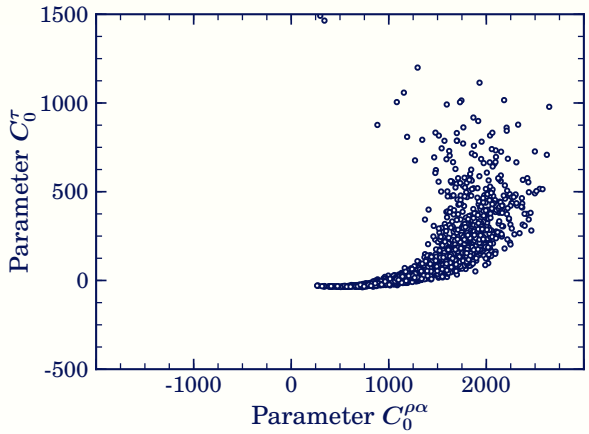


Illustration analogous to the preceding one; here Skyrme Hartree-Fock; notice two types of parametric correlations [B. Szpak, PhD thesis]

Correlation matrix for the Skyrme-Hartree-Fock Hamiltonian parameters

	C_0^ρ	C_1^ρ	$C_0^{\rho\alpha}$	C_0^τ	C_1^τ	$C_0^{\nabla J}$
C_0^ρ	1.000	-0.948	-0.506	-0.902	0.952	0.965
C_1^ρ	-0.948	1.000	0.682	0.745	-0.838	-0.854
$C_0^{\rho\alpha}$	-0.506	0.682	1.000	0.102	-0.243	-0.290
C_0^τ	-0.902	0.745	0.102	1.000	-0.985	-0.977
C_1^τ	0.952	-0.838	-0.243	-0.985	1.000	0.993
$C_0^{\nabla J}$	0.965	-0.854	-0.290	-0.977	0.993	1.000

Parameter-Correlations in Skyrme-H-F

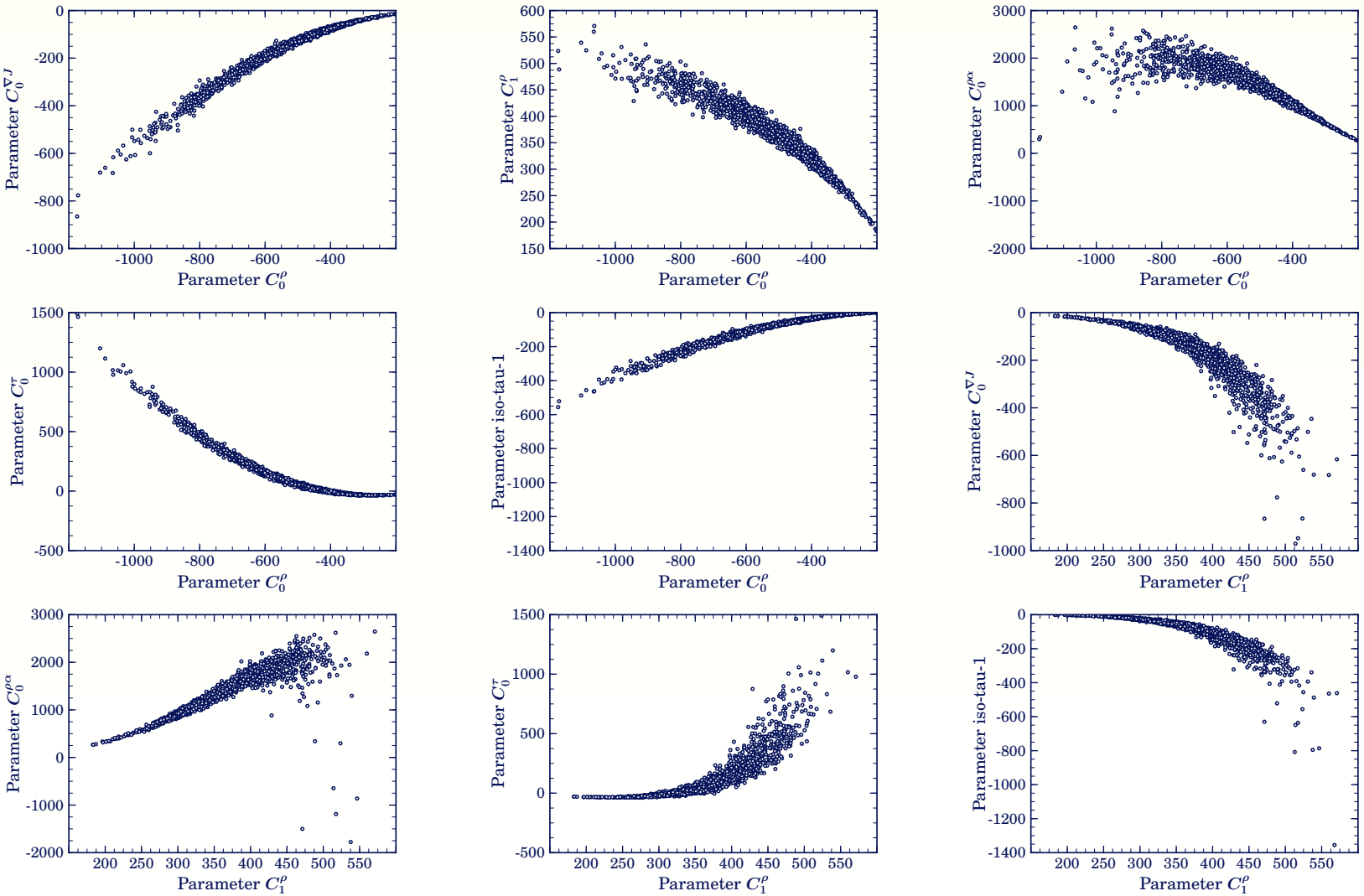


Illustration suggesting that majority of these parameters are strongly correlated excluding the prediction capacities of the model [B. Szpak, PhD thesis]

Parametric Correlations:

Strongly Present in the Nuclear Skyrme-Hartree-Fock Mean Fields

Parametric Correlations:

Strongly Present in the Nuclear Skyrme-Hartree-Fock Mean Fields

Parametric Correlations signify that no predictive power is possible to obtain with this type of the Hamiltonians

Parametric Correlations:

Strongly Present in the Nuclear Skyrme-Hartree-Fock Mean Fields

Parametric Correlations signify that no predictive power is possible to obtain with this type of the Hamiltonians

In other words: This Hamiltonian may very well allow to fit the data - but by no means predict[*)]

[*)] **J. Rikovska-Stone, J. Phys. G31 (2005) R211-R230: Cites over 100 distinct, non-equivalent parameterisations of the Skyrme Hartree-Fock Hamiltonian so far published in the literature**

Attention! A JOKE:

The Following Messages

Attention! A JOKE:

The Following Messages are intended

Attention! A JOKE:

The Following Messages are intended for Mature Audiences

Attention! A JOKE:

The Following Messages are intended for Mature Audiences

• **Observe: The 'standard' Skyrme Hartree-Fock Hamiltonian which was discussed above contains 12 terms with 12 adjustable coupling constants – of the so-called leading order (LO) – and shown to be largely very-correlated**

Leading Order (n=2) allows for 18 Hamiltonian terms maximum

Attention! A JOKE:

The Following Messages are intended for Mature Audiences

• **Observe: The 'standard' Skyrme Hartree-Fock Hamiltonian which was discussed above contains 12 terms with 12 adjustable coupling constants – of the so-called leading order (LO) – and shown to be largely very-correlated**

Leading Order (n=2) allows for 18 Hamiltonian terms maximum

• **The new approach mentioned next is an improvement of the method and contains terms of the next-to-next-to-next order i.e. 2632 vs. 12 terms...**

Skyrme-HF in the EDF Formulation up to N^3LO

• Numbers of terms depending on the time-even and time-odd densities are given below separately. The last two columns give numbers of terms when the Galilean or gauge[1] invariance symmetries are assumed, respectively.

Order	T-even	T-odd	Total	Galilean	Gauge
0	1	1	2	2	2
2	8	10	18	12	12
4	53	61	114	45	29
6	250	274	524	129	54
N^3LO	2x312	2x346	2x658	2x188	2x97
	624	692	1316	376	194

• Let us observe a very fast-growing number of terms. To take into account both isospin channels, the number of terms is multiplied by a factor of two

[1] *For comments about Skyrme HF gauge invariance cf. e.g. J. Dobaczewski and J. Dudek, PRC 52 (1995) 1827*

Selection of the Model Mean-Field Hamiltonian for the Project

Selection of Model Hamiltonian for the Project

- For the applications in this project we could have used the Skyrme Hartree-Fock approach and computer programs developed in Strasbourg:

[1] Solutions of the Skyrme-Hartree-Fock Equations: (I) The Method;
J. Dobaczewski and J. Dudek, *Comp. Phys. Comm.* **102 (1)** *(1997) 166-182*

[2] Solutions of the Skyrme-Hartree-Fock Equations. (II) The Program HF_ODD;
J. Dobaczewski and J. Dudek, *Comp. Phys. Comm.* **102 (1)** *(1997) 183-209*

Selection of Model Hamiltonian for the Project

• For the applications in this project we could have used the Skyrme Hartree-Fock approach and computer programs developed in Strasbourg:

[1] Solutions of the Skyrme-Hartree-Fock Equations: (I) The Method;
J. Dobaczewski and J. Dudek, *Comp. Phys. Comm.* **102 (1)** *(1997) 166-182*

[2] Solutions of the Skyrme-Hartree-Fock Equations. (II) The Program HF_ODD;
J. Dobaczewski and J. Dudek, *Comp. Phys. Comm.* **102 (1)** *(1997) 183-209*

• We decided not to use the Skyrme because of the overwhelmingly present parametric correlations and the implied issues of missing predictive power

Selection of Model Hamiltonian for the Project

• For the applications in this project we could have used the Skyrme Hartree-Fock approach and computer programs developed in Strasbourg:

[1] Solutions of the Skyrme-Hartree-Fock Equations: (I) The Method;
J. Dobaczewski and J. Dudek, *Comp. Phys. Comm.* **102 (1)** *(1997) 166-182*

[2] Solutions of the Skyrme-Hartree-Fock Equations. (II) The Program HF_ODD;
J. Dobaczewski and J. Dudek, *Comp. Phys. Comm.* **102 (1)** *(1997) 183-209*

• We decided not to use the Skyrme because of the overwhelmingly present parametric correlations and the implied issues of missing predictive power

• **Alternative: Phenomenological Woods-Saxon Universal mean-field**

[A] J. Dudek and T. Werner 1978, J. Phys. G4 1543
[B] J. Dudek and collaborators, 1979 J. Phys. G5 1359
[C] J. Dudek, Z. Szymański and T. Werner 1981, Phys. Rev. C23 920
and summarized in
[D] S. Ćwiok, J. Dudek, W. Nazarewicz, J. Skalski, T. Werner, 1987, CPC 46, 379

Selection of Model Hamiltonian for the Project

• For the applications in this project we could have used the Skyrme Hartree-Fock approach and computer programs developed in Strasbourg:

[1] Solutions of the Skyrme-Hartree-Fock Equations: (I) The Method;
J. Dobaczewski and J. Dudek, *Comp. Phys. Comm.* **102 (1)** *(1997) 166-182*

[2] Solutions of the Skyrme-Hartree-Fock Equations. (II) The Program HF_ODD;
J. Dobaczewski and J. Dudek, *Comp. Phys. Comm.* **102 (1)** *(1997) 183-209*

• We decided not to use the Skyrme because of the overwhelmingly present parametric correlations and the implied issues of missing predictive power

• **Alternative: Phenomenological Woods-Saxon Universal mean-field**

[A] J. Dudek and T. Werner 1978, J. Phys. G4 1543
[B] J. Dudek and collaborators, 1979 J. Phys. G5 1359
[C] J. Dudek, Z. Szymański and T. Werner 1981, Phys. Rev. C23 920
and summarized in
[D] S. Ćwiok, J. Dudek, W. Nazarewicz, J. Skalski, T. Werner, 1987, CPC 46, 379

• 'Woods-Saxon Universal' is used today by many-many articles every year

W-S Universal: Among Popular Realistic Models

W-S Universal: Among Popular Realistic Models

• To give an illustration of the use-frequency we quote below the articles which appeared only in 2013 and only in one journal - The Physical Review:

W-S Universal: Among Popular Realistic Models

• To give an illustration of the use-frequency we quote below the articles which appeared only in 2013 and only in one journal - The Physical Review:

[1] Phys. Rev. C 88, 044313 (2013); J. Rissanen et al.,

W-S Universal: Among Popular Realistic Models

• To give an illustration of the use-frequency we quote below the articles which appeared only in 2013 and only in one journal - The Physical Review:

[1] Phys. Rev. C 88, 044313 (2013); J. Rissanen et al.,
[2] Phys. Rev. C 88, 044307 (2013); W. Brodziński et al.,

W-S Universal: Among Popular Realistic Models

• To give an illustration of the use-frequency we quote below the articles which appeared only in 2013 and only in one journal - The Physical Review:

[1] Phys. Rev. C 88, 044313 (2013); J. Rissanen et al.,
[2] Phys. Rev. C 88, 044307 (2013); W. Brodziński et al.,
[3] Phys. Rev. C 88, 024302 (2013); S. Lalkowski et al.,

W-S Universal: Among Popular Realistic Models

• To give an illustration of the use-frequency we quote below the articles which appeared only in 2013 and only in one journal - The Physical Review:

[1] Phys. Rev. C 88, 044313 (2013); J. Rissanen et al.,
[2] Phys. Rev. C 88, 044307 (2013); W. Brodziński et al.,
[3] Phys. Rev. C 88, 024302 (2013); S. Lalkowski et al.,
[4] Phys. Rev. C 87, 067304 (2013); H. L. Liu et al.,

W-S Universal: Among Popular Realistic Models

• To give an illustration of the use-frequency we quote below the articles which appeared only in 2013 and only in one journal - The Physical Review:

[1] Phys. Rev. C 88, 044313 (2013); J. Rissanen et al.,
[2] Phys. Rev. C 88, 044307 (2013); W. Brodziński et al.,
[3] Phys. Rev. C 88, 024302 (2013); S. Lalkowski et al.,
[4] Phys. Rev. C 87, 067304 (2013); H. L. Liu et al.,
[5] Phys. Rev. C 87, 041302 (2013); D. S. Delion et al.,

W-S Universal: Among Popular Realistic Models

• To give an illustration of the use-frequency we quote below the articles which appeared only in 2013 and only in one journal - The Physical Review:

[1] Phys. Rev. C 88, 044313 (2013); J. Rissanen et al.,
[2] Phys. Rev. C 88, 044307 (2013); W. Brodziński et al.,
[3] Phys. Rev. C 88, 024302 (2013); S. Lalkowski et al.,
[4] Phys. Rev. C 87, 067304 (2013); H. L. Liu et al.,
[5] Phys. Rev. C 87, 041302 (2013); D. S. Delion et al.,
[6] Phys. Rev. C 87, 034328 (2013); D. S. Delion et al.,

W-S Universal: Among Popular Realistic Models

• To give an illustration of the use-frequency we quote below the articles which appeared only in 2013 and only in one journal - The Physical Review:

[1] Phys. Rev. C 88, 044313 (2013); J. Rissanen et al.,
[2] Phys. Rev. C 88, 044307 (2013); W. Brodziński et al.,
[3] Phys. Rev. C 88, 024302 (2013); S. Lalkowski et al.,
[4] Phys. Rev. C 87, 067304 (2013); H. L. Liu et al.,
[5] Phys. Rev. C 87, 041302 (2013); D. S. Delion et al.,
[6] Phys. Rev. C 87, 034328 (2013); D. S. Delion et al.,
[7] Phys. Rev. C 87, 024309 (2013); D. S. Delion et al.,

W-S Universal: Among Popular Realistic Models

• To give an illustration of the use-frequency we quote below the articles which appeared only in 2013 and only in one journal - The Physical Review:

[1] Phys. Rev. C 88, 044313 (2013); J. Rissanen et al.,
[2] Phys. Rev. C 88, 044307 (2013); W. Brodziński et al.,
[3] Phys. Rev. C 88, 024302 (2013); S. Lalkowski et al.,
[4] Phys. Rev. C 87, 067304 (2013); H. L. Liu et al.,
[5] Phys. Rev. C 87, 041302 (2013); D. S. Delion et al.,
[6] Phys. Rev. C 87, 034328 (2013); D. S. Delion et al.,
[7] Phys. Rev. C 87, 024309 (2013); D. S. Delion et al.,
[8] Phys. Rev. C 87, 014329 (2013); D. Deleanu et al.,

W-S Universal: Among Popular Realistic Models

• To give an illustration of the use-frequency we quote below the articles which appeared only in 2013 and only in one journal - The Physical Review:

[1] Phys. Rev. C 88, 044313 (2013); J. Rissanen et al.,
[2] Phys. Rev. C 88, 044307 (2013); W. Brodziński et al.,
[3] Phys. Rev. C 88, 024302 (2013); S. Lalkowski et al.,
[4] Phys. Rev. C 87, 067304 (2013); H. L. Liu et al.,
[5] Phys. Rev. C 87, 041302 (2013); D. S. Delion et al.,
[6] Phys. Rev. C 87, 034328 (2013); D. S. Delion et al.,
[7] Phys. Rev. C 87, 024309 (2013); D. S. Delion et al.,
[8] Phys. Rev. C 87, 014329 (2013); D. Deleanu et al.,
[9] Phys. Rev. C 86, 064323 (2013); S. Takahara et al.,

- We present here only the spherical variant of the Woods-Saxon potential

$$V_{cent}^{\mathrm{WS}} = \frac{V_c}{1 + \exp\left[\left(r - R_c\right)/a_c\right]}; \quad R_c = r_c A^{1/3}.$$

It has unique features among most of the mean field models, namely, each parameter is related to an independent class of experiments:

- V_c - depth parameter; specific transfer reactions
- r_c - radius parameter; electron scattering
- a_c - diffuseness parameter; hadron scattering

- In principle each of these parameters can be determined separately thus helping to counteract certain parametric correlations

- The importance – This potential is broadly used for deformed nuclei:

$$V_{cent}^{\mathrm{WS}} = \frac{V_c}{1 + \exp\left[\mathrm{dist}_{\Sigma}(\vec{r}; R_0)/a_c\right]}$$

with a fixed parameter set for thousands of nuclei $\Rightarrow$ Thus **'universal'**

Woods-Saxon Hamiltonian: Spin-Orbit Potential

The spherical Woods-Saxon spin-orbit potential has the form

$$V_{so}^{ws} = \frac{\lambda_{so}}{r}\frac{d}{dr}\left[\frac{1}{1+\exp\left[\left(r-R_{so}\right)/a_{so}\right]}\right]\hat{\ell}\cdot\hat{s}; \quad R_{so} = r_{so}A^{1/3}$$

- λ_{so} - strength parameter
- r_{so} - radius parameter
- a_{so} - diffuseness parameter

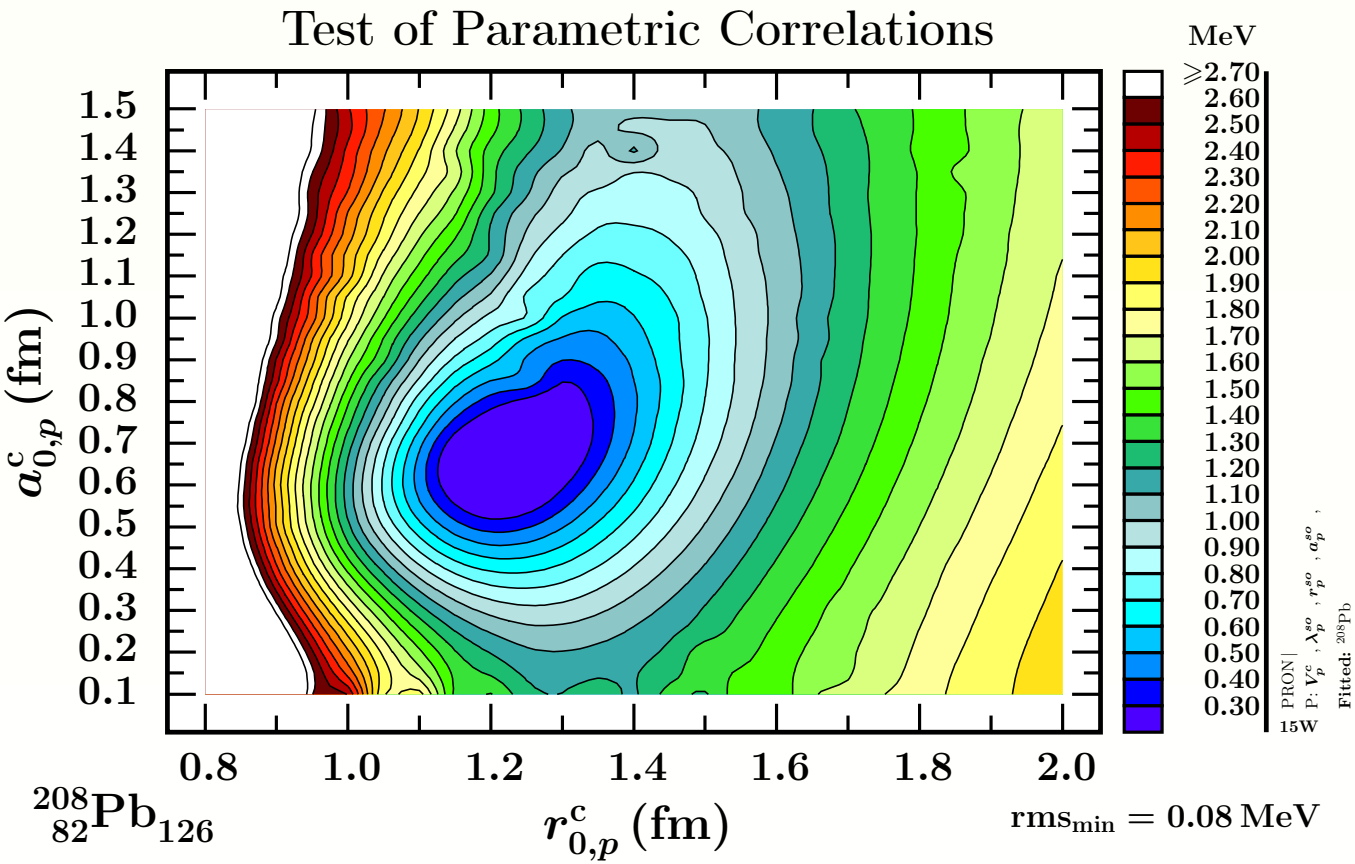
In total two sets of six parameters $\{V_c, r_c, a_c; \lambda_{so}, r_{so}, a_{so}\}_{\pi,\nu}$

Back to the Parametric Correlation Problem

- **One can show that the parametric correlations can be detected through projecting the $\chi^2(p)$ onto a (p_j, p_k)-plane:** $\min_{i\neq j,k} \chi^2(p_1, p_2, \ldots p_m)$

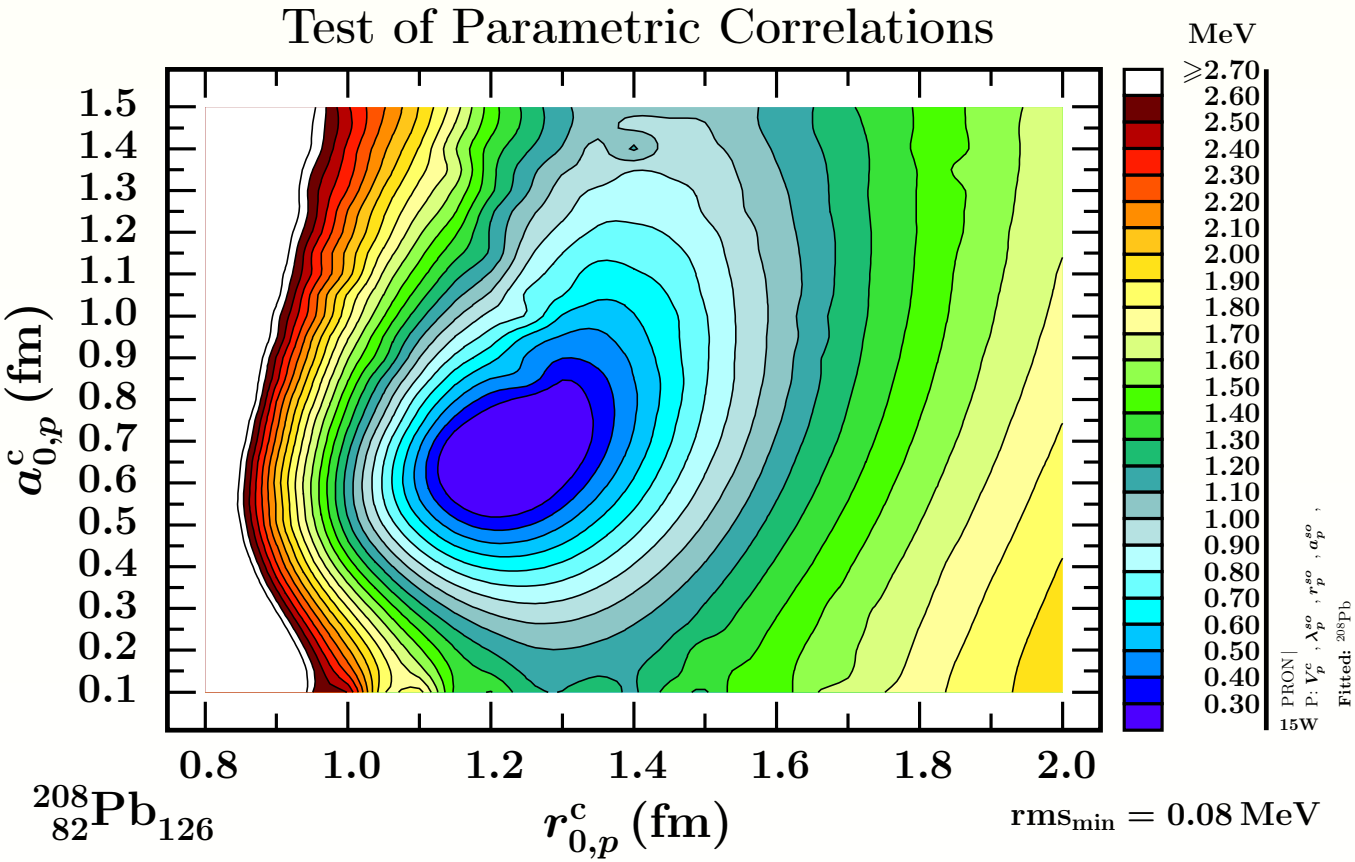
Back to the Parametric Correlation Problem

- **One can show that the parametric correlations can be detected through projecting the $\chi^2(p)$ onto a (p_j, p_k)-plane:** $\min_{i\neq j,k}\chi^2(p_1, p_2, \ldots p_m)$



Back to the Parametric Correlation Problem

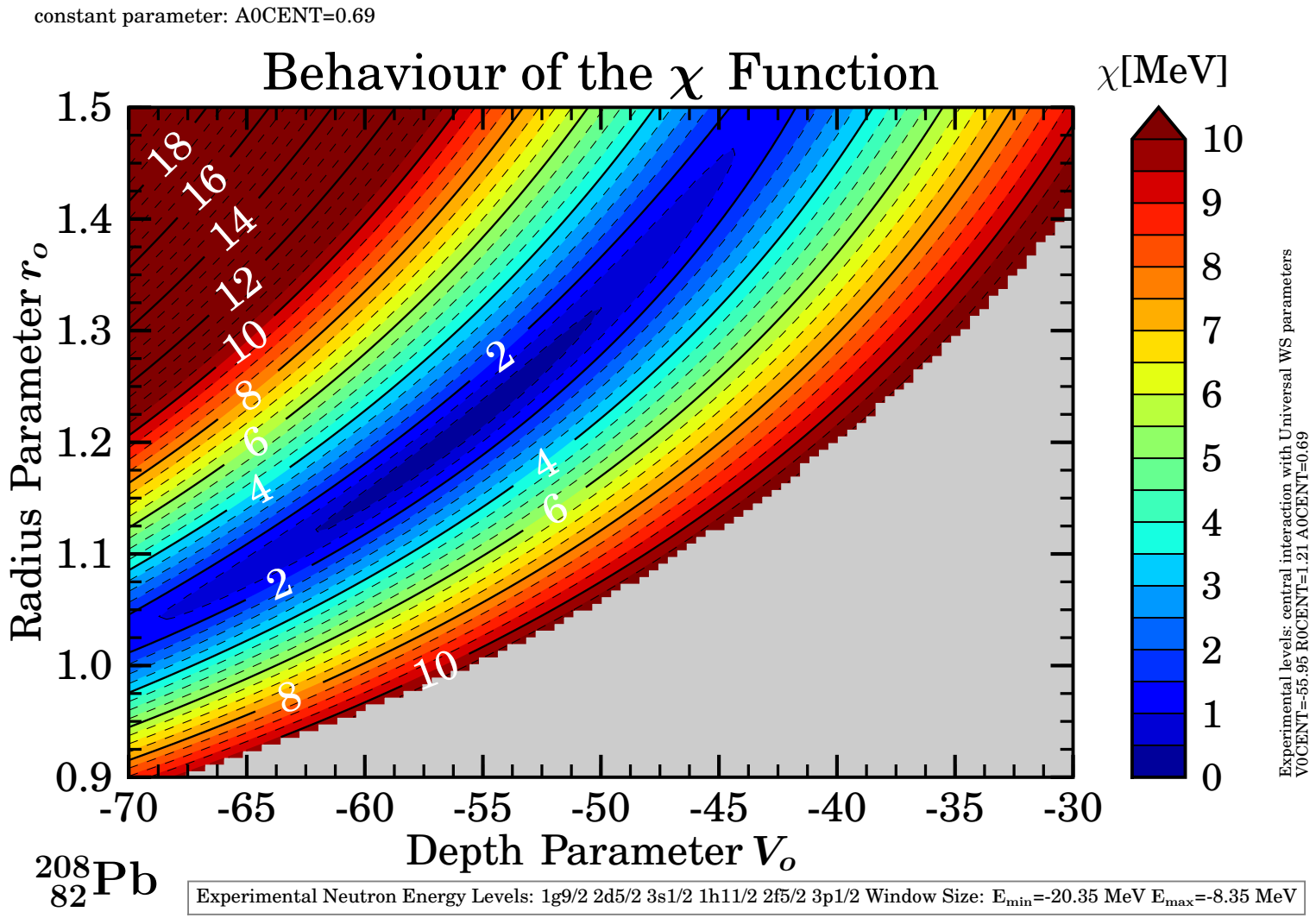
- **One can show that the parametric correlations can be detected through projecting the $\chi^2(p)$ onto a (p_j, p_k)-plane:** $\min_{i\neq j,k}\chi^2(p_1, p_2, \ldots p_m)$



- **As the approximate circular symmetry of this diagram shows, the central potential radius and central potential diffuseness are not correlated - thus no danger to the predictive power**

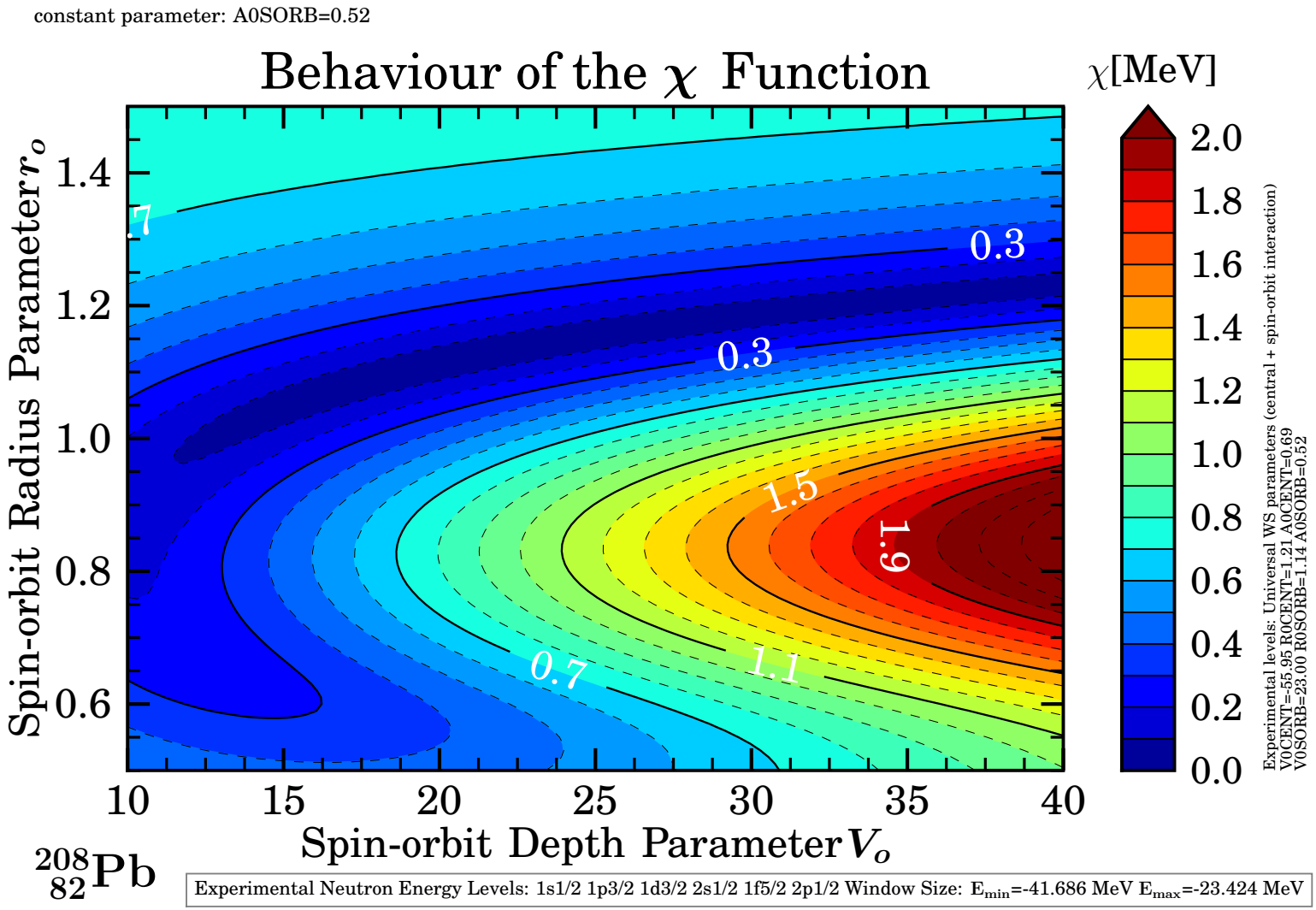
Undesired Parametric Correlations: Illustrative Examples

Begin with a Well Known: V_o vs. r_o Are Correlated



A map of χ^2 from the fit based on six levels close to the Fermi level.

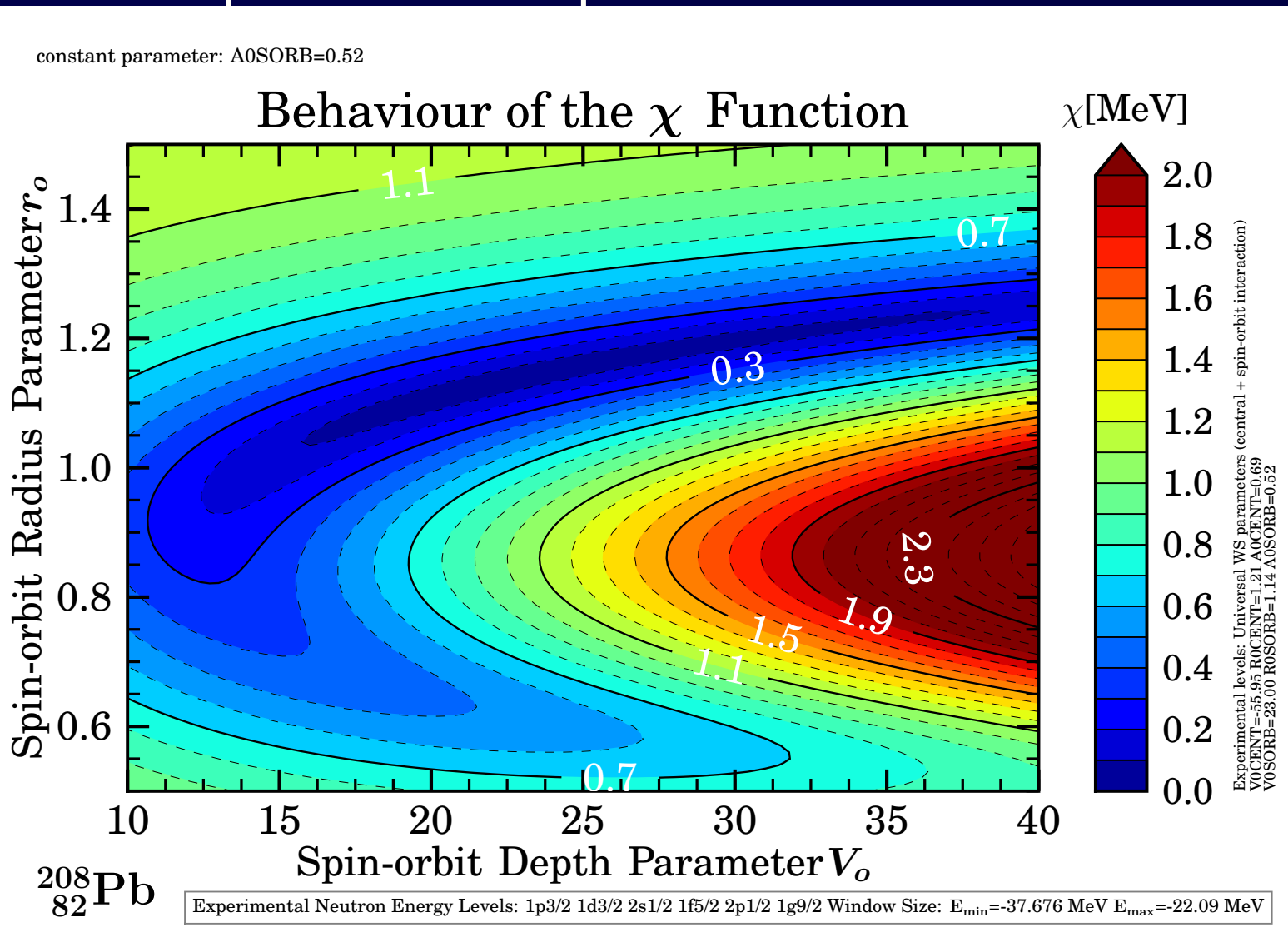
Parametric Correlations and Their Consequences



We start with six very lowest levels. Very important observation: no way to fix reliably the spin-orbit strength in the interval from 15 to 40 units.

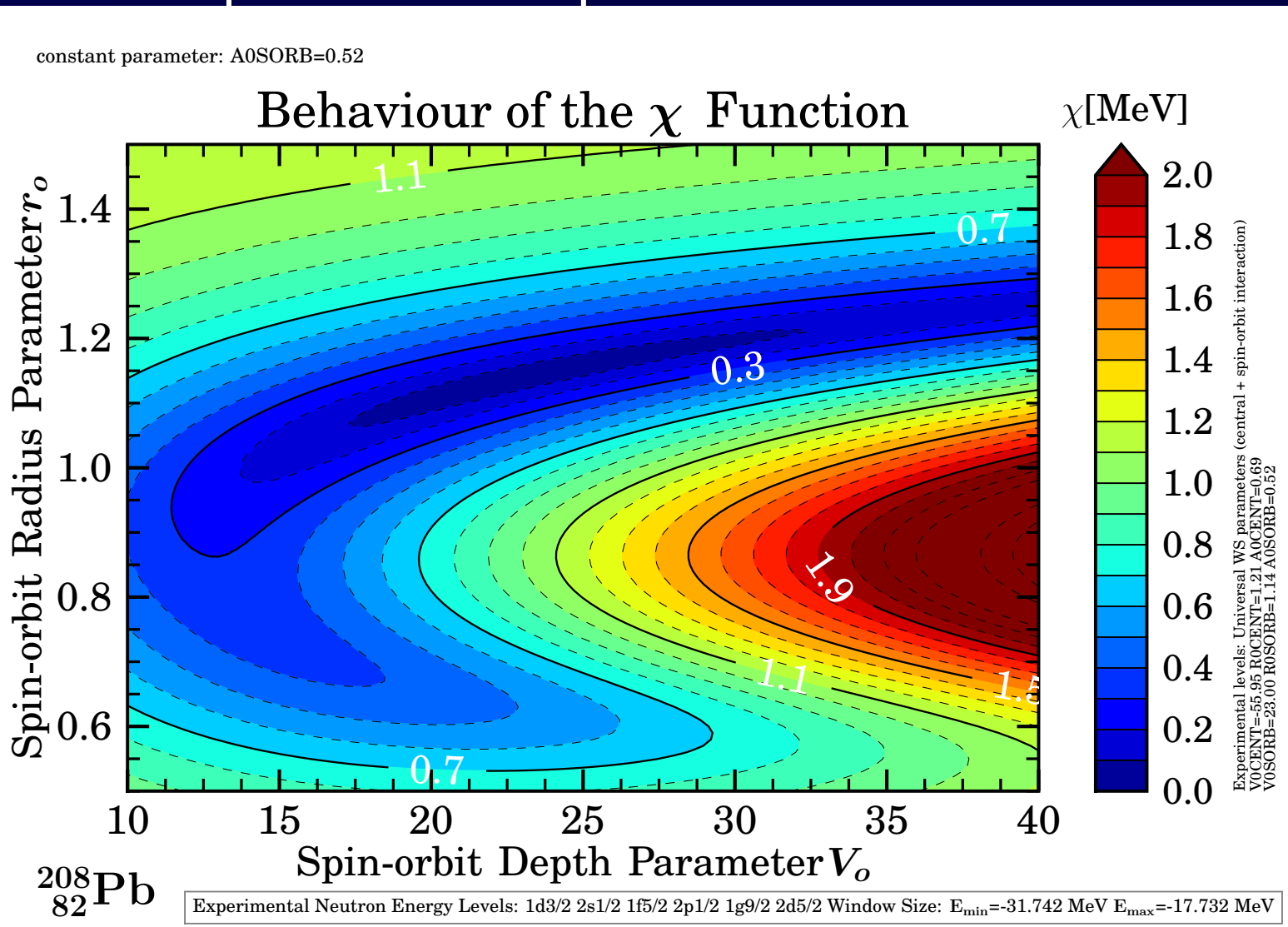
We will gradually increase the energy of the six-level window to approach the nucleon binding region and thus simulate the present-day experimental situation

Limited Experimental Input: How Little is Sufficient?



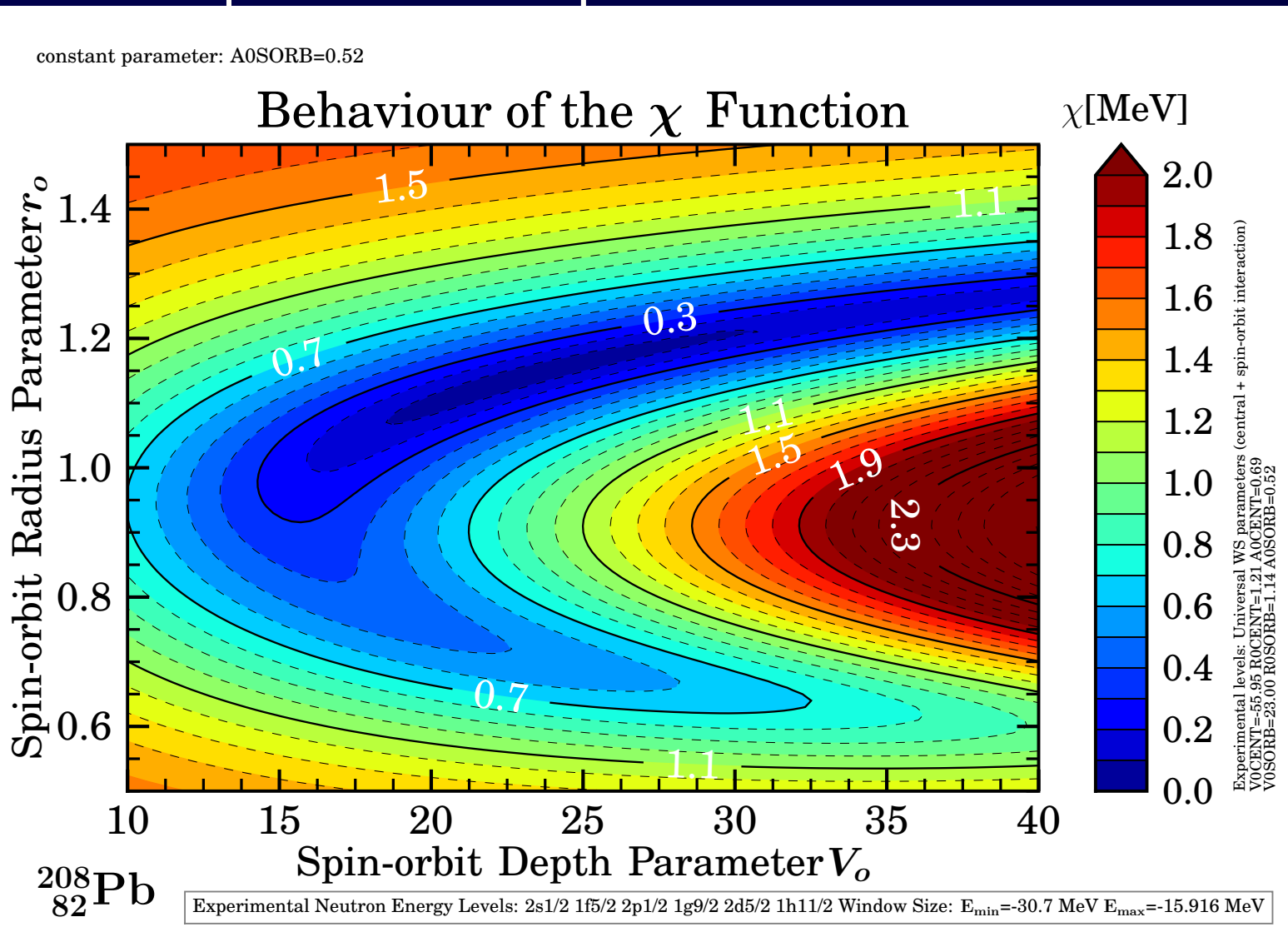
Increasing energy of six levels helps localising the spin-orbit strength slowly!

Limited Experimental Input: How Little is Sufficient?



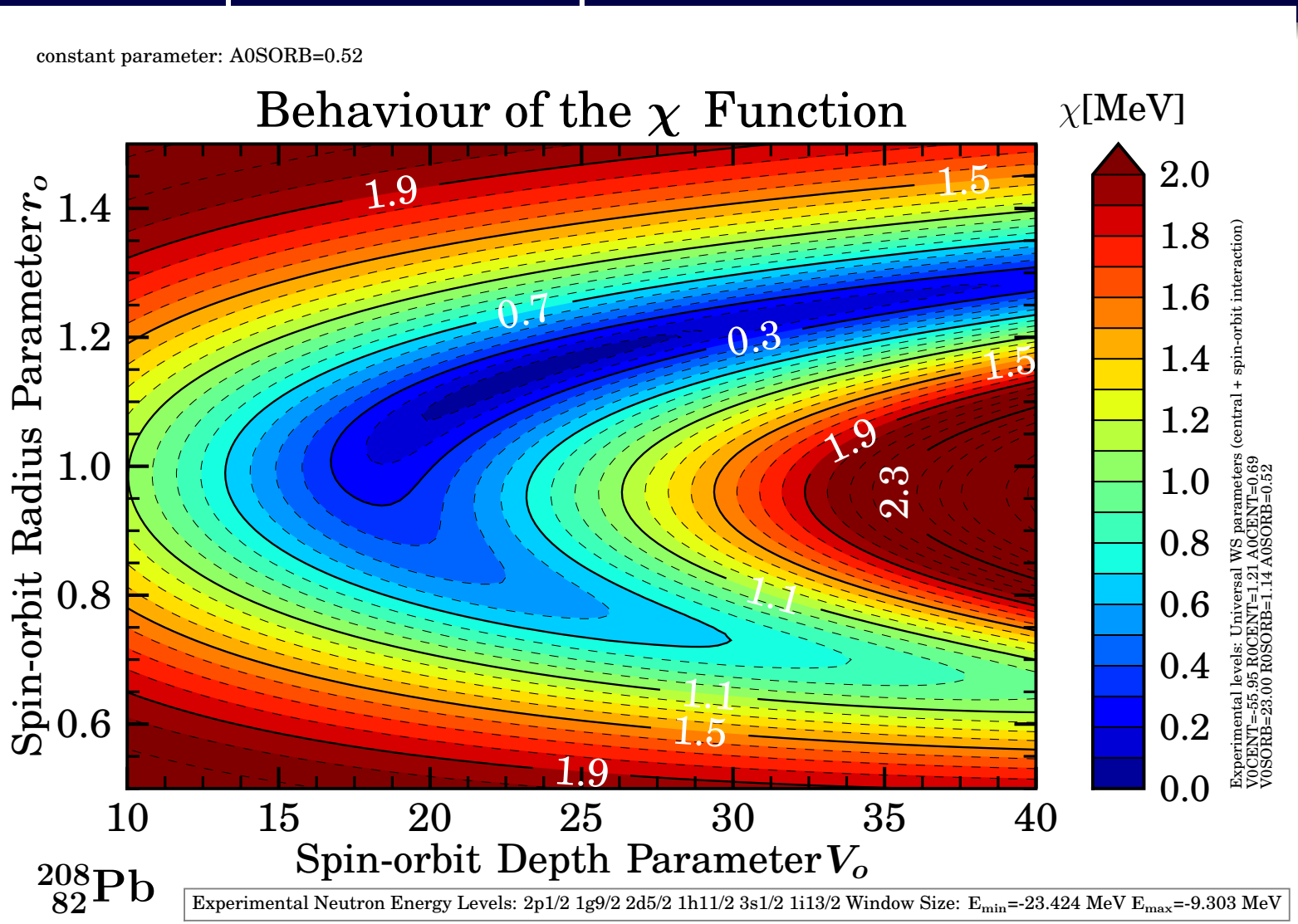
Increasing energy of six levels helps localising the spin-orbit strength slowly...

Limited Experimental Input: How Little is Sufficient?



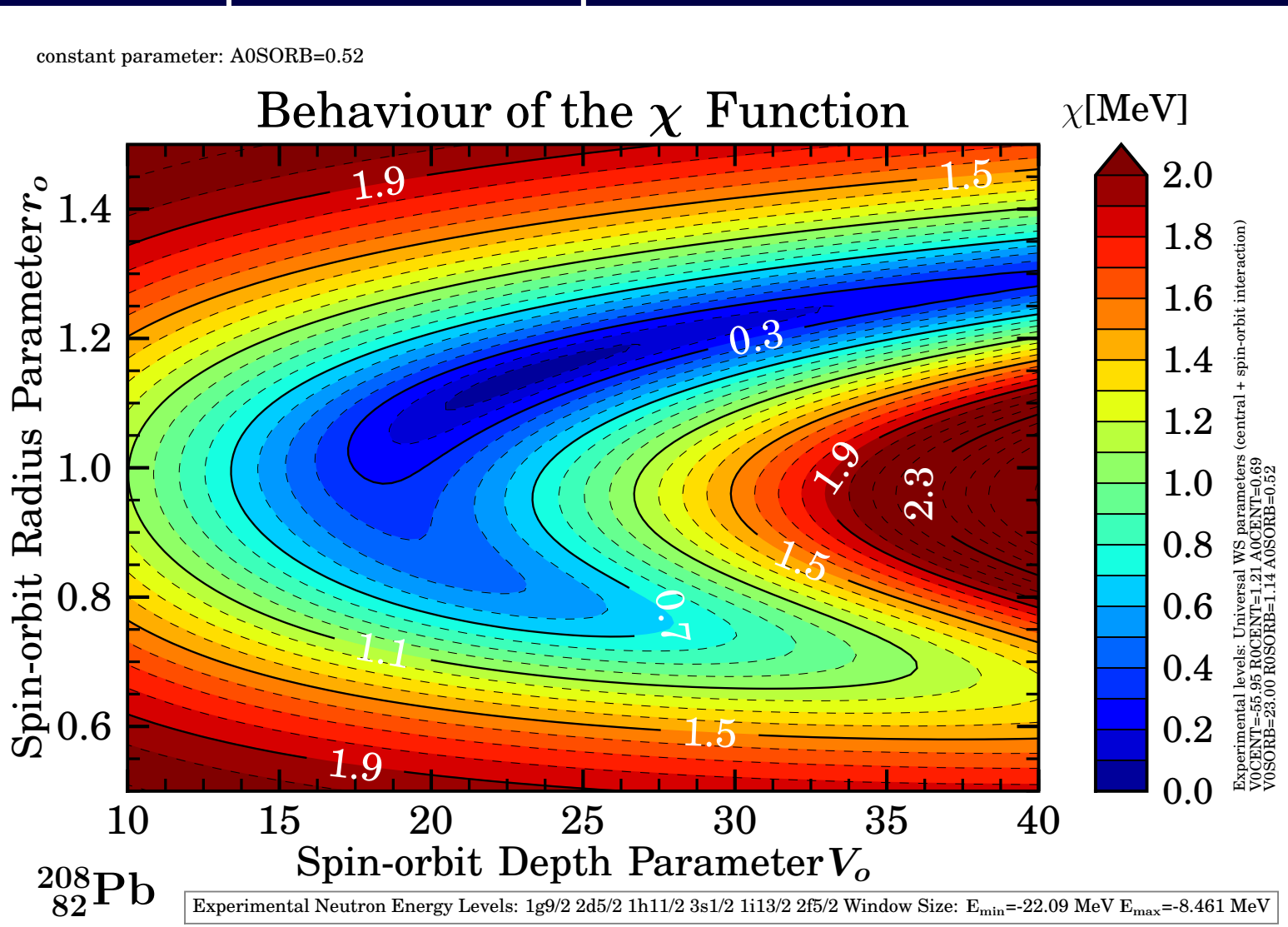
Increasing energy of six levels helps localising the spin-orbit strength slowly...

Limited Experimental Input: How Little is Sufficient?



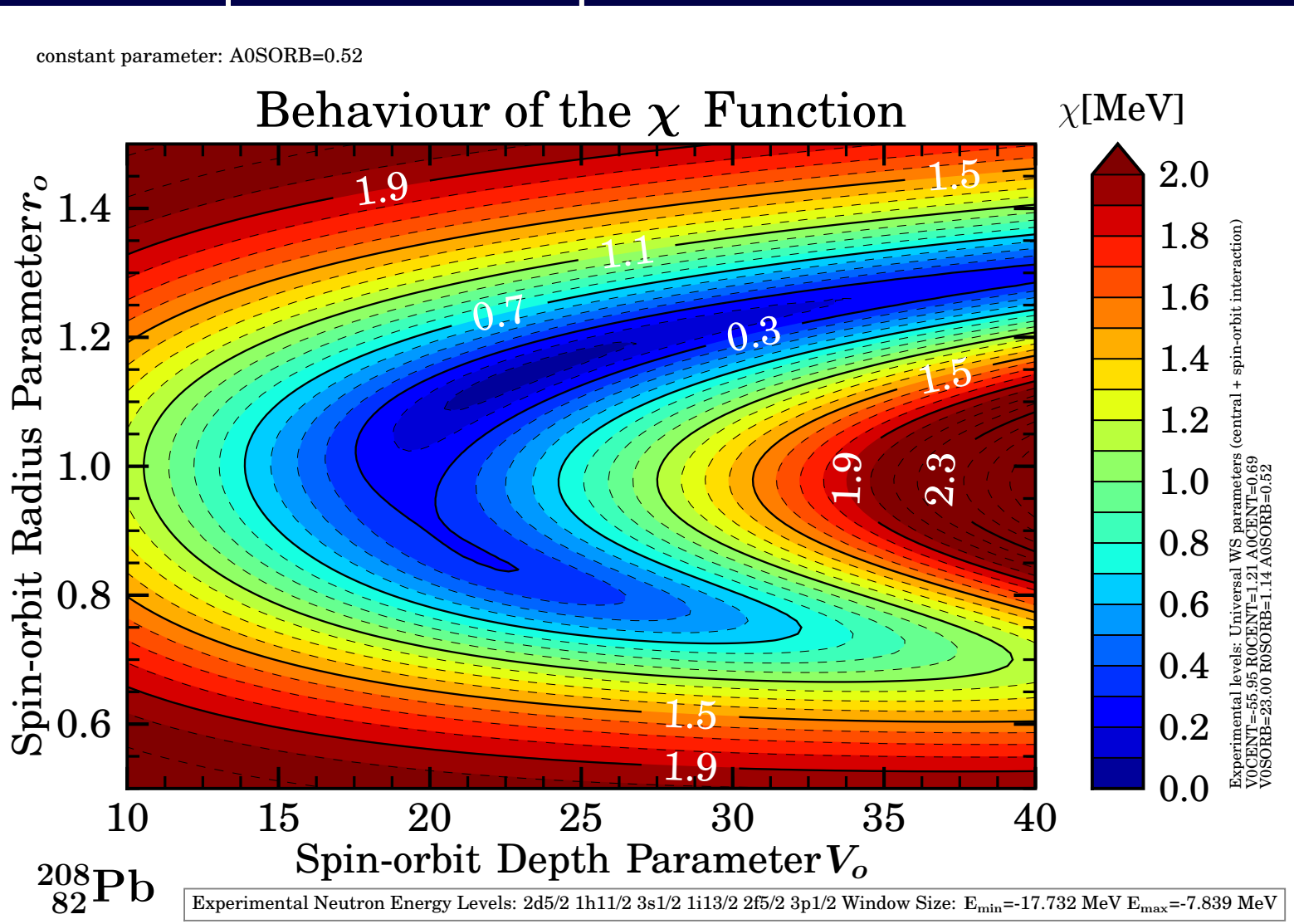
Increasing energy of six levels helps localising the spin-orbit strength slowly...

Limited Experimental Input: How Little is Sufficient?



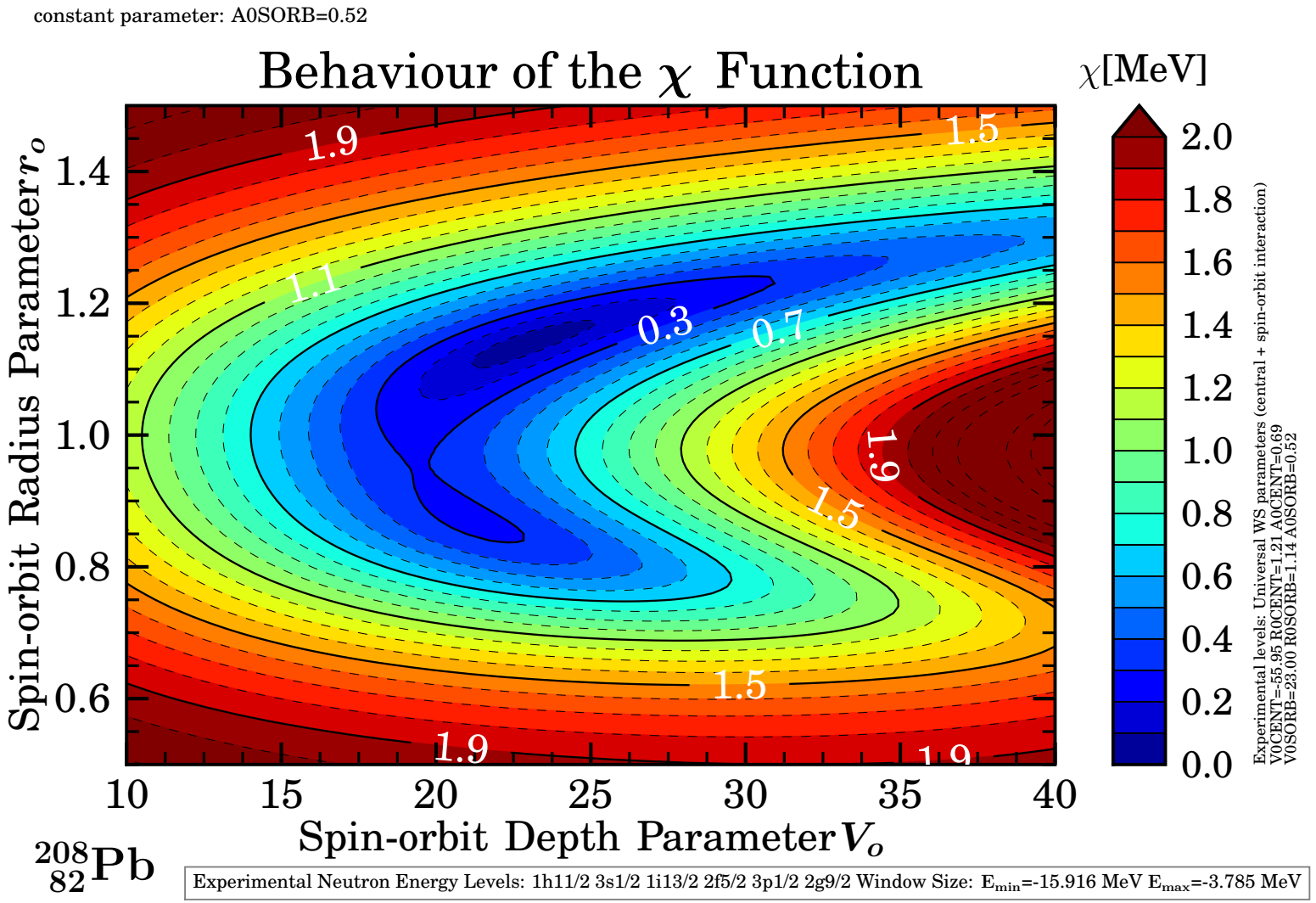
Increasing energy of six levels helps localising the spin-orbit strength slowly...

Limited Experimental Input: How Little is Sufficient?



Increasing energy of six levels helps localising the spin-orbit strength slowly...

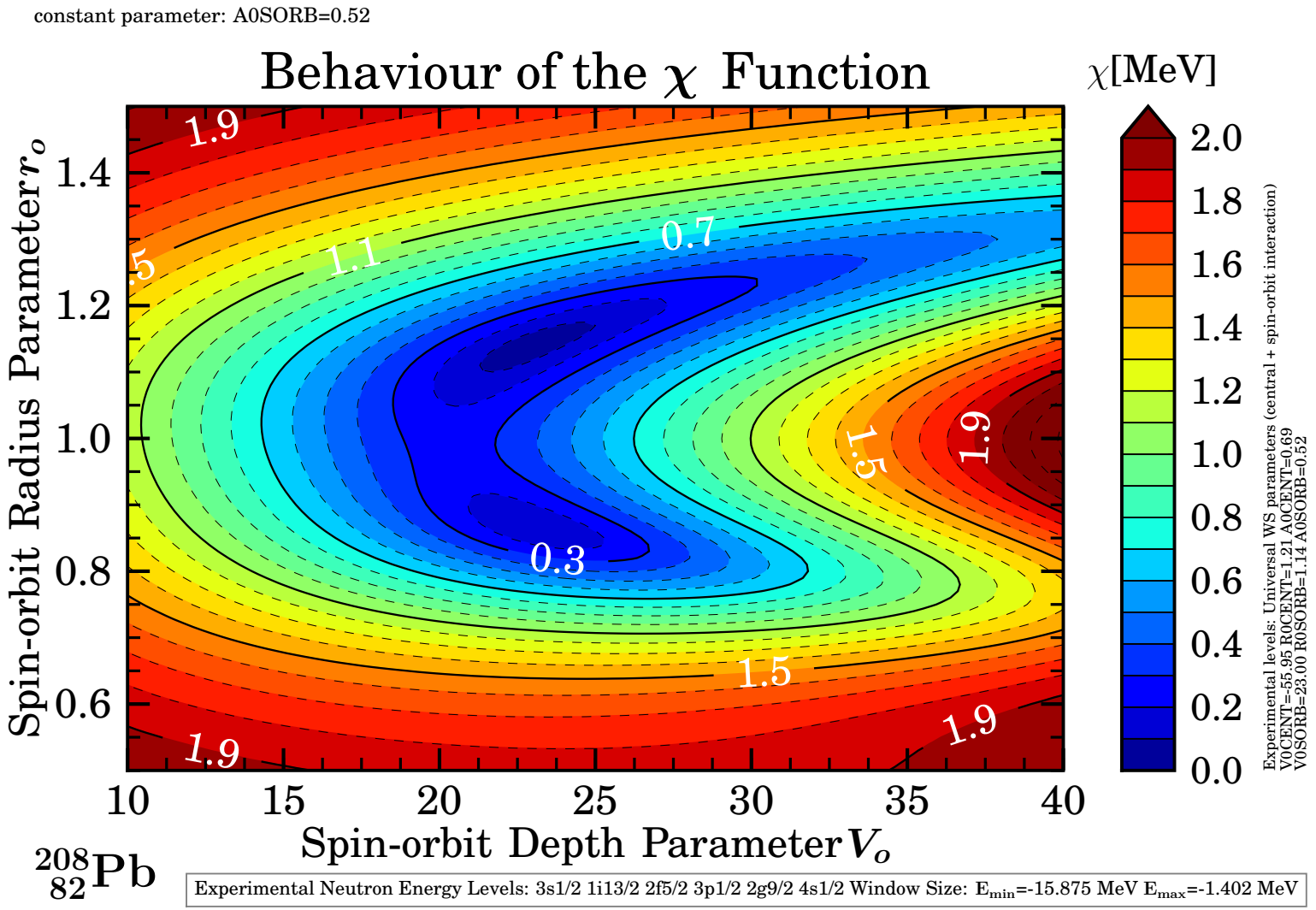
Limited Experimental Input: How Little is Sufficient?



Increasing energy of six levels helps localising the spin-orbit strength slowly...

Attention: Second solution is coming !

Limited Experimental Input: How Little is Sufficient?



ATTENTION: Here we discover the existence of two solutions with very different radii – Traditionally we call them compact and non-compact.

What Can We Conclude From This Set of Tests?

- **First of all, the fitted spin-orbit strength may vary widely from one doubly-magic nucleus to another - there exists a considerable softness in χ^2 dependence on λ_{so}**

What Can We Conclude From This Set of Tests?

- **First of all, the fitted spin-orbit strength may vary widely from one doubly-magic nucleus to another - there exists a considerable softness in χ^2 dependence on λ_{so}**

- **Secondly - there are correlations between the parameters: two relatively distant sets of parameters may be, what we call spectroscopically equivalent ('iso-spectroscopic')**

What Can We Conclude From This Set of Tests?

- **First of all, the fitted spin-orbit strength may vary widely from one doubly-magic nucleus to another - there exists a considerable softness in χ^2 dependence on λ_{so}**

- **Secondly - there are correlations between the parameters: two relatively distant sets of parameters may be, what we call spectroscopically equivalent ('iso-spectroscopic')**

- **Clearly: The 'spectroscopic predictive power' is in danger !!! In particular results depend on the sampling and thus possibly on experimentalist's choice - with all the implied subjectivity**

What Can We Conclude From This Set of Tests?

- **First of all, the fitted spin-orbit strength may vary widely from one doubly-magic nucleus to another - there exists a considerable softness in χ^2 dependence on λ_{so}**

- **Secondly - there are correlations between the parameters: two relatively distant sets of parameters may be, what we call spectroscopically equivalent ('iso-spectroscopic')**

- **Clearly: The 'spectroscopic predictive power' is in danger !!! In particular results depend on the sampling and thus possibly on experimentalist's choice - with all the implied subjectivity**

- **We discover a possibility of double-valued solutions giving rise to compact and non-compact spin-orbit parametrisation**

What Can We Conclude From This Set of Tests?

- **First of all, the fitted spin-orbit strength may vary widely from one doubly-magic nucleus to another - there exists a considerable softness in χ^2 dependence on λ_{so}**

- **Secondly - there are correlations between the parameters: two relatively distant sets of parameters may be, what we call spectroscopically equivalent ('iso-spectroscopic')**

- **Clearly: The 'spectroscopic predictive power' is in danger !!! In particular results depend on the sampling and thus possibly on experimentalist's choice - with all the implied subjectivity**

- **We discover a possibility of double-valued solutions giving rise to compact and non-compact spin-orbit parametrisation**

- **We confirm the presence of the mechanism of iso-spectral lines - also in the space of the spin-orbit potential parameters**

Elementary Conclusions about Correlation Removal:

Elementary Conclusions about Correlation Removal:

- Suppose that Monte Carlo simulation provides a χ^2-valley on r_0-vs.-V_0 plane.

- It will be sufficient to parametrise it by defining function f in the relation $r_0 = f(V_0)$

Elementary Conclusions about Correlation Removal:

- Suppose that Monte Carlo simulation provides a χ^2-valley on r_0-vs.-V_0 plane.
- It will be sufficient to parametrise it by defining function f in the relation $r_0 = f(V_0)$
- A possible alternative: Using regularisation methods for instance: Truncated Singular Value Decomposition Theorem

Elementary Conclusions about Correlation Removal:

- Suppose that Monte Carlo simulation provides a χ^2-valley on r_0-vs.-V_0 plane.
- It will be sufficient to parametrise it by defining function f in the relation $r_0 = f(V_0)$
- A possible alternative: Using regularisation methods for instance: Truncated Singular Value Decomposition Theorem
- However, here we will explore yet another, physics approach

Section 6

Density-Dependent spin-orbit interaction potential

Physics-Guided Improvements of WS Universal

- It is well known that the microscopic structure of the mean field, $\hat{V}_{\rm mf}$, is based on the 2-body interactions, $\hat{v}_2$:

$$\hat{v}_2 \leftrightarrow \hat{v}_{\rm two-body}(\vec{r}_i - \vec{r}_j) \rightarrow V_{\rm mean-field}(\vec{r}_i) \leftrightarrow \hat{V}_{\rm mf}(\vec{r}_i)$$

$$\hat{V}_{\rm mf}(\vec{r}_i) \propto \sum_{j \neq i} \int \psi_j^*(\vec{r}_j)\, \hat{v}_2(\vec{r}_i - \vec{r}_j)\, \psi_j(\vec{r}_j)\, d^3\vec{r}_j, \qquad \sum_j \psi_j^*(\vec{r}_j)\, \psi_j(\vec{r}_j) \equiv \rho(\vec{r})$$

- Here we follow the 'microscopic generalisation of the W-S-universal' in:

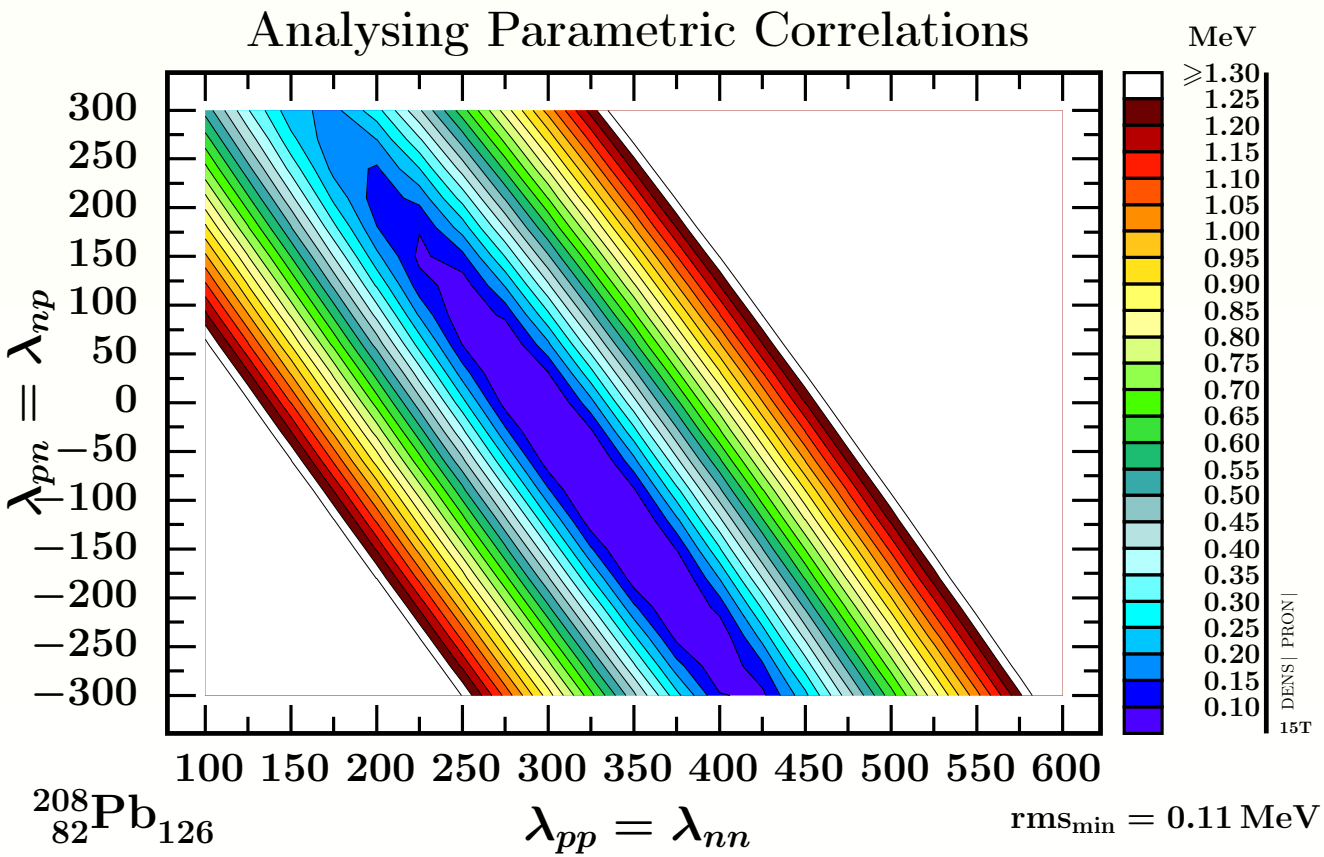
Realistic Nuclear Mean Field Approach with the Density-Dependent Spin-Orbit Term;
B. Belgoumène, J. Dudek and T. Werner, *Phys. Lett.* **B267 (4)** *(1991) 431-437* $\Rightarrow$

$$\hat{V}_{so}^{\pi} \leftrightarrow \lambda_{\pi\pi} \frac{1}{r} \frac{d\rho_\pi}{dr} + \lambda_{\pi\nu} \frac{1}{r} \frac{d\rho_\nu}{dr} \qquad \textbf{Eq.(A)}$$

$$\hat{V}_{so}^{\nu} \leftrightarrow \lambda_{\nu\pi} \frac{1}{r} \frac{d\rho_\pi}{dr} + \lambda_{\nu\nu} \frac{1}{r} \frac{d\rho_\nu}{dr} \qquad \textbf{Eq.(B)}$$

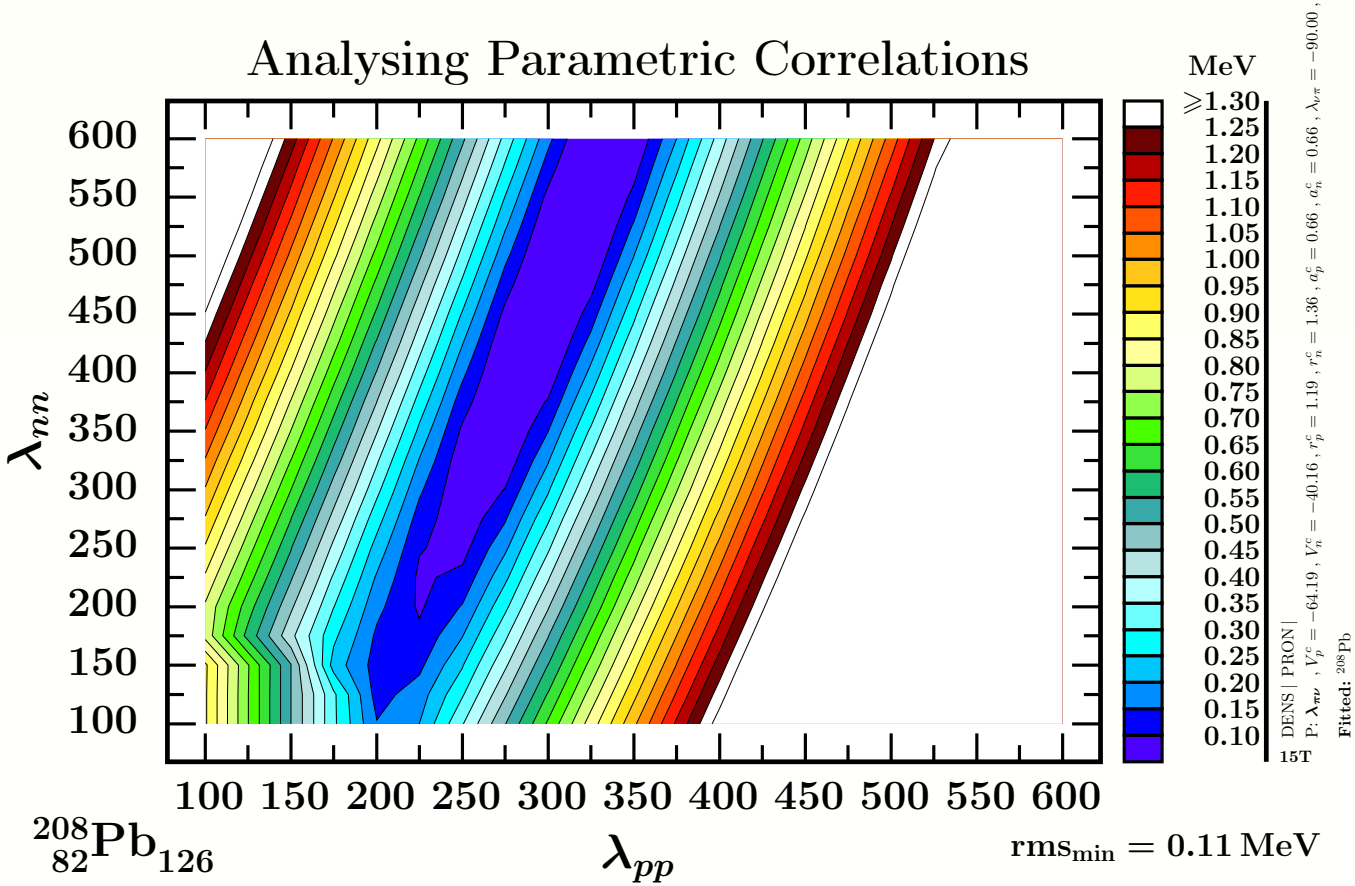
Advantages: The new expression includes the microscopic HF approach rather than pure phenomenology and contains 4 parameters rather than 6. What are their correlations?

- **The pilot-project tests show that $\lambda_{\pi\nu} \approx \lambda_{\nu\pi}$ and $\lambda_{\pi\pi} \approx \lambda_{\nu\nu}$ - then:**



- **Realistic calculations indicate that the density-dependent spin-orbit potential parameters are correlated – but the correlations are perfectly linear**

- **Another variant: Correlations λ_{pp} *vs.* $\lambda_{\nu\nu}$ at fixed, optimal $\lambda_{pn} = \lambda_{np}$**



- **Again: Calculations show that the density-dependent spin-orbit potential parameters are correlated – but the correlations are perfectly linear**

Conclusion:

We may significantly decrease the number of spin-orbit potential parameters

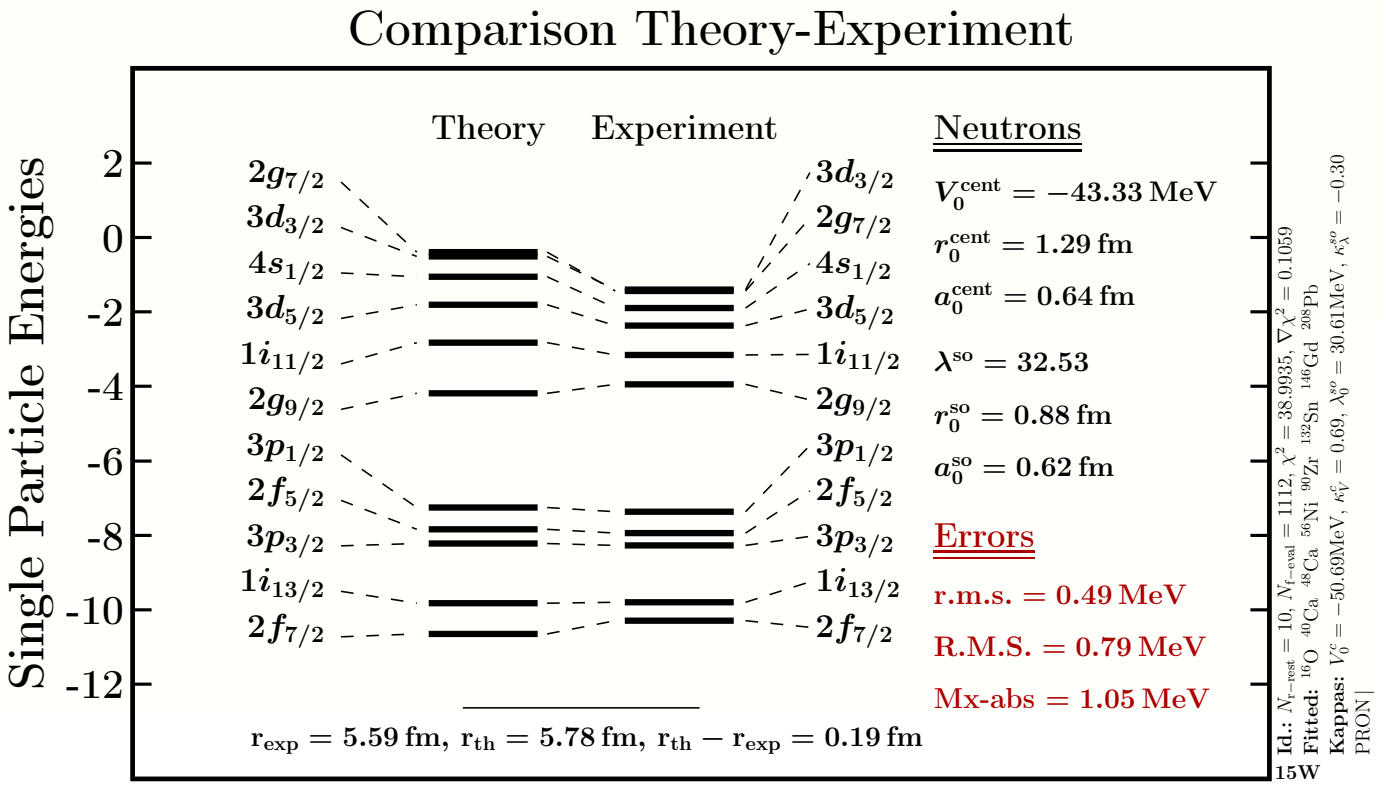
Conclusion:

We may significantly decrease the number of spin-orbit potential parameters

But: Do we loose something? At which aspect? What?

How Many Degrees of Freedom the V_{so} Has?

- **We fit all the traditional WS potential parameters to several nuclei**

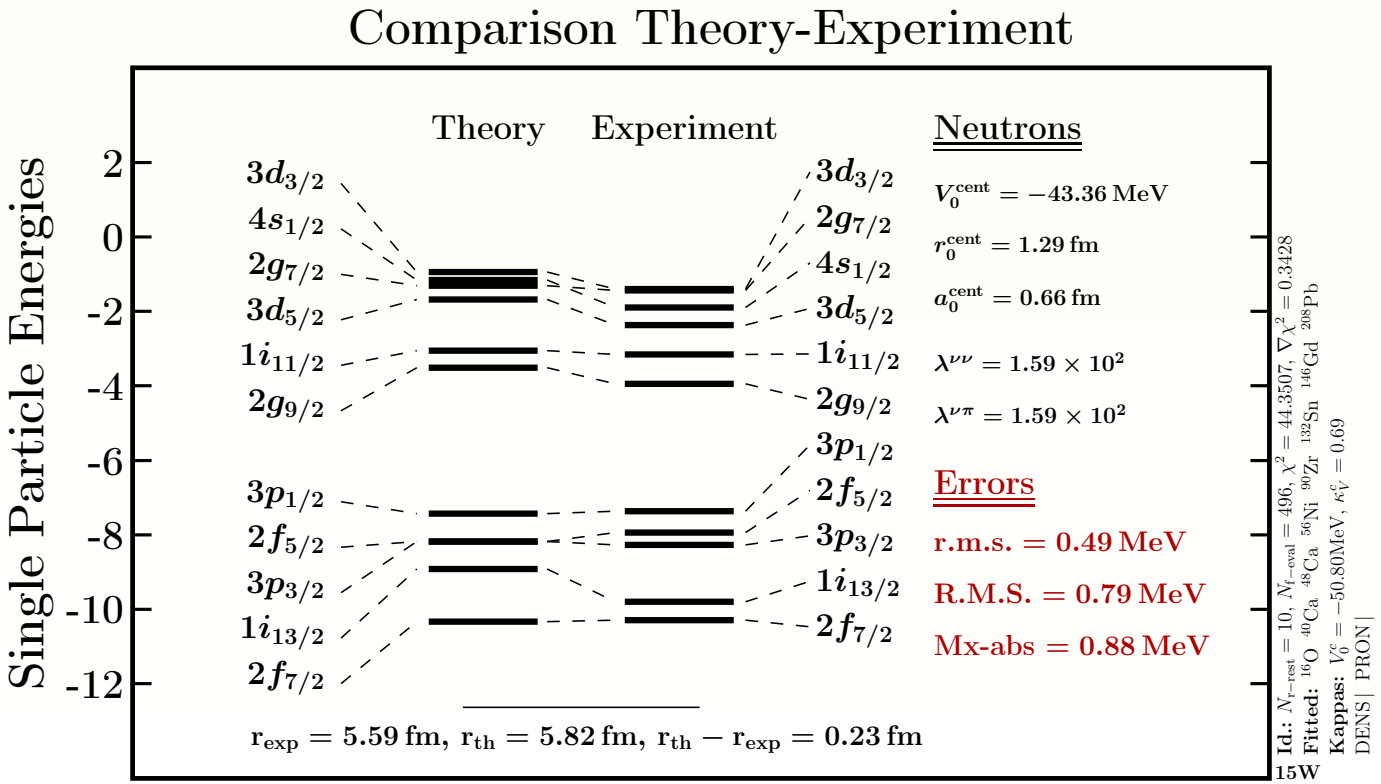


$^{208}_{82}\mathrm{Pb}_{126}$ Spherical Woods-Saxon Hamiltonian

- **We illustrate the results for ^{208}Pb-neutrons – Solution r.m.s.=0.49 MeV**
- **The answer: 6 - $\{\lambda^{so}, r_0^{so}, a_0^{so}\}$ for protons and $\{\lambda^{so}, r_0^{so}, a_0^{so}\}$ for neutrons**

How Many Degrees of Freedom the V_{so} Has?

- **We fit the density-dependent spin-orbit: $\lambda_{nn} = \lambda_{np} = \lambda_{pn} = \lambda_{pp} \equiv \lambda$**



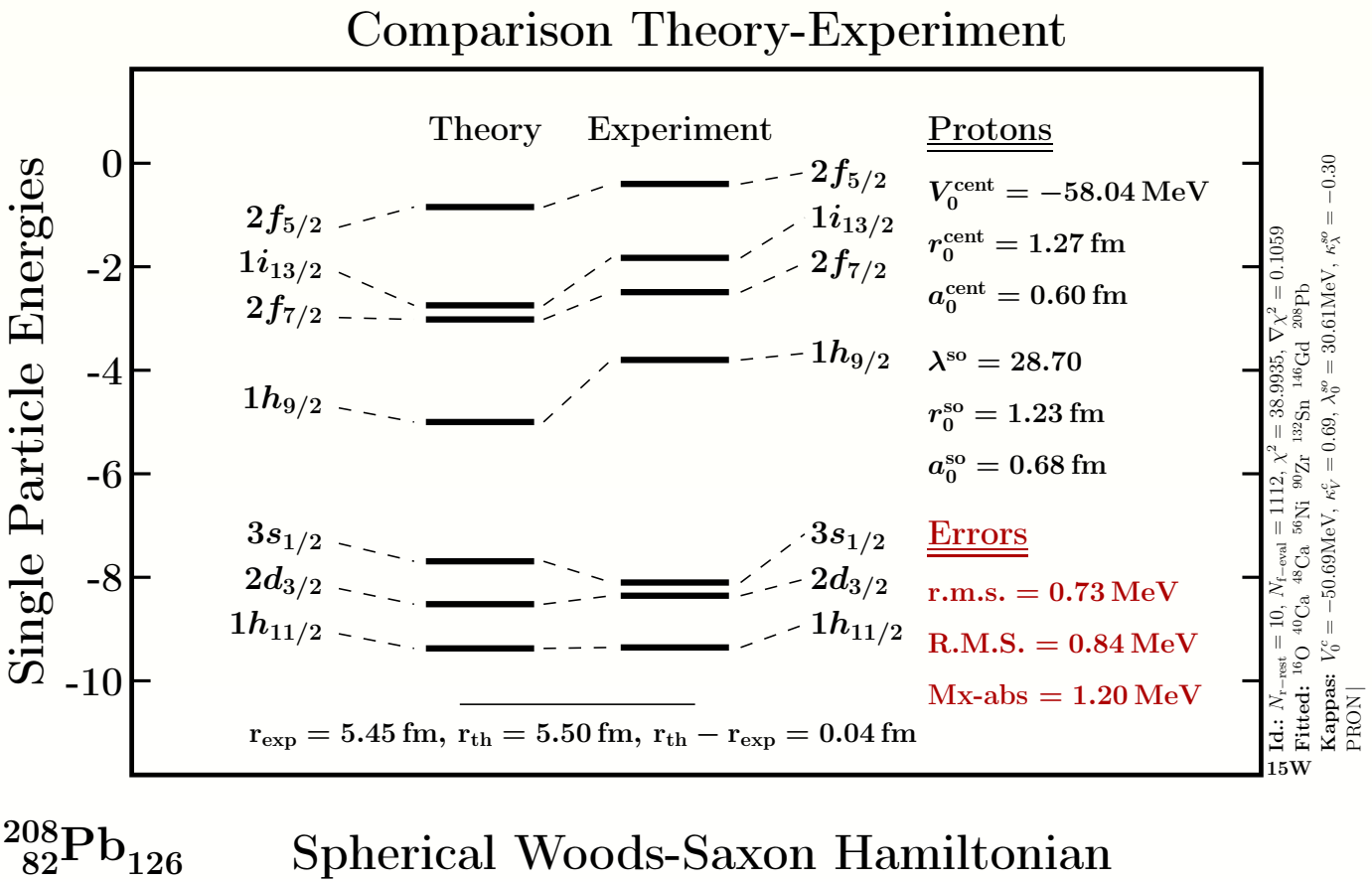
$^{208}_{82}\mathrm{Pb}_{126}$ Spherical Woods-Saxon Hamiltonian

- **The results for ^{208}Pb-neutrons – Solution r.m.s.=0.49 MeV is unchanged**
- **The answer: 1 parameter - common for the protons and for the neutrons**

We repeat the test for the protons

How Many Degrees of Freedom the V_{so} Has?

- **We fit all the traditional WS potential parameters to several nuclei**

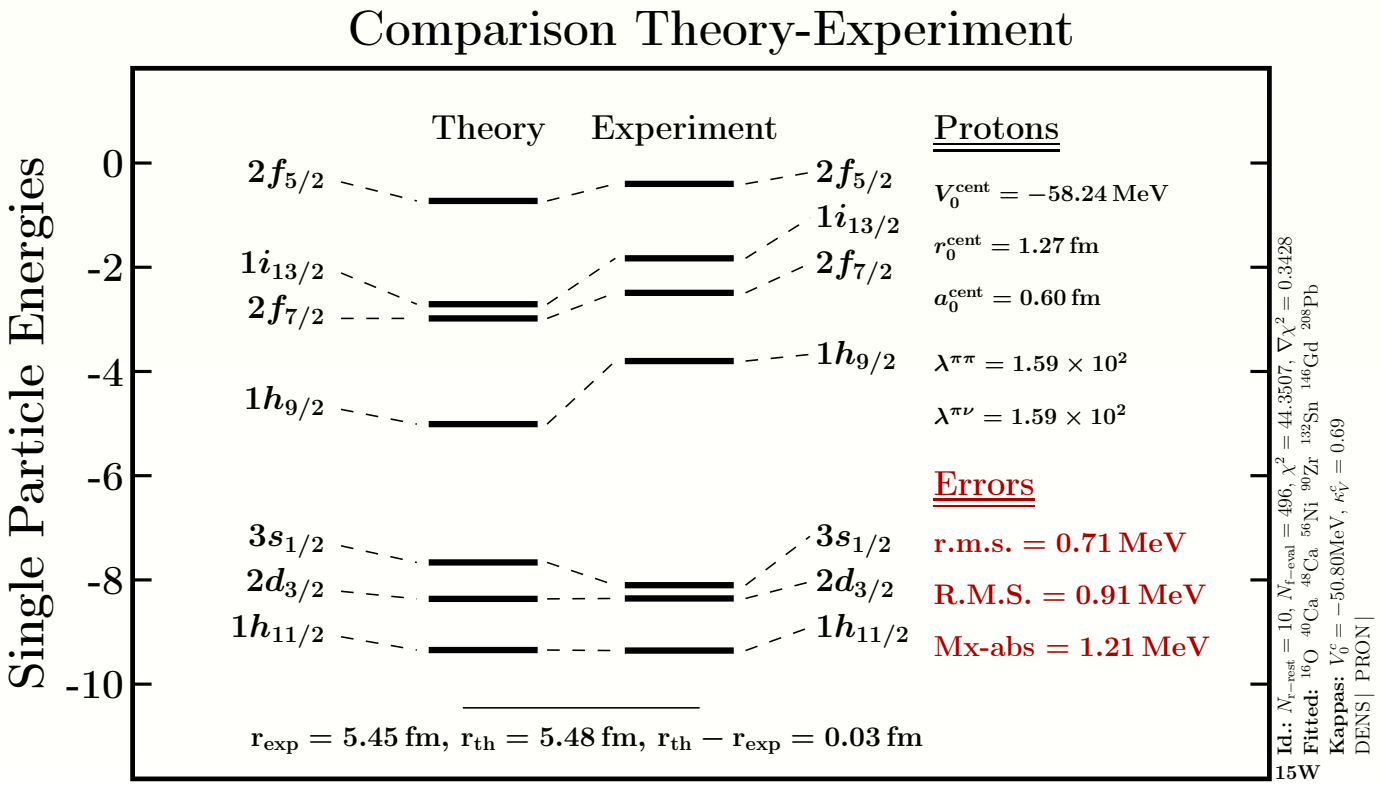


$^{208}_{82}\mathrm{Pb}_{126}$ Spherical Woods-Saxon Hamiltonian

- **We illustrate the results for ^{208}Pb-protons – Solution r.m.s.=0.73 MeV**

How Many Degrees of Freedom the V_{so} Has?

- **We repeat the test under the constraint: $\lambda_{nn} = \lambda_{np} = \lambda_{pn} = \lambda_{pp} \equiv \lambda$**



$^{208}_{82}\mathrm{Pb}_{126}$ Spherical Woods-Saxon Hamiltonian

- **^{208}Pb-protons – The r.m.s. decreased from r.m.s.=0.73 MeV to 0.71 MeV**
- **We decreased the number of spin-orbit potential parameters – and this from 6 to 1 and the r.m.s. slightly improved. Conclusions for the project?**

$\Rightarrow$

How Many Degrees of Freedom the V_{so} Has?

Conclusions:

The density-dependent, thus more microscopic spin-orbit potential, depends effectively on one parameter rather than six

- **We obtain better or equal quality of comparison with experiment**
- **We arrive at the eliminating of all parametric correlation problems**

The Notion of Over-Parameterised Hamiltonians

Basic conclusion for this domain of research

The Notion of Over-Parameterised Hamiltonians

Basic conclusion for this domain of research

We may use the physicist's intuition to invent more and more complex interactions containing more and more parameters
[e.g. 2632 parameters, see above]

The Notion of Over-Parameterised Hamiltonians

Basic conclusion for this domain of research

We may use the physicist's intuition to invent more and more complex interactions containing more and more parameters
[e.g. 2632 parameters, see above]

but if the number of effective degrees of freedom is close to 1 – no wonder that the parametric correlations will be of the type "everyone-with-everyone"

The Notion of Over-Parameterised Hamiltonians

Basic conclusion for this domain of research

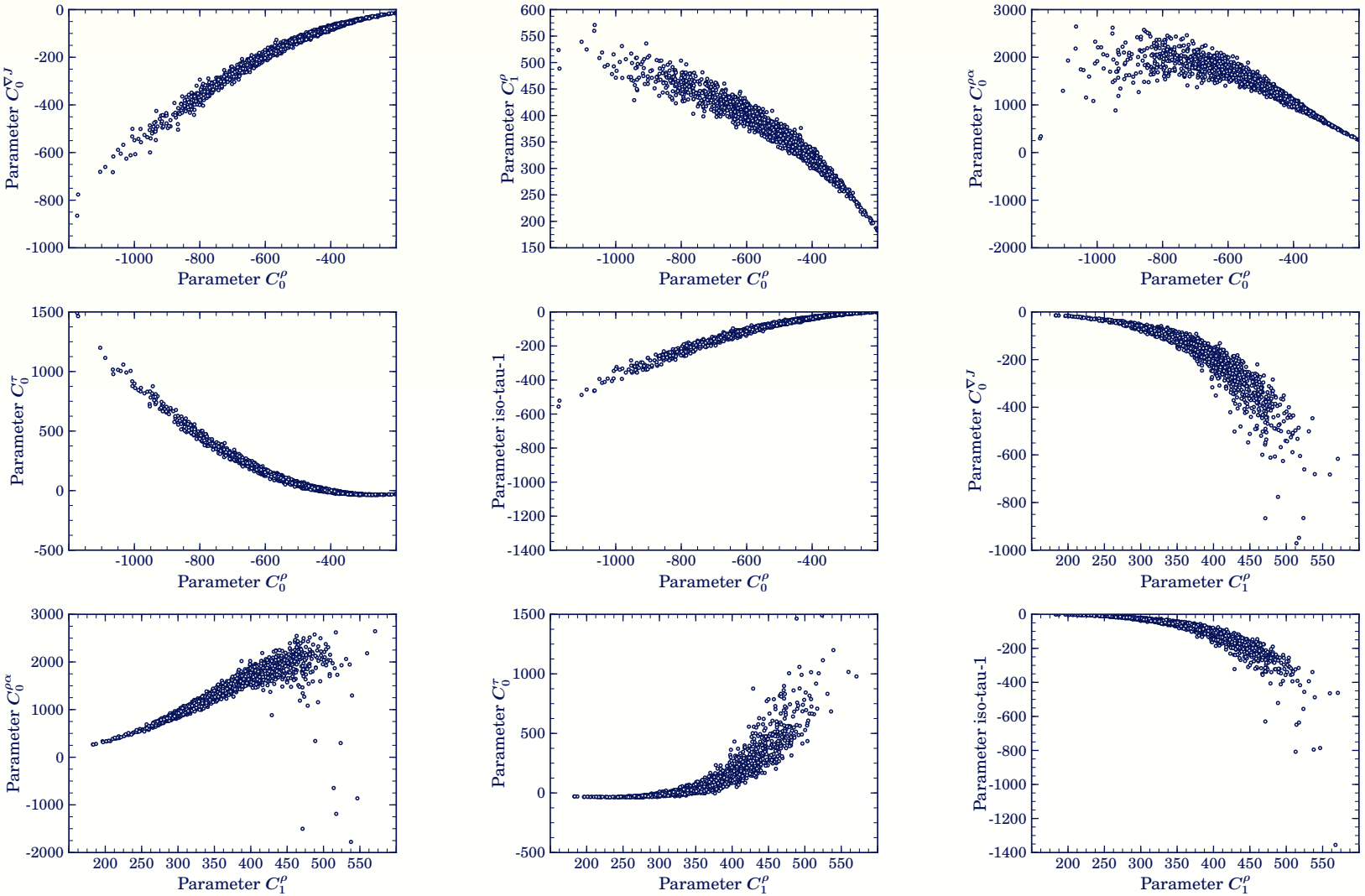
We may use the physicist's intuition to invent more and more complex interactions containing more and more parameters [e.g. 2632 parameters, see above]

but if the number of effective degrees of freedom is close to 1 – no wonder that the parametric correlations will be of the type "everyone-with-everyone"

We arrive in this way at the notion of "Over-Parameterised Hamiltonians"

In such cases the very definition of the Hamiltonian currently excludes applications to the modelling with prediction capacities

We Can Interpret this Diagram from a New Perspective



Majority of these parameters are strongly correlated because the model is over-parameterised thus excluding the prediction capacities

[B. Szpak, PhD thesis]

Strategy and Strategical Goals

With this strategy in mind:

What are the actualised research directions for the project?

Strategy and Strategical Goals

With this strategy in mind:

What are the actualised research directions for the project?

Recall. We have two strategical goals:

• Eliminate parametric correlations and model over-parametrisation in order not to "kill" the predictive power at the start [as presented]

Strategy and Strategical Goals

With this strategy in mind:

What are the actualised research directions for the project?

Recall. We have two strategical goals:

- Eliminate parametric correlations and model over-parametrisation in order not to "kill" the predictive power at the start [as presented]
- Determine quantitative limitations from the today's constraints such as experimental and theory errors which we cannot bypass today

Strategy and Strategical Goals

In other words:

Strategy and Strategical Goals

In other words:

We can neither increase the number of data points (volume of sampling) nor the quality of the sampling.

Strategy and Strategical Goals

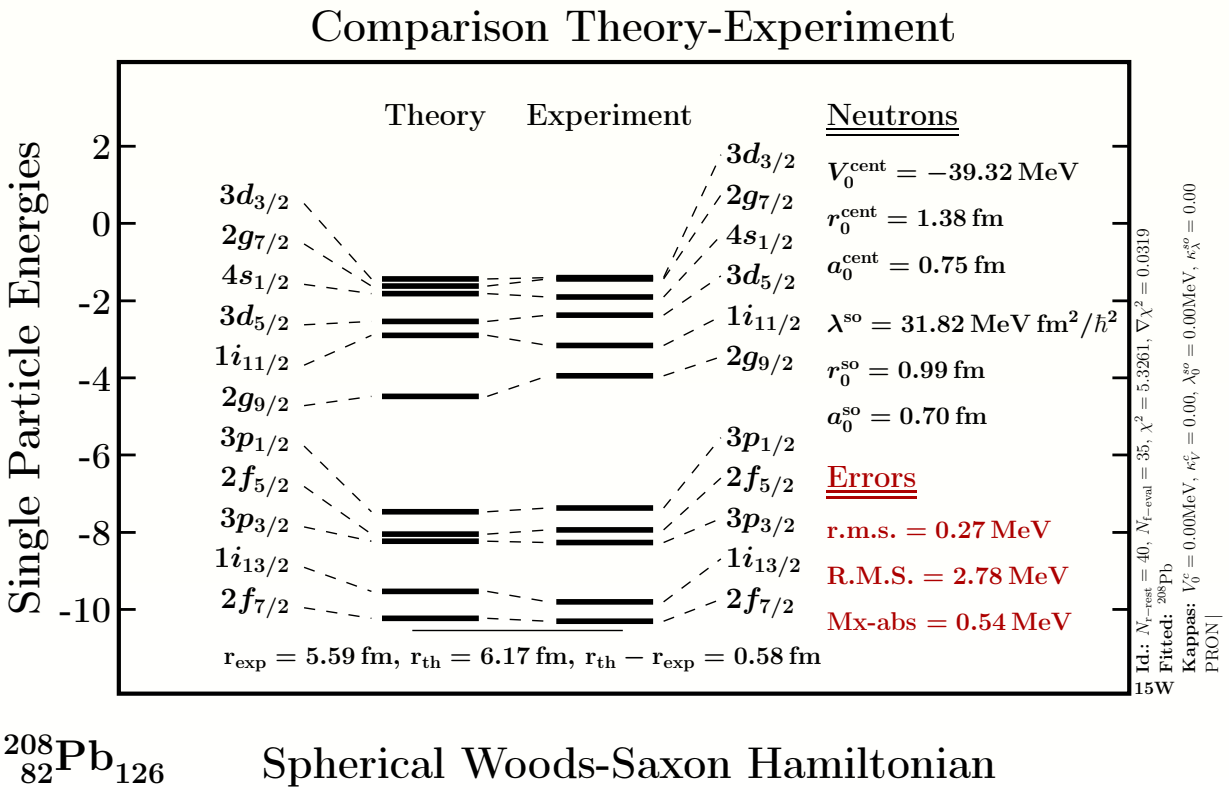
In other words:

We can neither increase the number of data points (volume of sampling) nor the quality of the sampling.

Under these objective constraints we wish to know how (un)certain is what we calculate with our very complex/advanced computer programs?

Uncertainties of Calculated Nucleon Energies

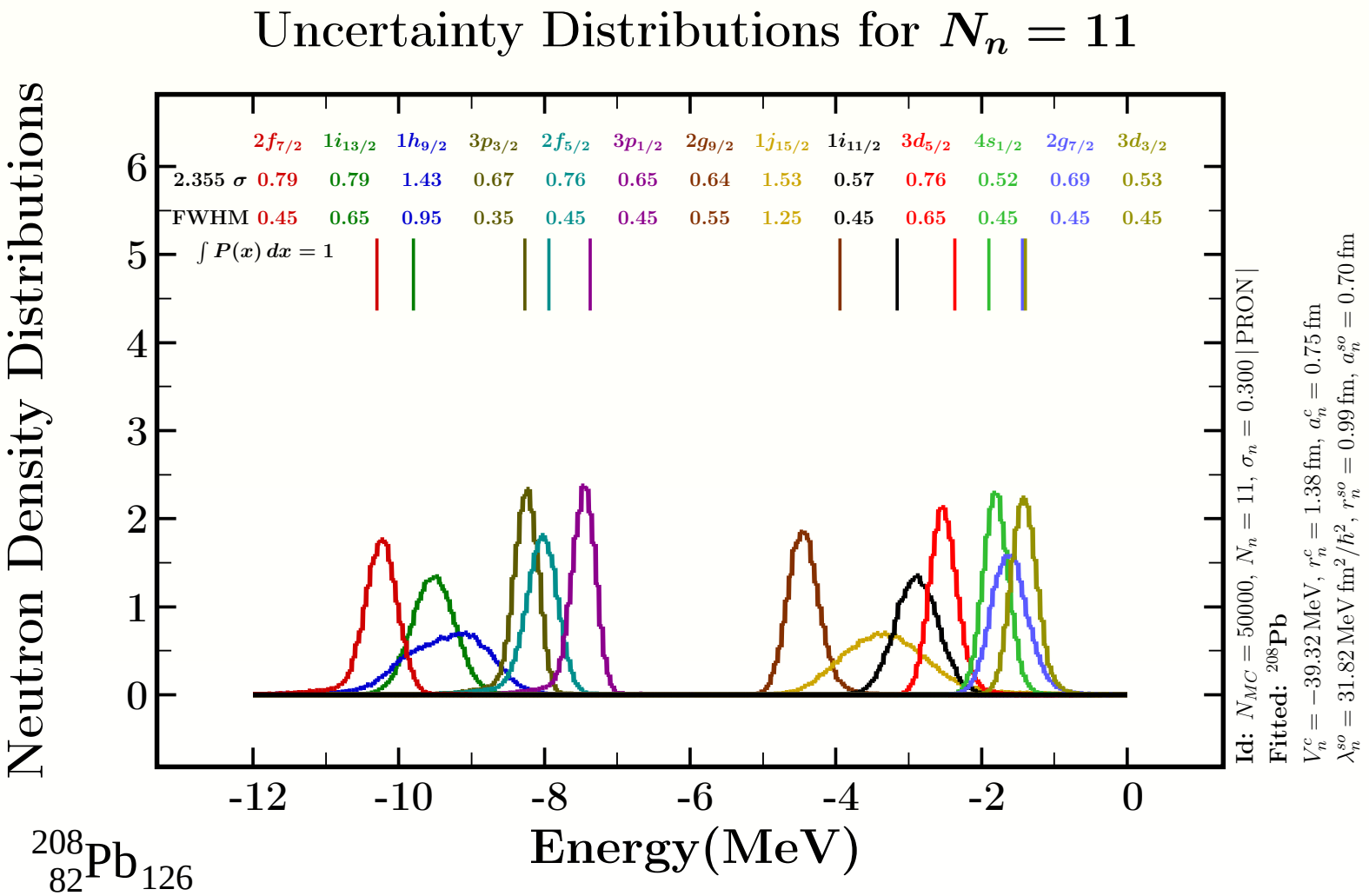
- The concept of pseudo-experimental levels: Optimise Hamiltonian under some plausible conditions $\longrightarrow$ Replace experimental levels by the model energies $\longrightarrow$ Construct in this way an exact model $\longrightarrow$ Now we can modify the 'sampling'



- LEFT: ^{208}Pb levels after a fit which will be treated as pseudo-experimental

Uncertainties of Calculated Nucleon Energies

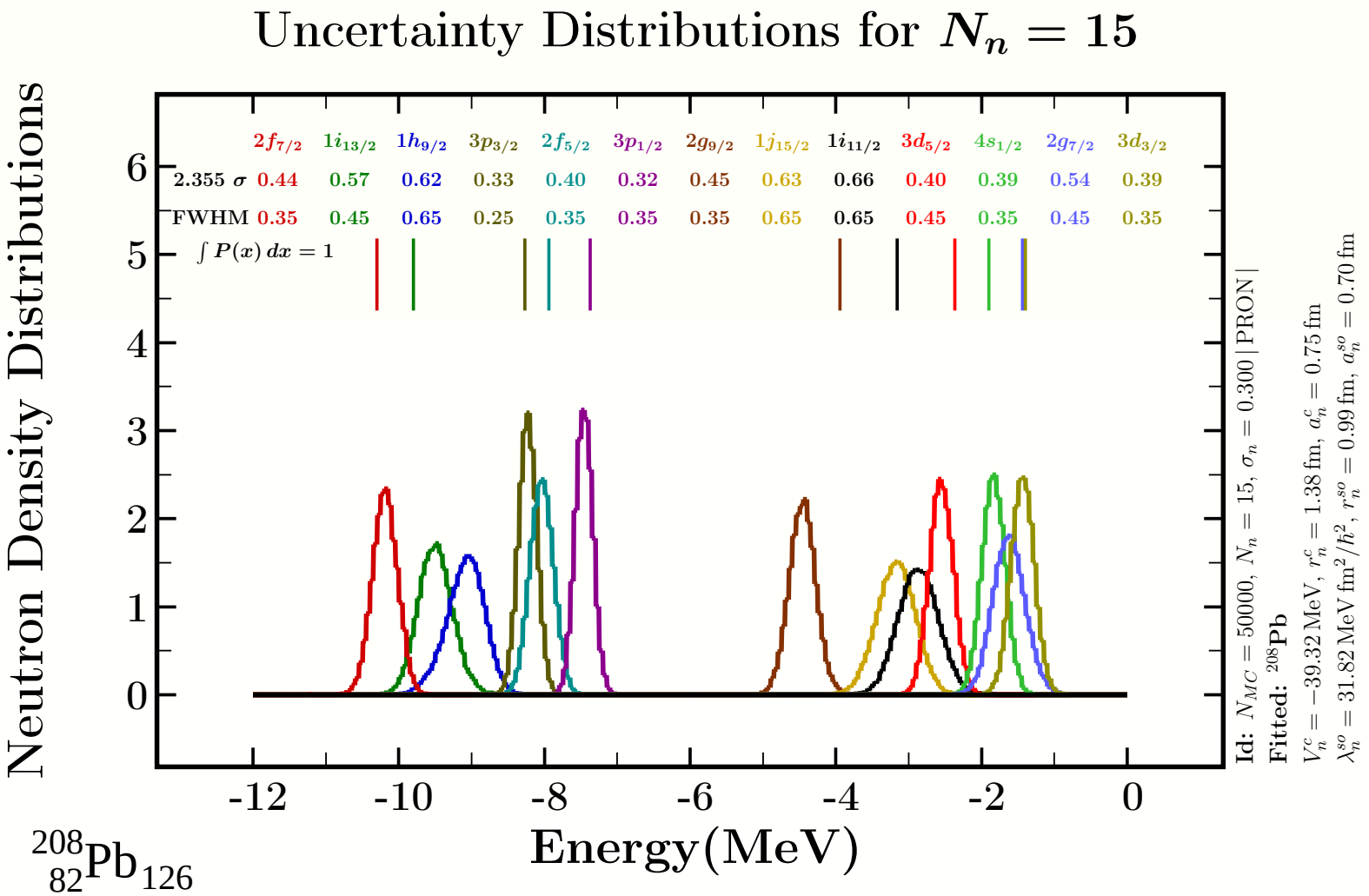
- The pseudo-experimental levels: Now we can modify/increase the 'sampling'



- Definitions: $\sigma = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(e_i - \bar{e})^2}$ $\qquad \bar{e} = \frac{1}{n}\sum_{i=1}^{n}(e_i)$

Uncertainties of Calculated Nucleon Energies

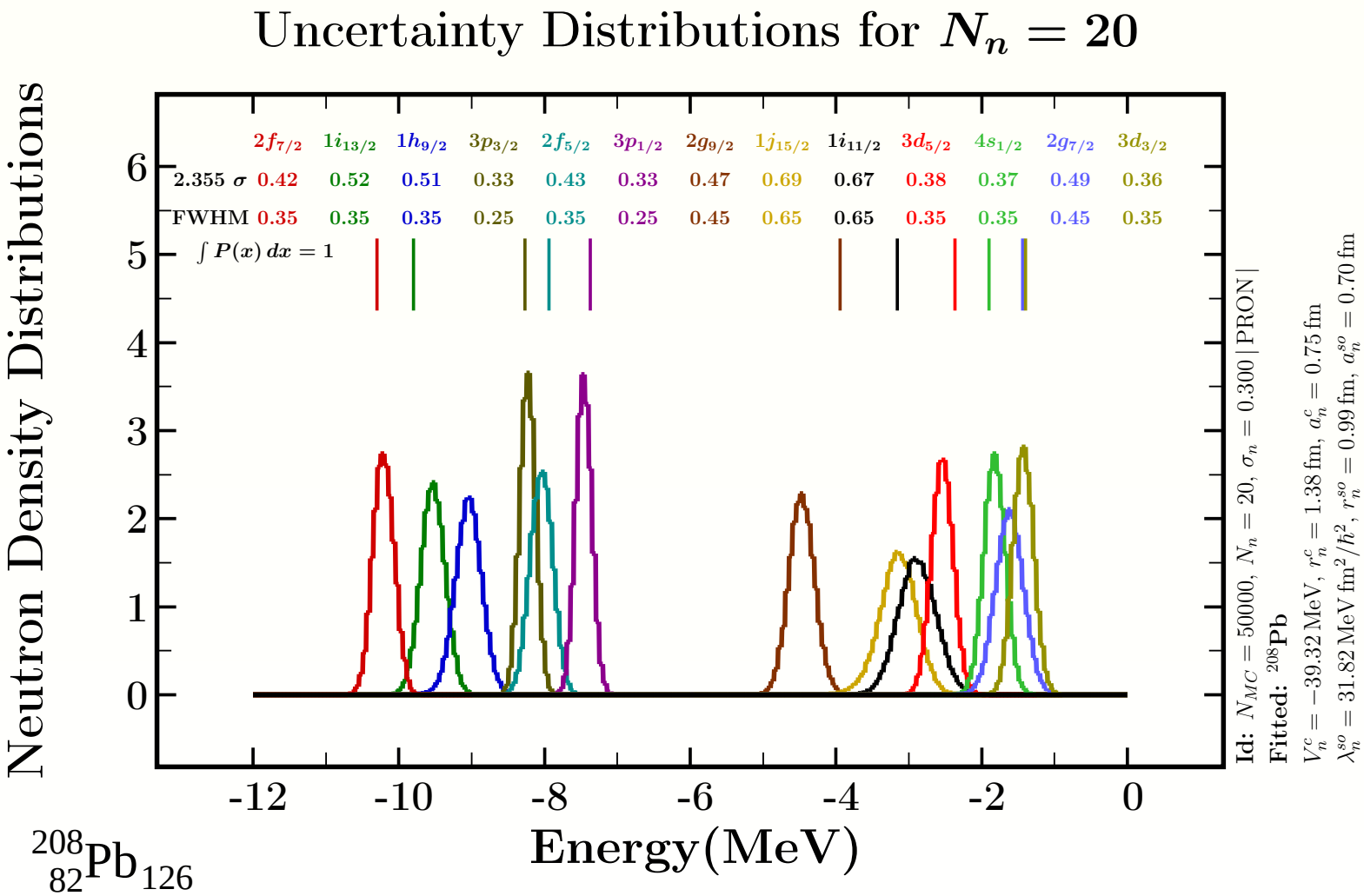
- The pseudo-experimental levels: Now we can modify/increase the 'sampling'



- Definitions: $\sigma = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(e_i - \bar{e})^2}$ $\qquad \bar{e} = \frac{1}{n}\sum_{i=1}^{n}(e_i)$

Uncertainties of Calculated Nucleon Energies

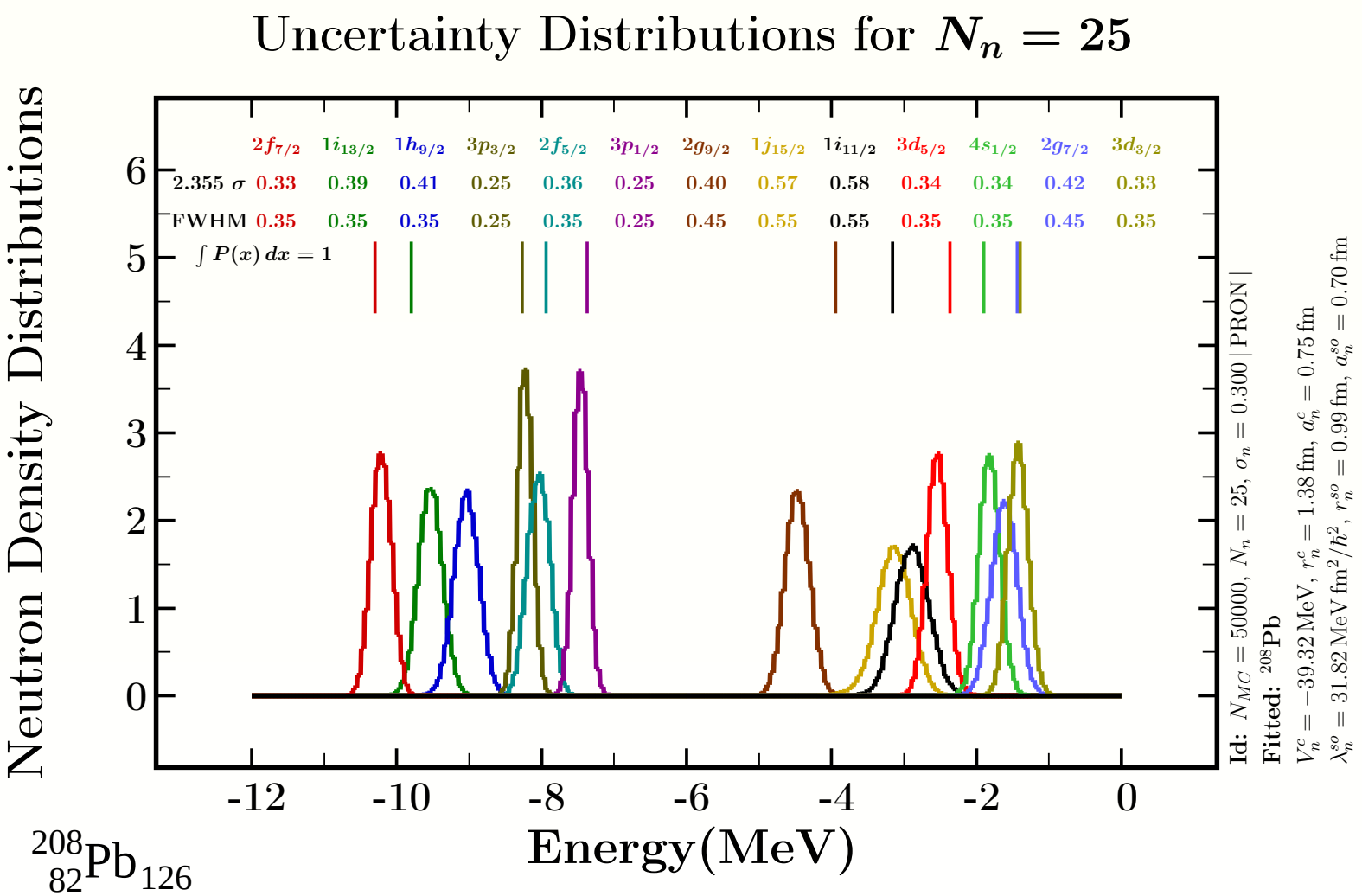
- The pseudo-experimental levels: Now we can modify/increase the 'sampling'



- Definitions: $\sigma = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(e_i - \bar{e})^2}$ $\qquad \bar{e} = \frac{1}{n}\sum_{i=1}^{n}(e_i)$

Uncertainties of Calculated Nucleon Energies

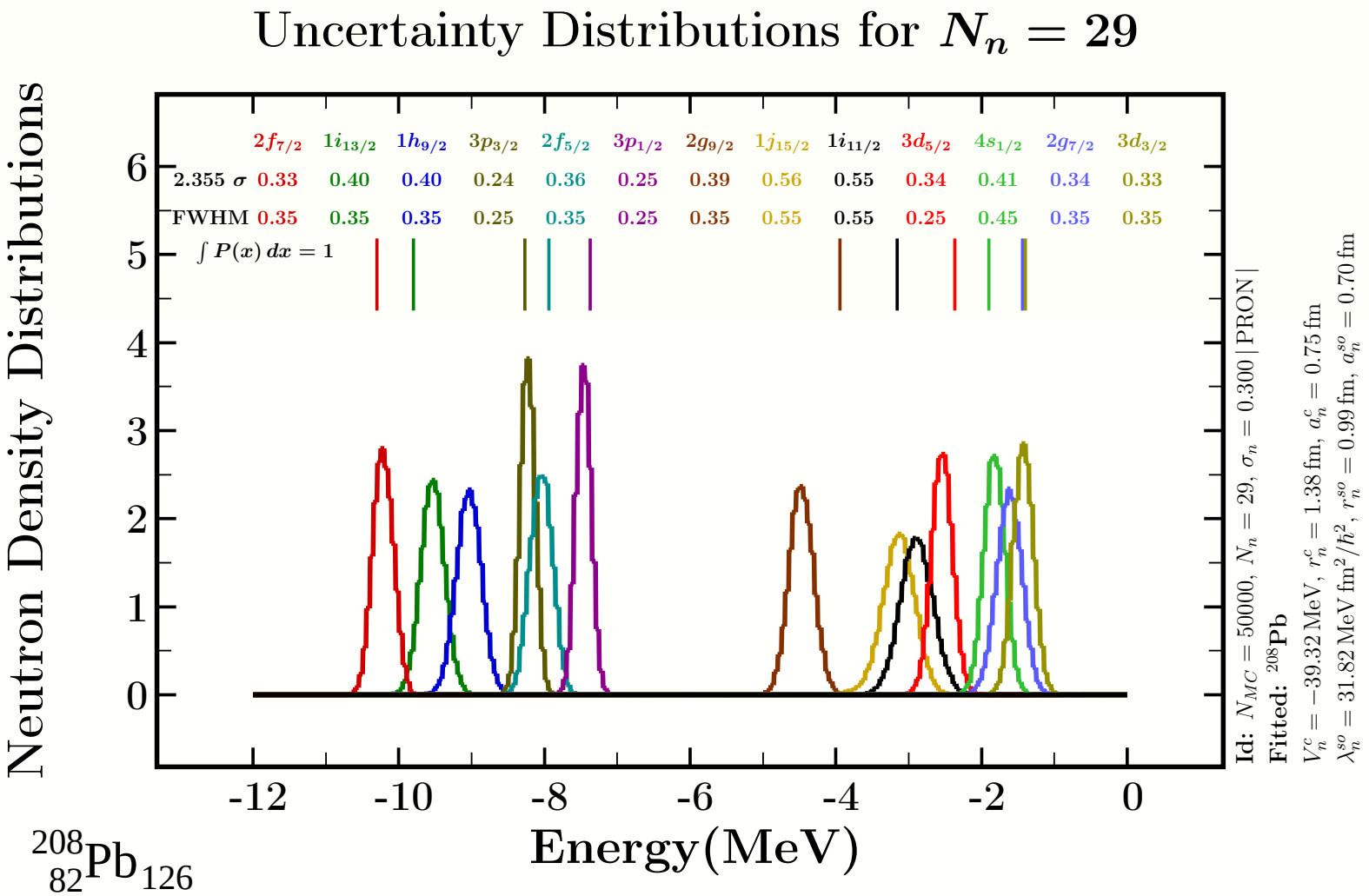
- The pseudo-experimental levels: Now we can modify/increase the 'sampling'



- Definitions: $\sigma = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(e_i - \bar{e})^2}$ $\qquad \bar{e} = \frac{1}{n}\sum_{i=1}^{n}(e_i)$

Uncertainties of Calculated Nucleon Energies

- The pseudo-experimental levels: Now we can modify/increase the 'sampling'

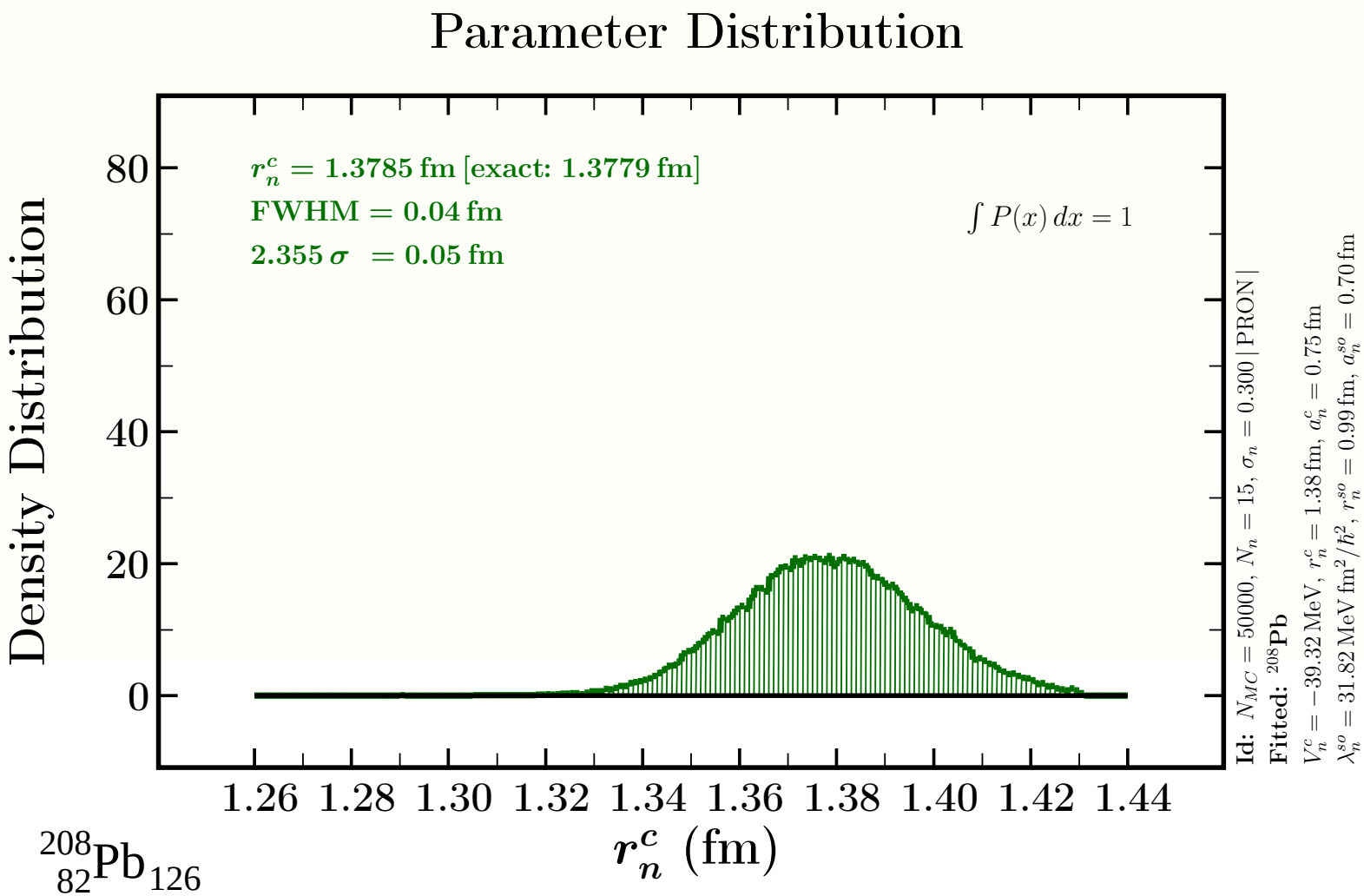


- Definitions: $\sigma = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(e_i - \bar{e})^2}$ $\qquad \bar{e} = \frac{1}{n}\sum_{i=1}^{n}(e_i)$

Central Radius Uncertainties

Uncertainties of the Optimal Parameters: r_n^c

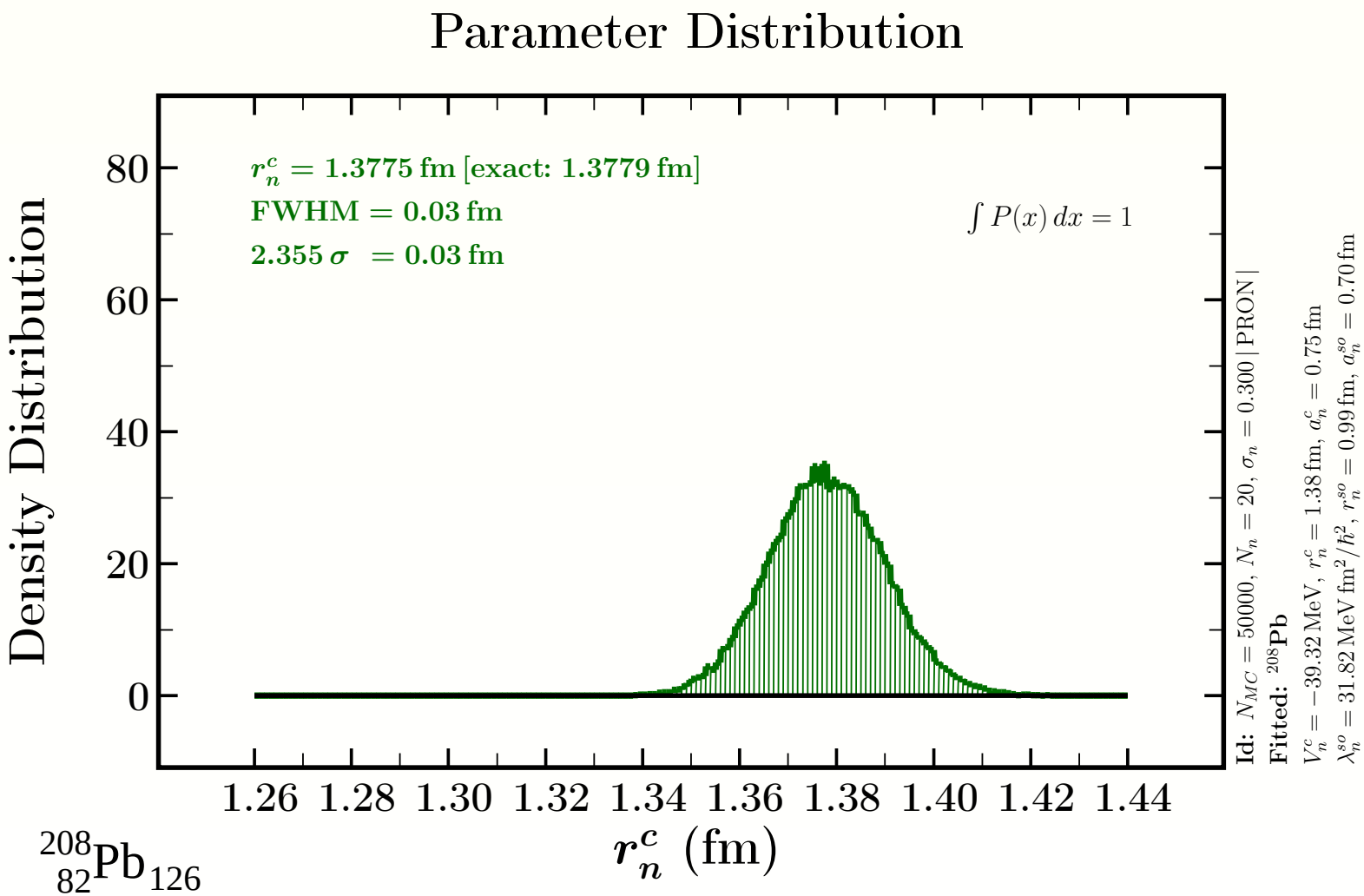
- Pseudo-experimental levels: Parameter uncertainties ← increasing 'sampling'



- Here: Sampling composed of 15 levels around the Fermi level

Uncertainties of the Optimal Parameters: r_n^c

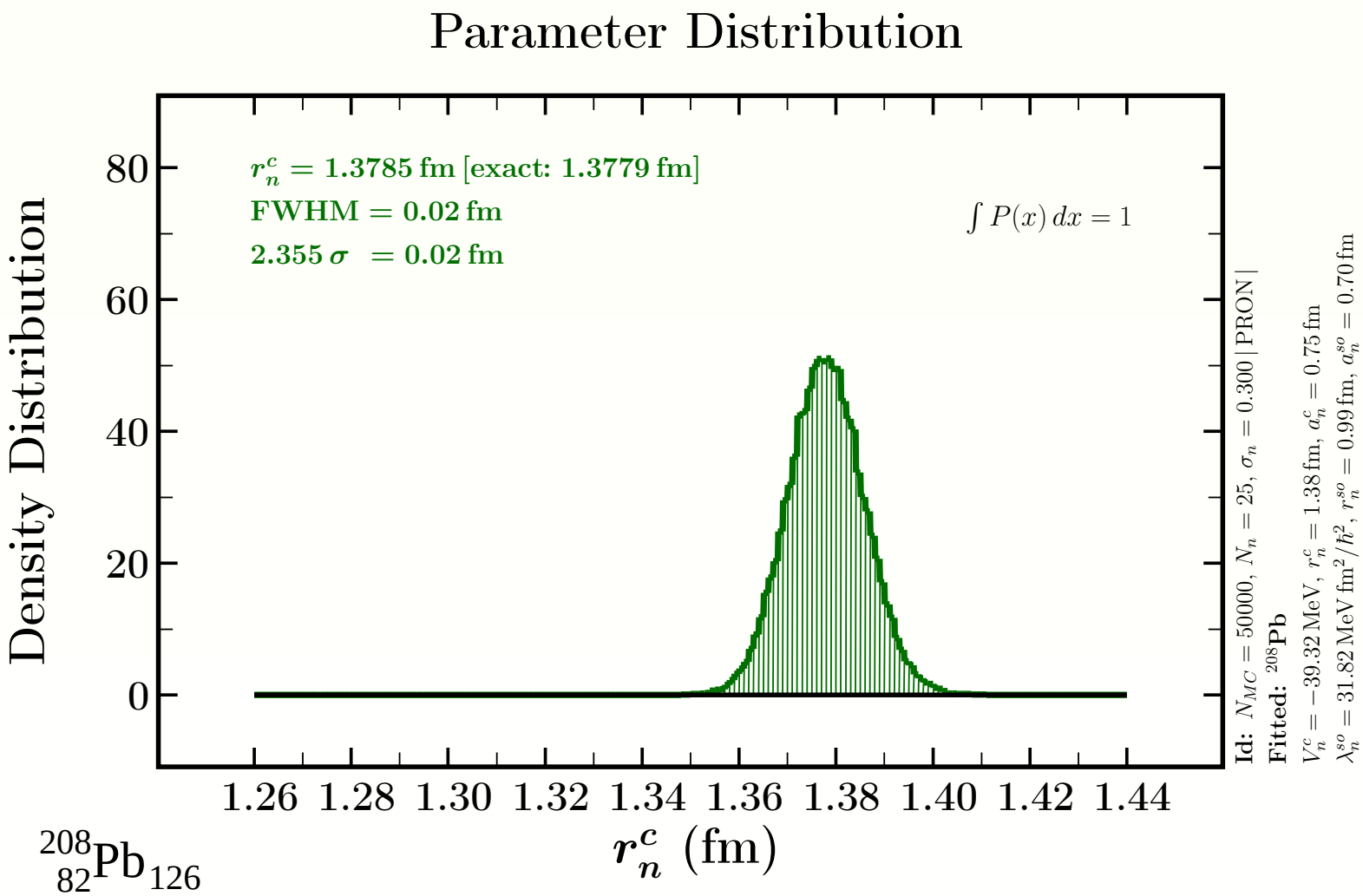
- Pseudo-experimental levels: Parameter uncertainties ← increasing 'sampling'



- Here: Sampling composed of 20 levels around the Fermi level

Uncertainties of the Optimal Parameters: r_n^c

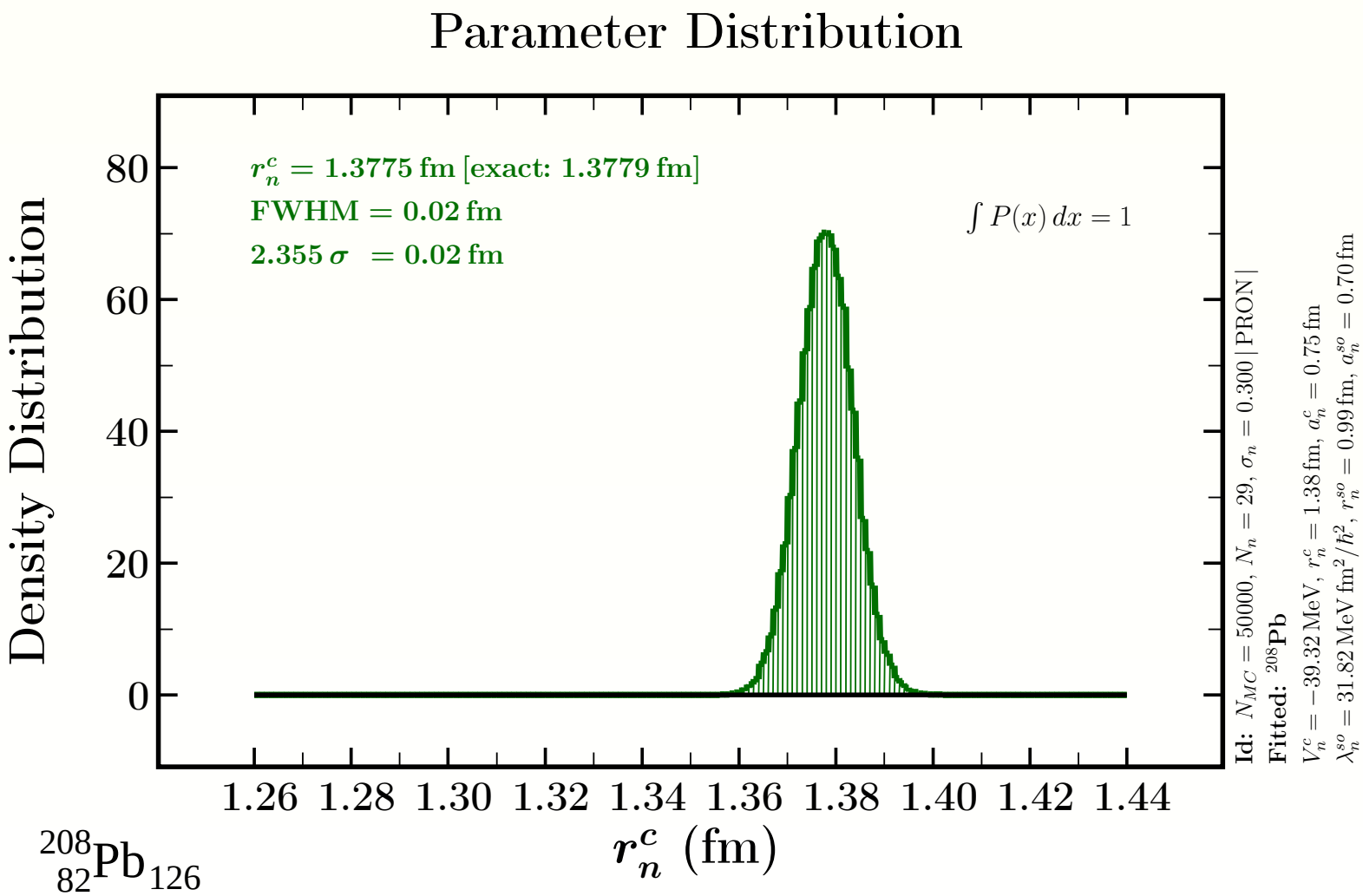
- Pseudo-experimental levels: Parameter uncertainties ← increasing 'sampling'



- Here: Sampling composed of 25 levels around the Fermi level

Uncertainties of the Optimal Parameters: r_n^c

- Pseudo-experimental levels: Parameter uncertainties ← increasing 'sampling'

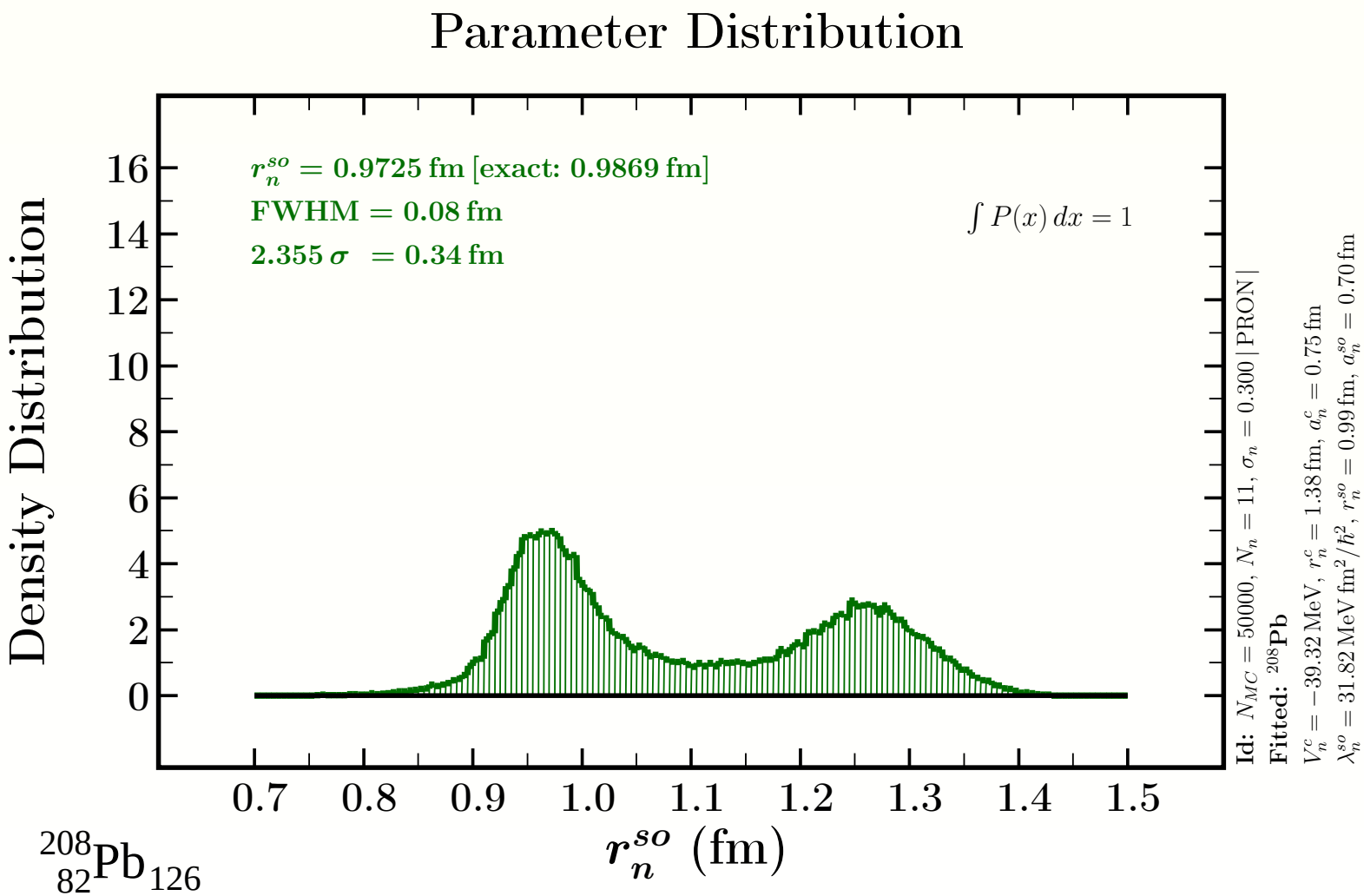


- Here: Sampling composed of 29 levels around the Fermi level

Spin-Orbit Radius Uncertainties

Uncertainties of the Optimal Parameters: r_n^{so}

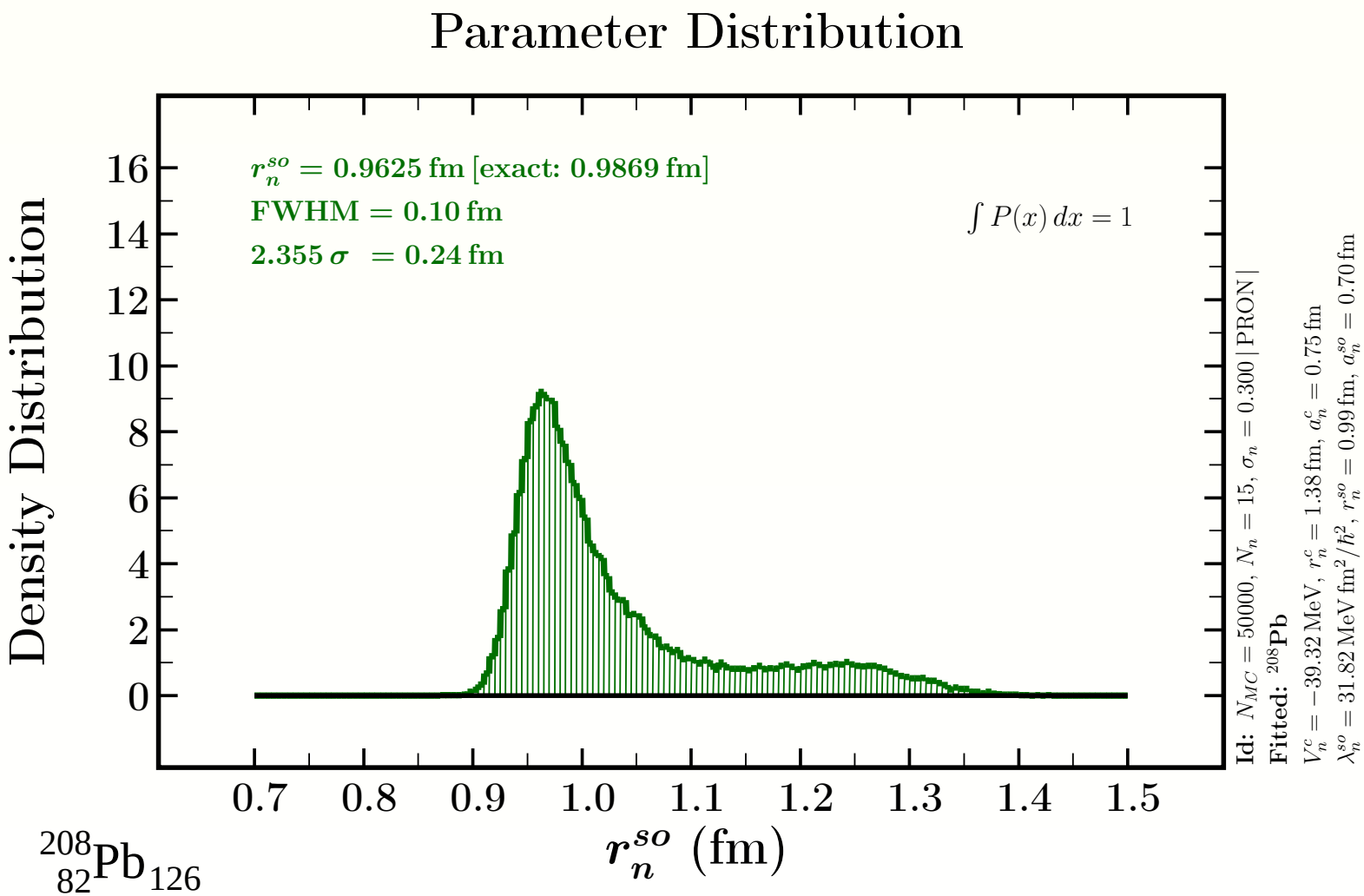
- Pseudo-experimental levels: Parameter uncertainties ← increasing 'sampling'



- Here: Sampling composed of 11 levels around the Fermi level

Uncertainties of the Optimal Parameters: r_n^{so}

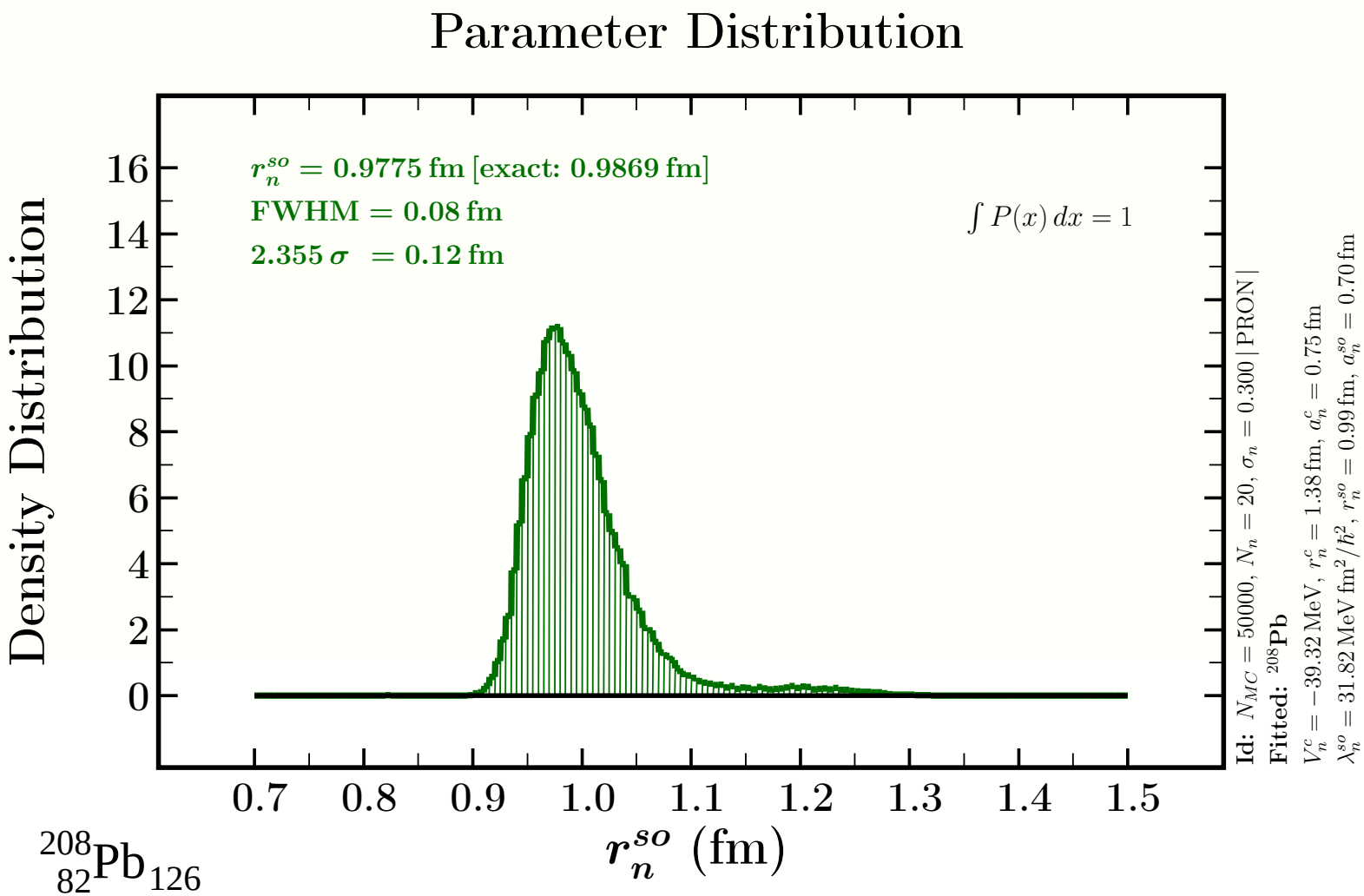
- Pseudo-experimental levels: Parameter uncertainties ← increasing 'sampling'



- Here: Sampling composed of 15 levels around the Fermi level

Uncertainties of the Optimal Parameters: r_n^{so}

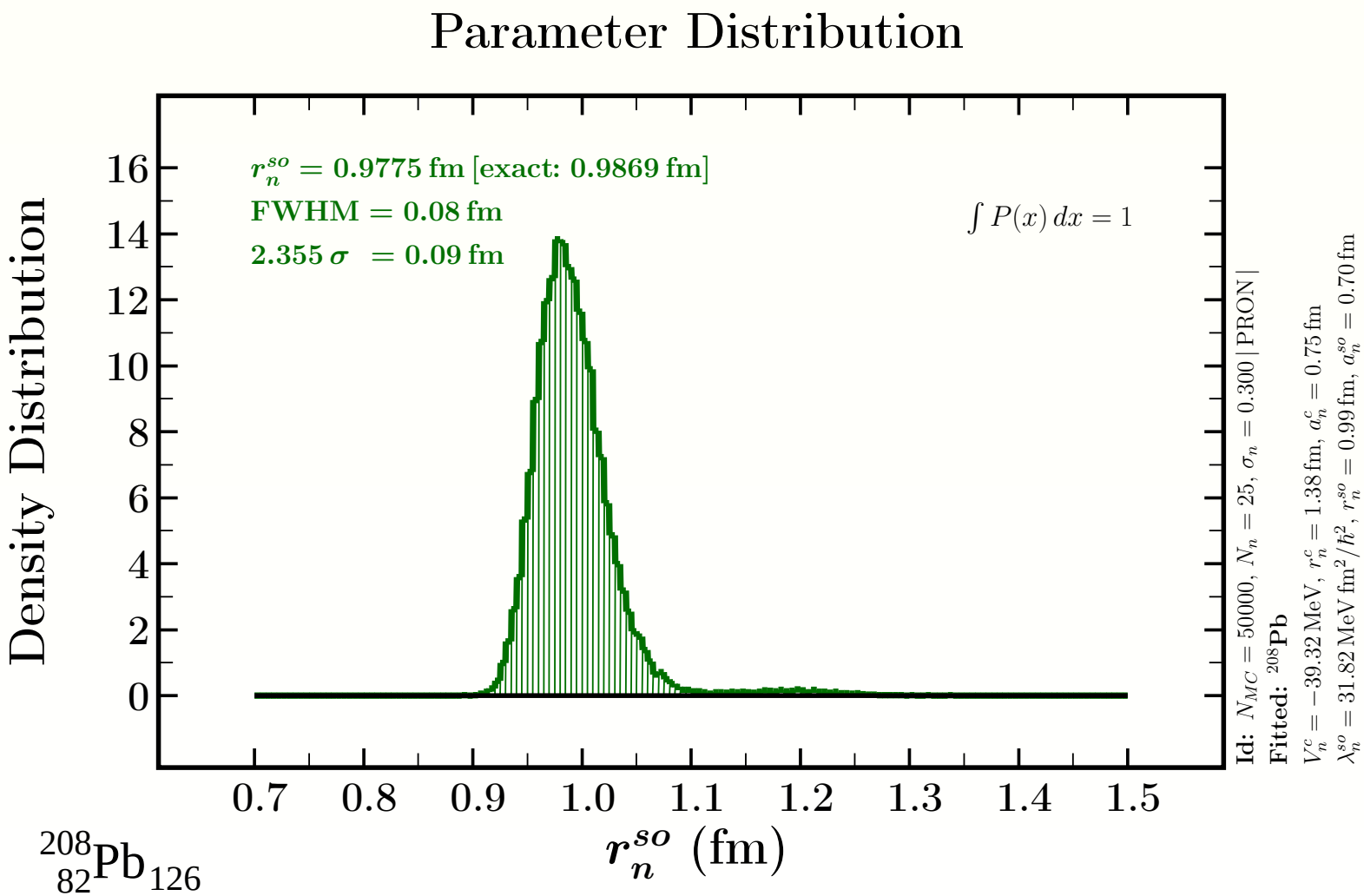
- Pseudo-experimental levels: Parameter uncertainties ← increasing 'sampling'



- Here: Sampling composed of 20 levels around the Fermi level

Uncertainties of the Optimal Parameters: r_n^{so}

- Pseudo-experimental levels: Parameter uncertainties ← increasing 'sampling'

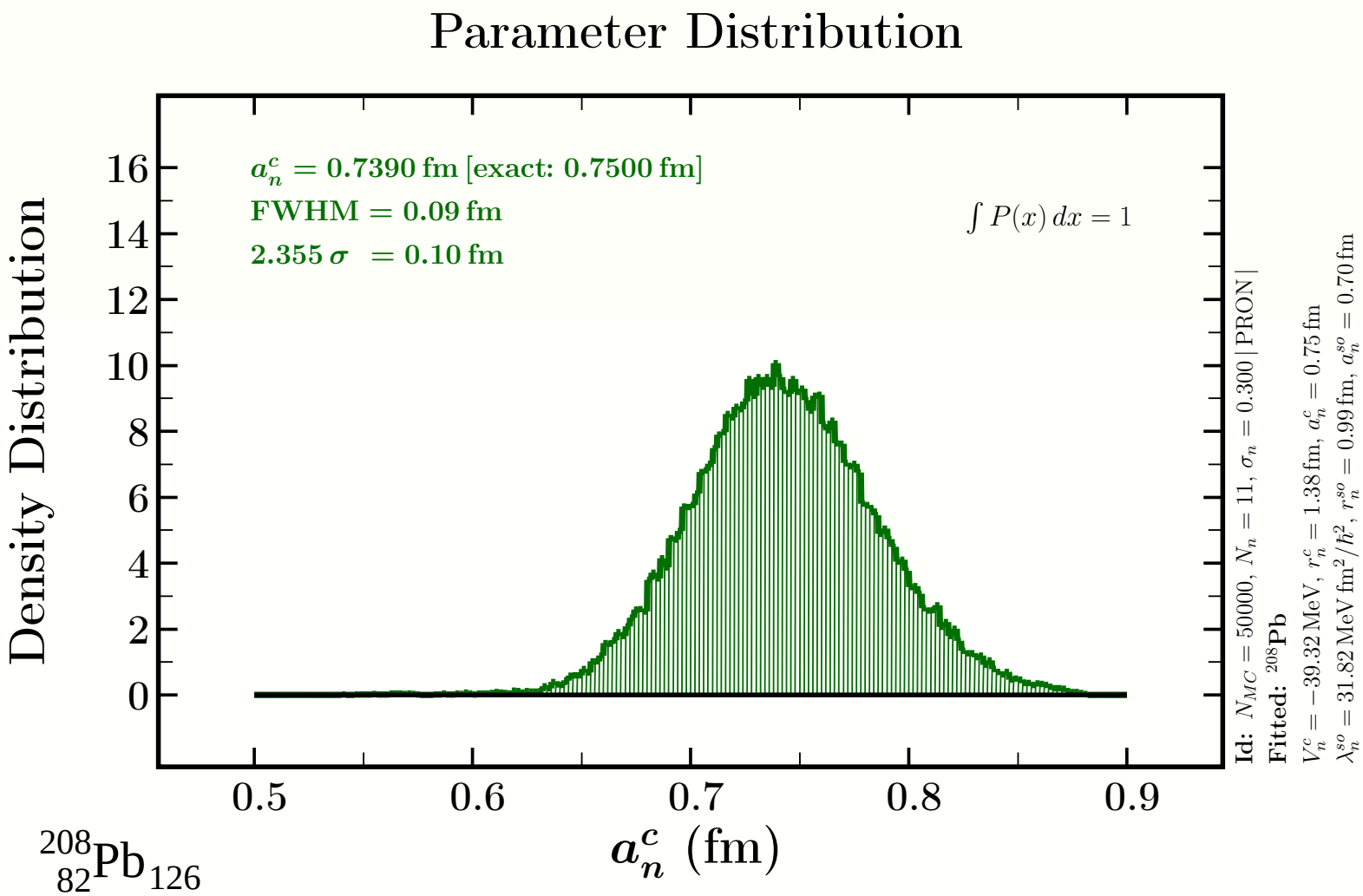


- Here: Sampling composed of 25 levels around the Fermi level

Diffusivity Parameter Uncertainties

Uncertainties of the Optimal Parameters: a_n^c

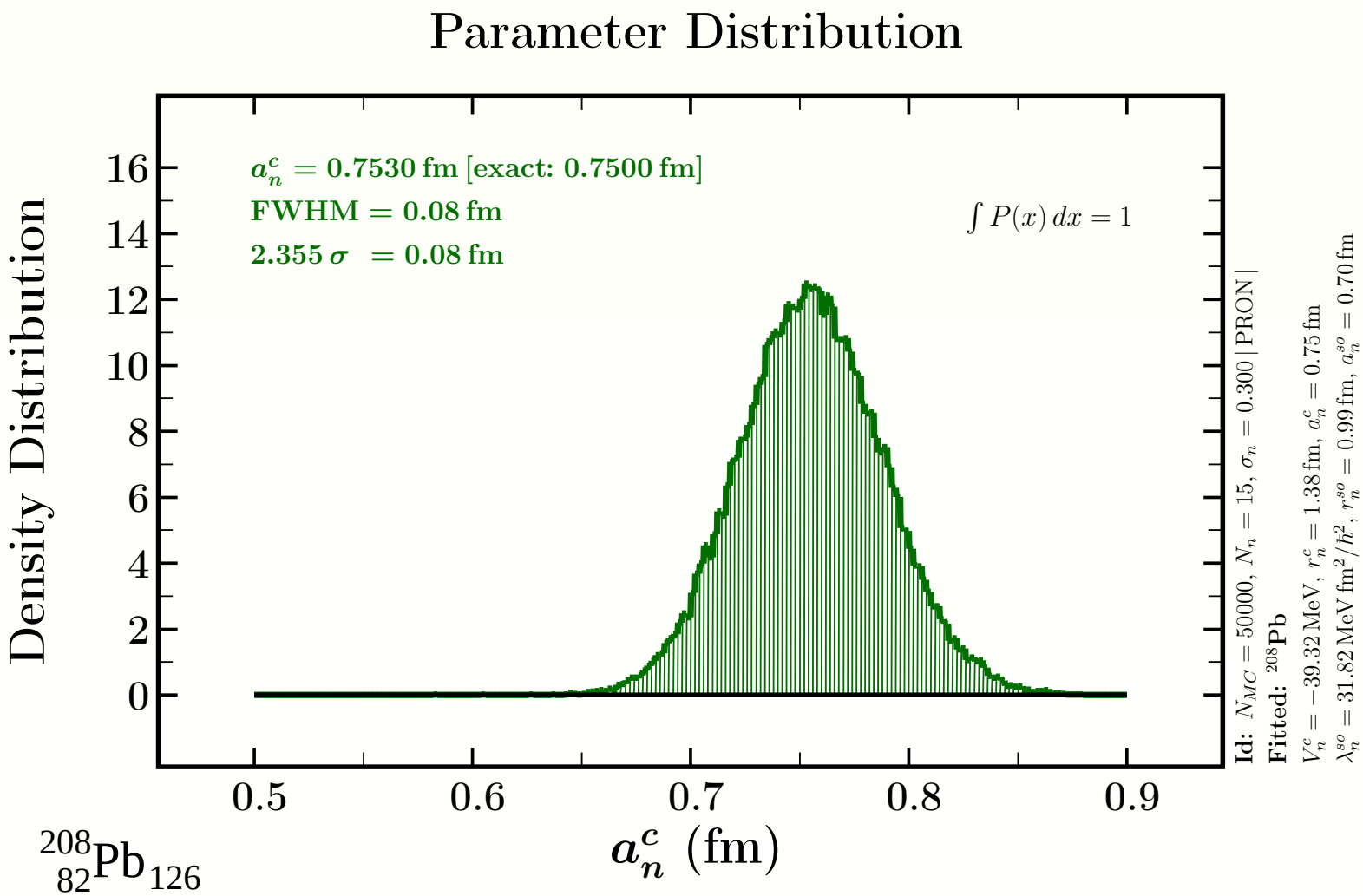
- Pseudo-experimental levels: Parameter uncertainties ← increasing 'sampling'



- Here: Sampling composed of 11 levels around the Fermi level

Uncertainties of the Optimal Parameters: a_n^c

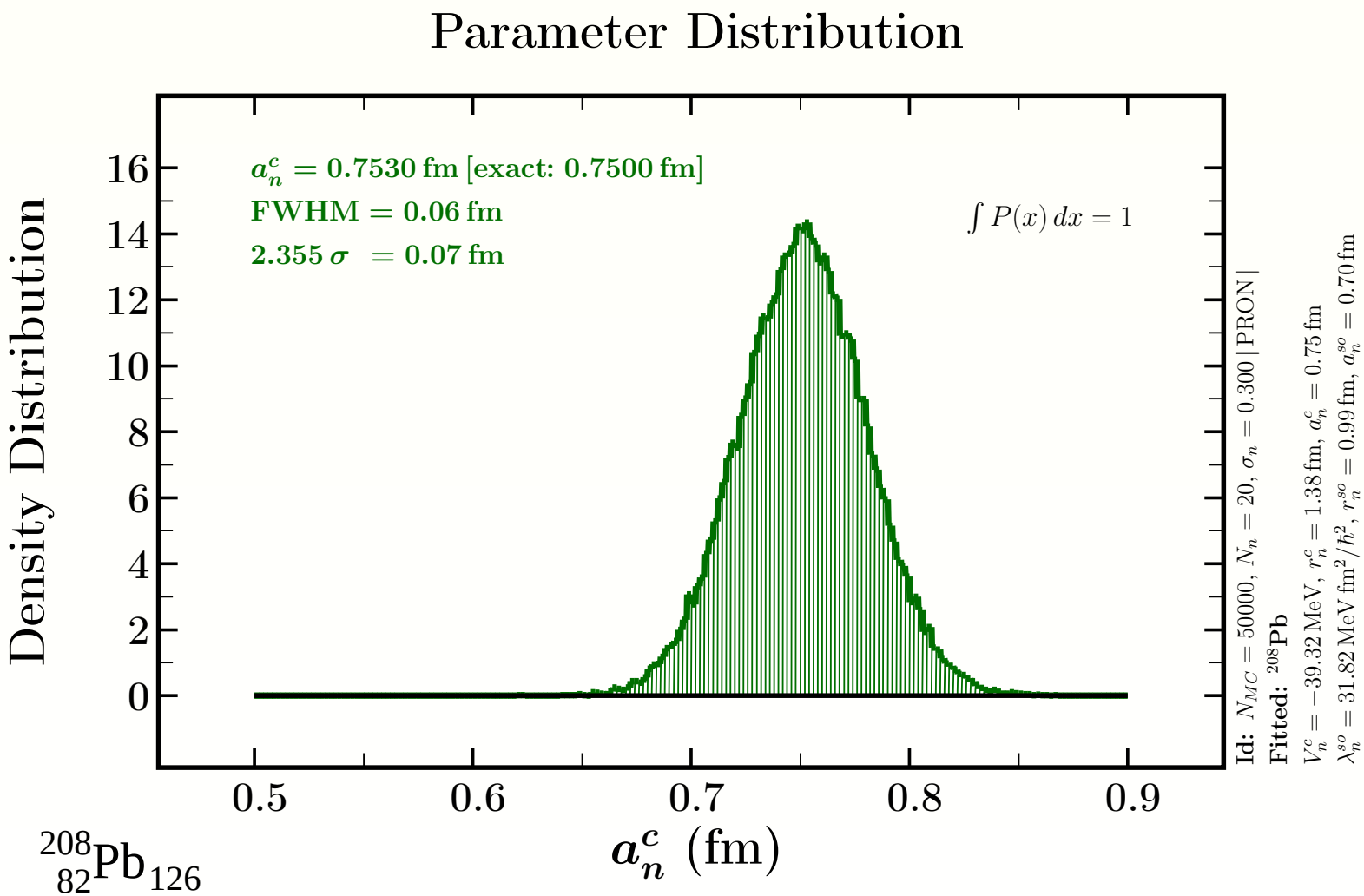
- Pseudo-experimental levels: Parameter uncertainties ← increasing 'sampling'



- Here: Sampling composed of 15 levels around the Fermi level

Uncertainties of the Optimal Parameters: a_n^c

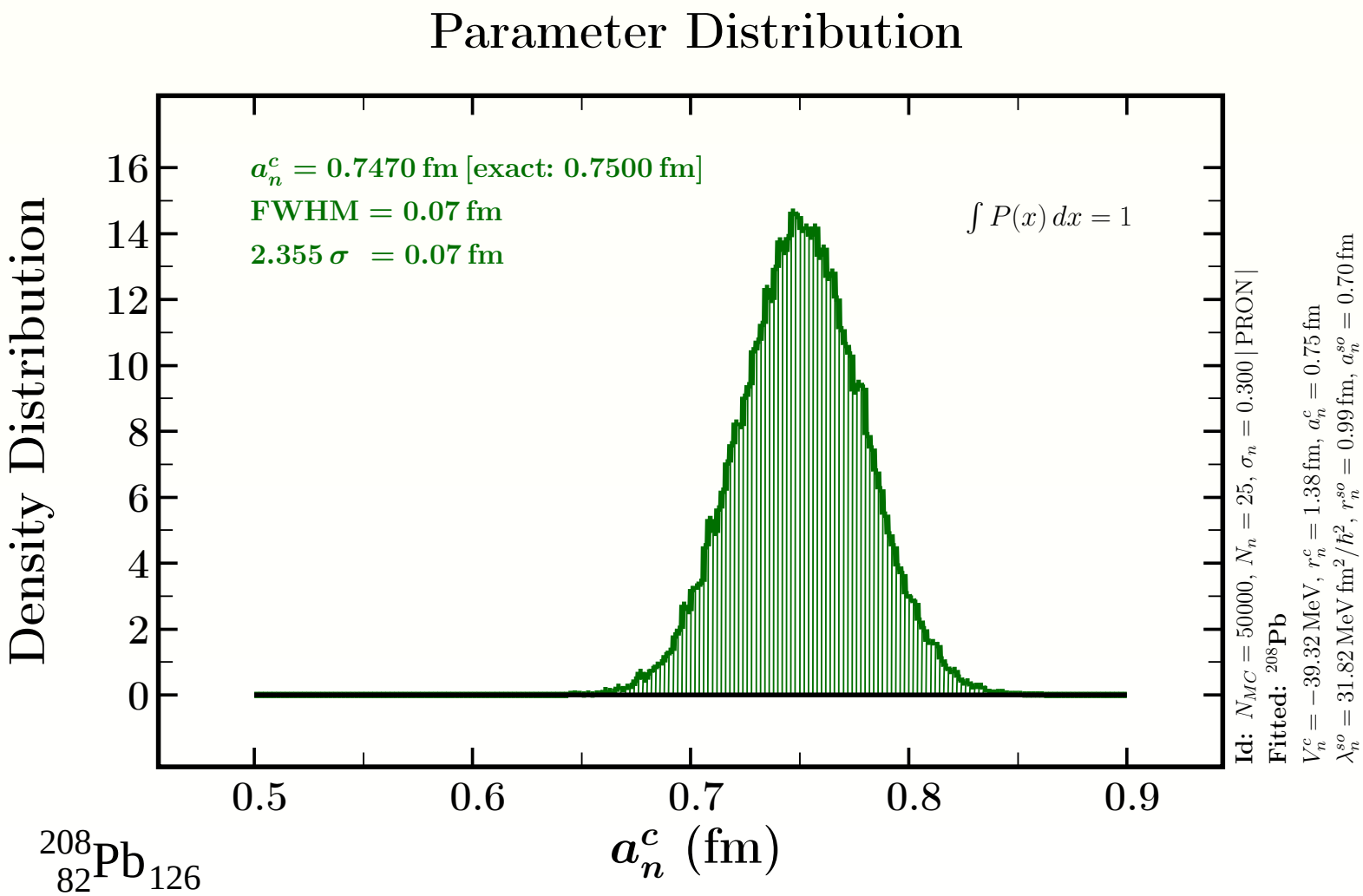
- Pseudo-experimental levels: Parameter uncertainties ← increasing 'sampling'



- Here: Sampling composed of 20 levels around the Fermi level

Uncertainties of the Optimal Parameters: a_n^c

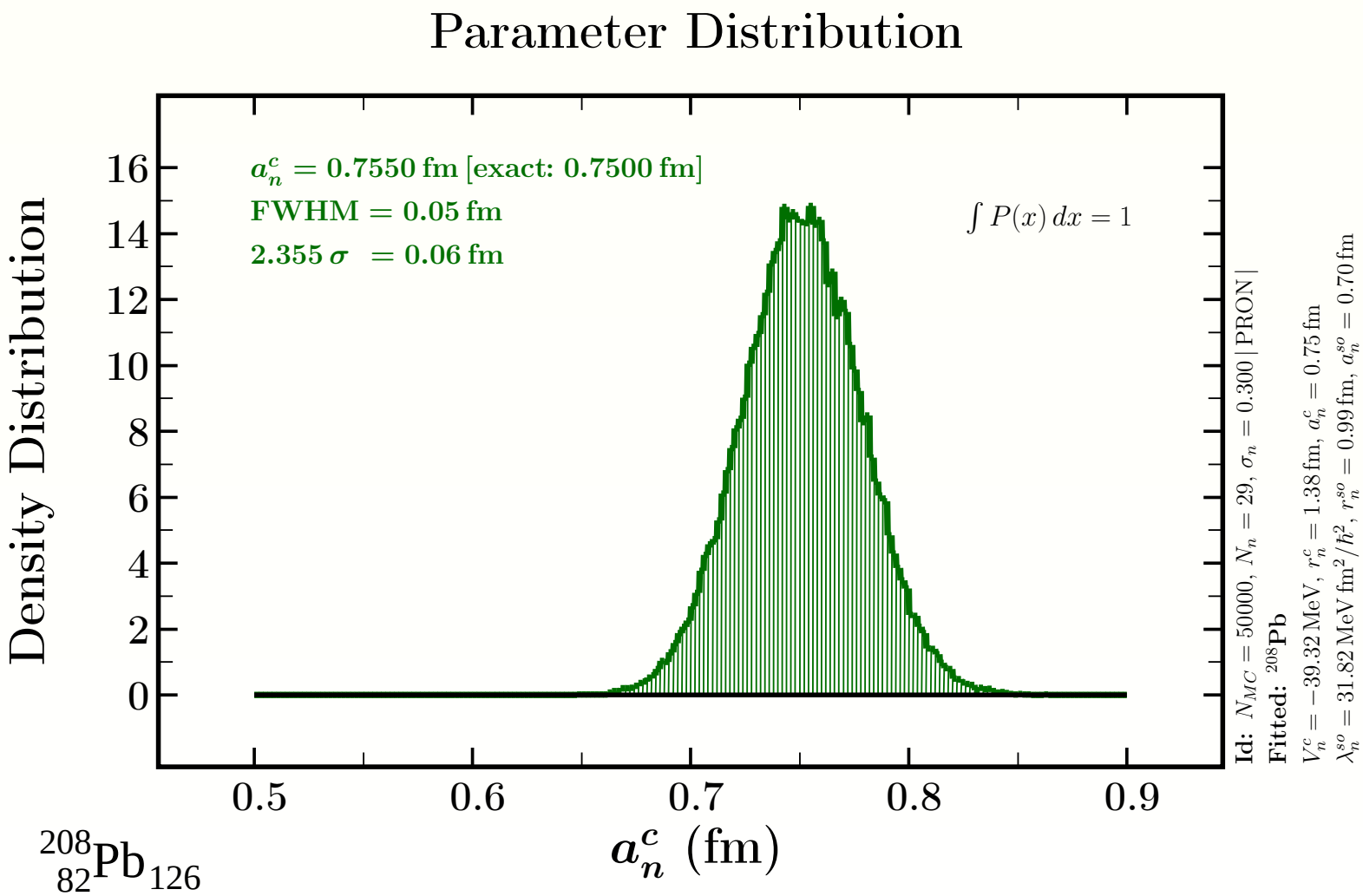
- Pseudo-experimental levels: Parameter uncertainties ← increasing 'sampling'



- Here: Sampling composed of 25 levels around the Fermi level

Uncertainties of the Optimal Parameters: a_n^c

- Pseudo-experimental levels: Parameter uncertainties ← increasing 'sampling'



- Here: Sampling composed of 29 levels around the Fermi level

Final Comments

Final Comments

• Fitting is usually easy: We obtain some "optimal" parameters and the "curve passes through the data"

Final Comments

- Fitting is usually easy: We obtain some "optimal" parameters and the "curve passes through the data"
- The very first test *sine qua non:* Are the parameters correlated?

Final Comments

• Fitting is usually easy: We obtain some "optimal" parameters and the "curve passes through the data"

• The very first test *sine qua non:* Are the parameters correlated?

• If they are we have decisions to take:

– Are we interested "just in fitting"?
or
– Are we interested also in predictions of new physics phenomena
and
– Are we interested in understanding the physics?

Final Comments

• Fitting is usually easy: We obtain some "optimal" parameters and the "curve passes through the data"

• The very first test *sine qua non:* Are the parameters correlated?

• If they are we have decisions to take:

– Are we interested "just in fitting"?
or
– Are we interested also in predictions of new physics phenomena
and
– Are we interested in understanding the physics?

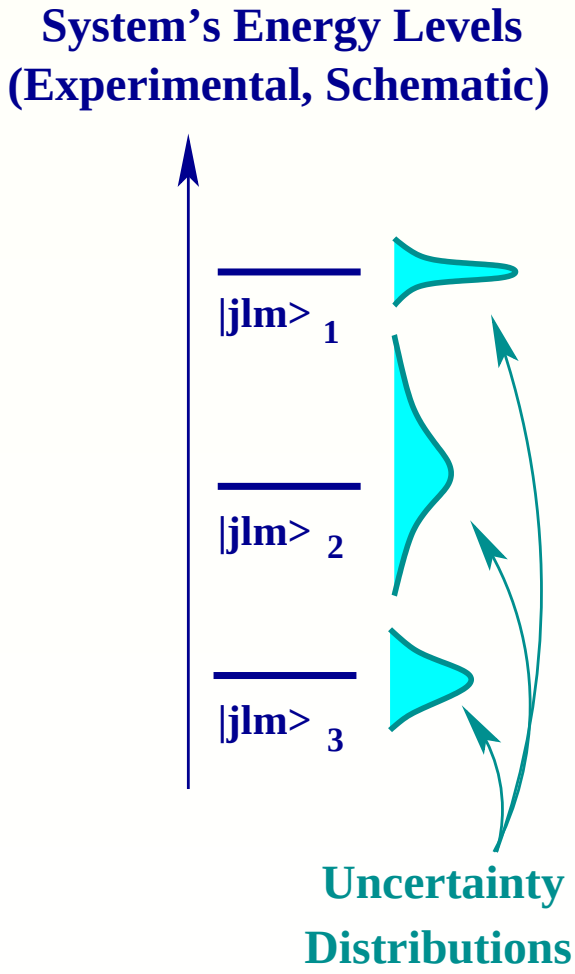
• If just in fitting: Everything may look fine... for those who chose!

ANNEX I

Experimental Uncertainties and Error-Probability Distributions

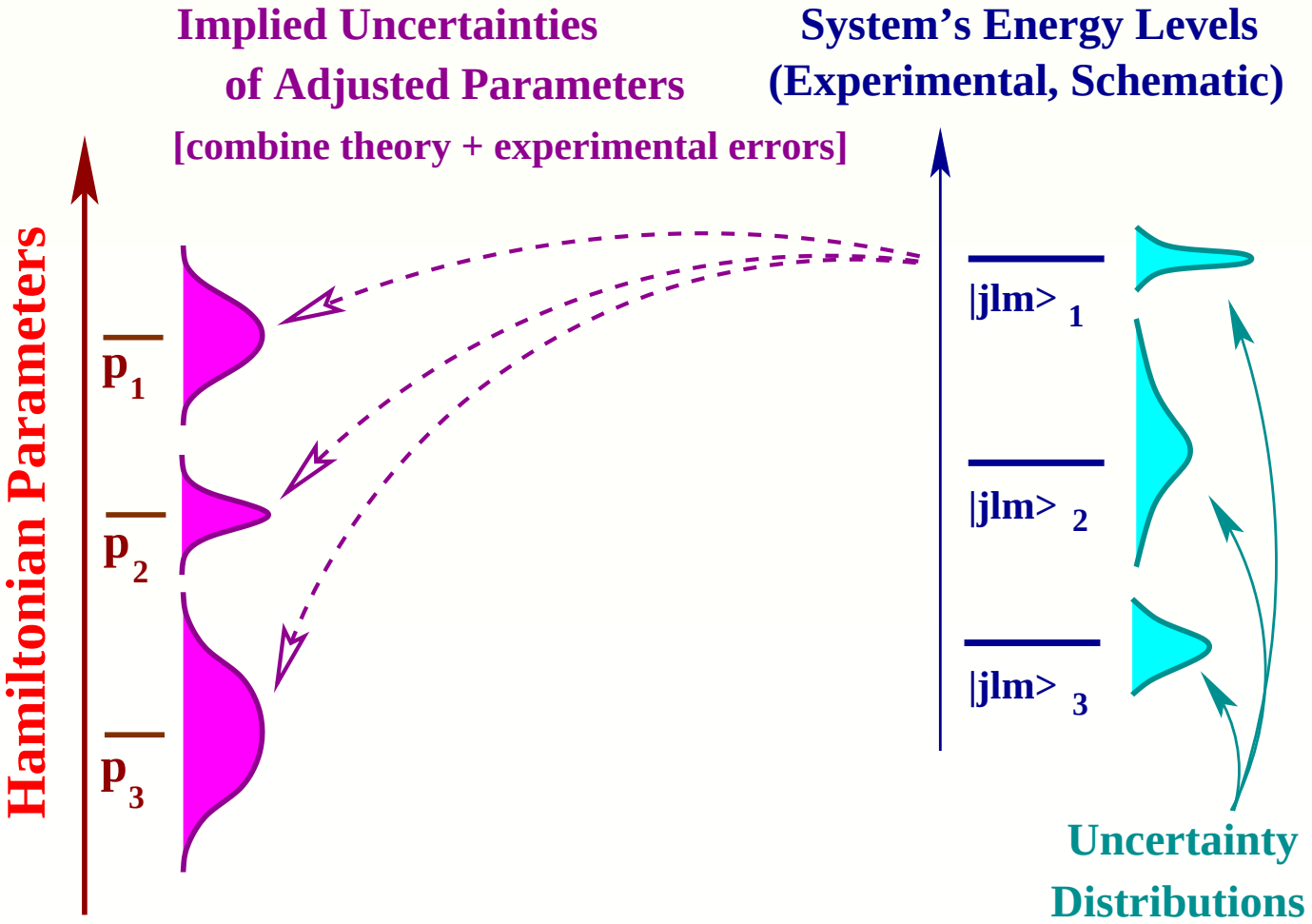
Single-Particle Levels as Probability Distributions

Experimental levels represent, from both quantum-mechanical and experimental points of view an ensemble of probability distributions



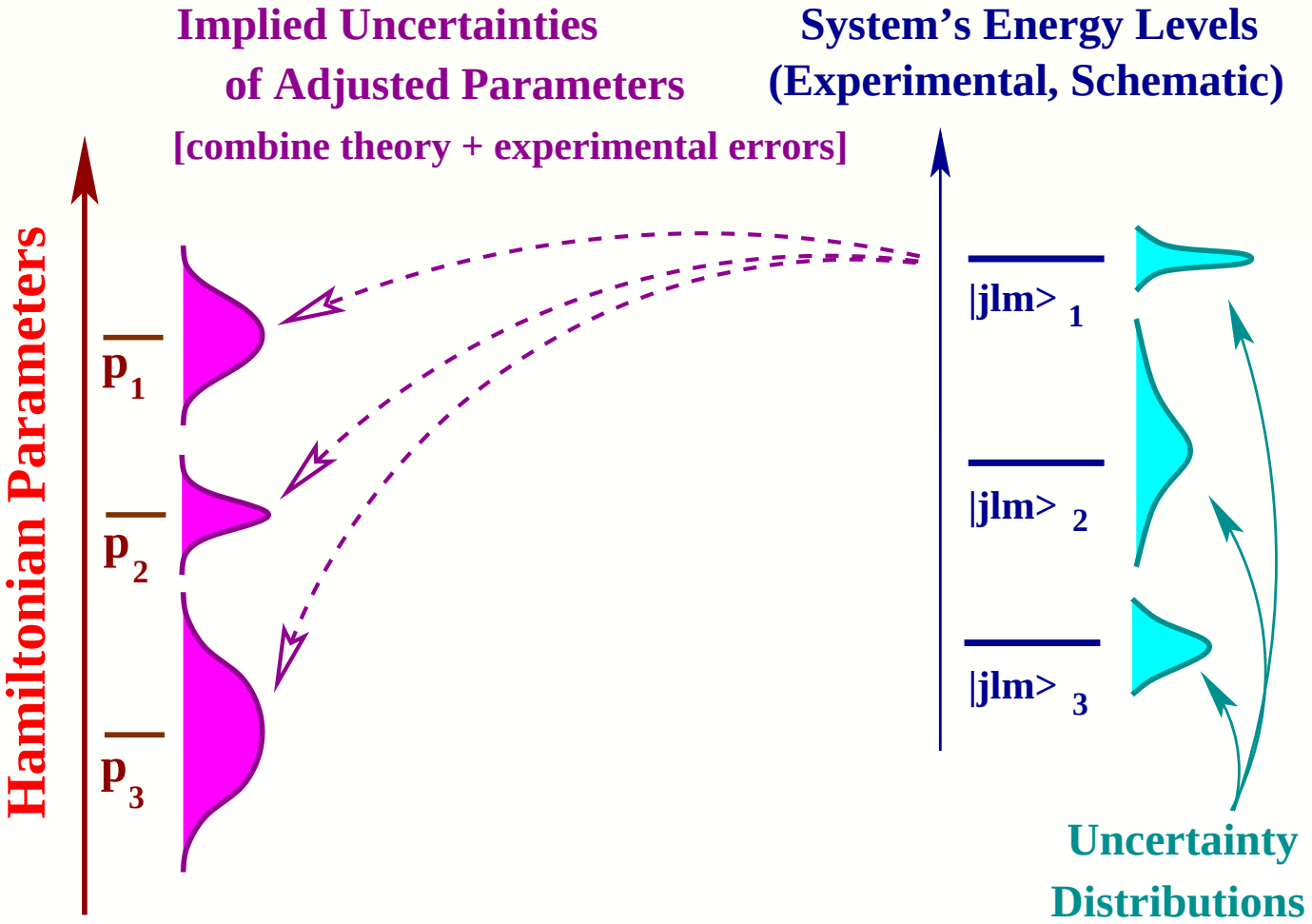
Single-Particle Levels as Probability Distributions

Uncertainties propagate to sought parameters $\{p_1, p_2, \ldots\} \equiv \{p\}$ in $\hat{H}(\hat{r}, \hat{p}; \{p\})\,\psi_n = e_n(p)\,\psi_n$: Parameters $\rightarrow$ Probability Distributions



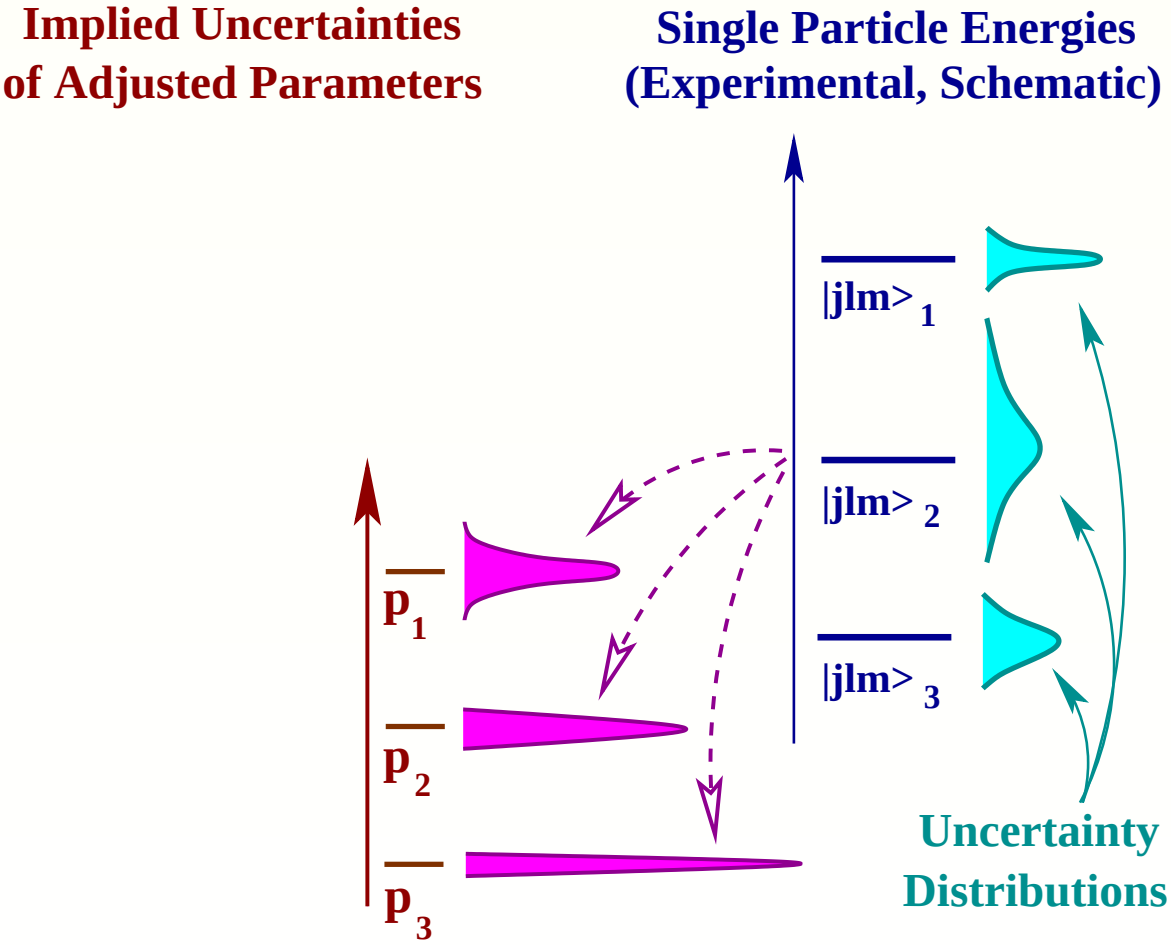
Single-Particle Levels as Probability Distributions

As it turns out, even small uncertainties on some experimental levels may cause very large uncertainties on the adjusted parameters ...



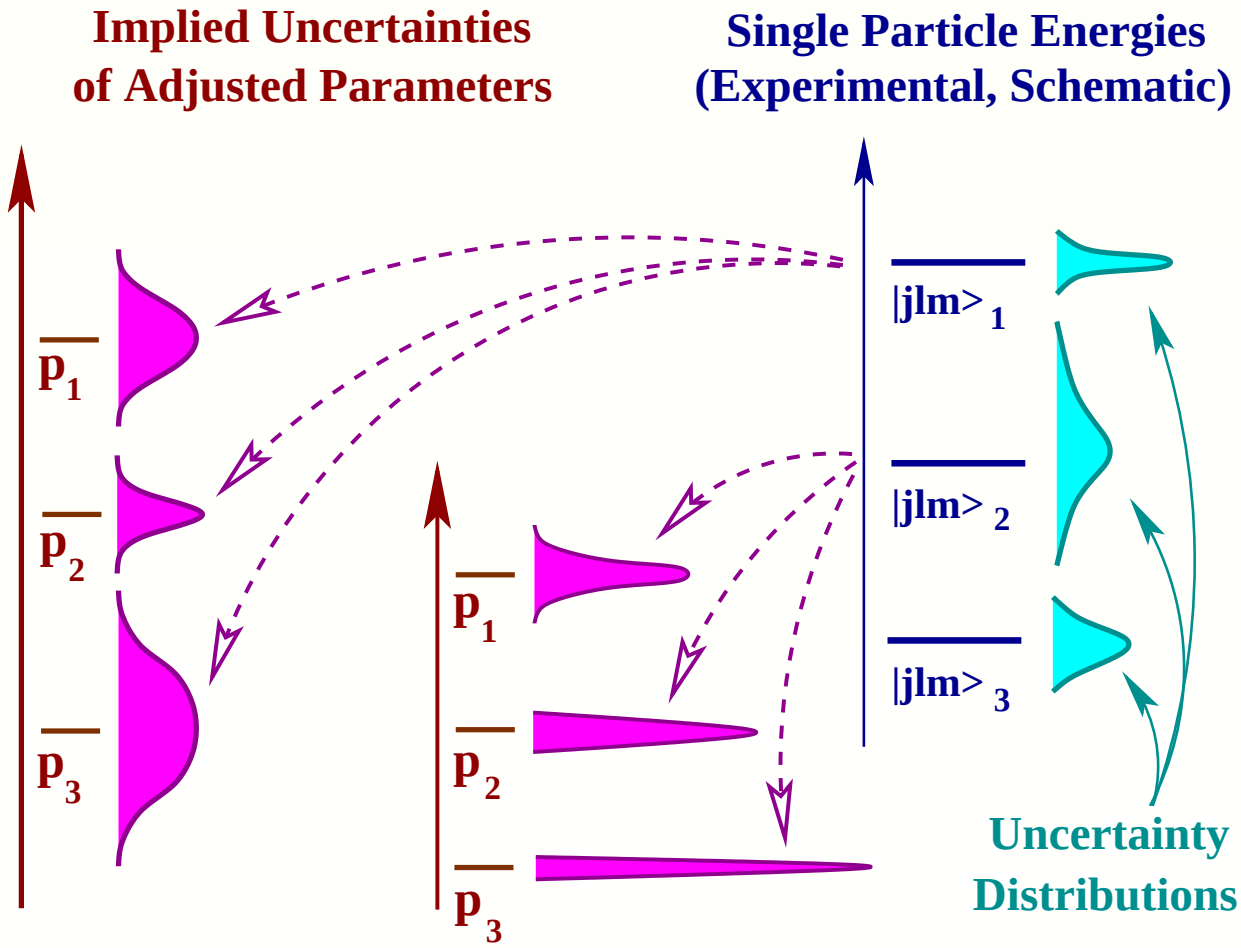
Single-Particle Levels as Probability Distributions

... while at the same time big uncertainties on other levels have a small impact: and this requires specialised case-by-case studies



Single-Particle Levels as Probability Distributions

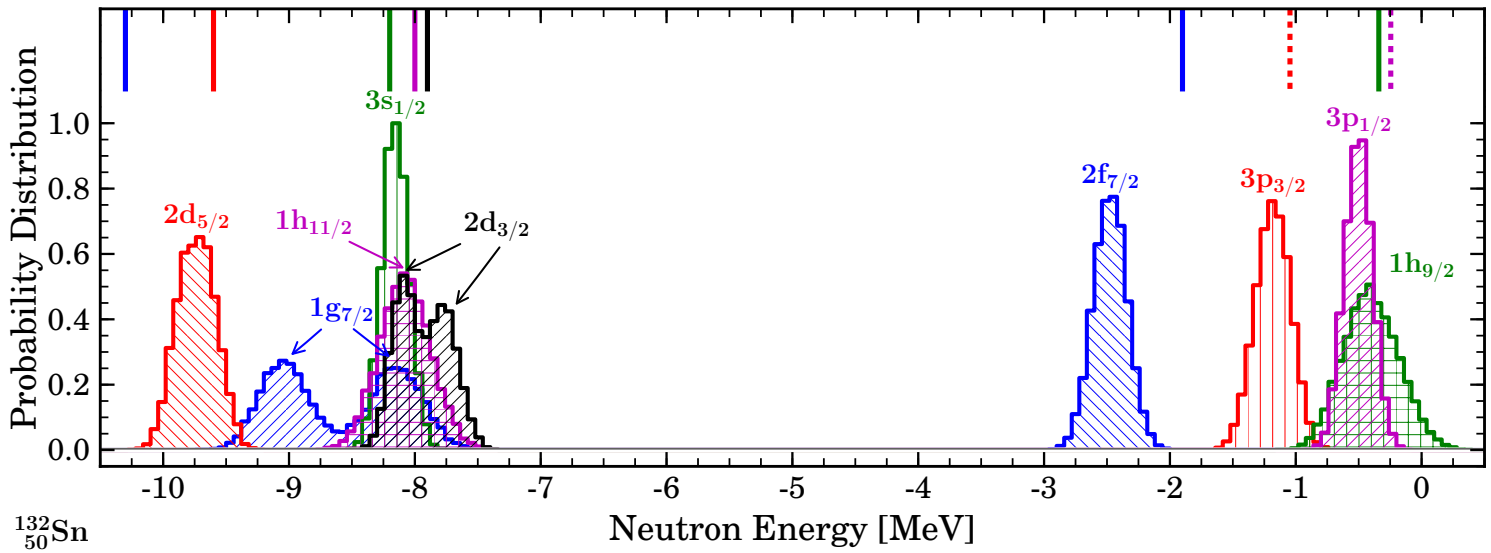
Conclusion: The parameter adjustment depends very strongly on the quality of the data implying the existence of theoretical error bars!!



ANNEX II

Examples of Stochastic Impact on Predicted Nucleon Energies

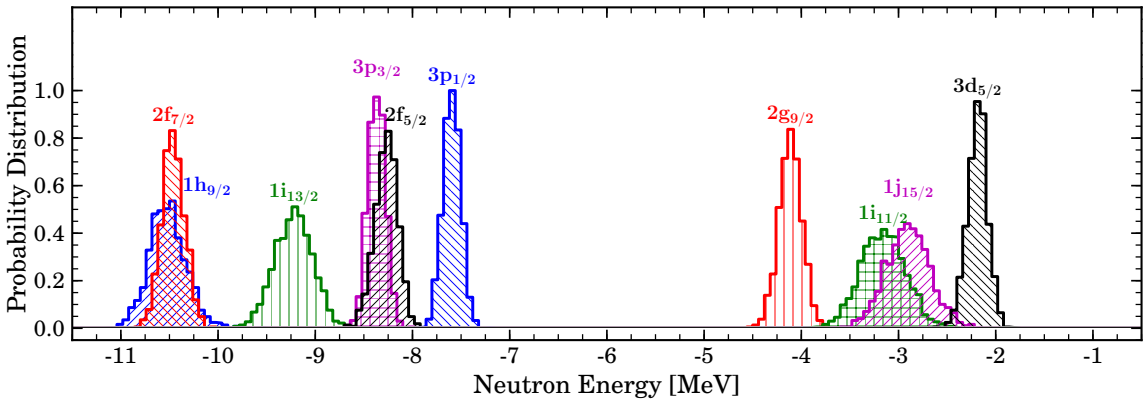
An Example of Stochastic Theory Predictions



Results of the extrapolation from the ^{208}Pb to the ^{132}Sn nucleus for the neutrons. Monte-Carlo simulation with N=20 000 Gaussian-distributed parameter sets, based on ^{208}Pb results; noise width σ=0.1 MeV. With each of the so obtained N=20 000 sets of parameters the results for the neutrons in ^{132}Sn nucleus have been obtained. Observe 'pathologies': Double-hump structures of $1g_{7/2}$ and $2d_{3/2}$.

An Example of Stochastic Theory Predictions

- Neutron levels for ^{208}Pb. Here: A realistic mean-field WS potential

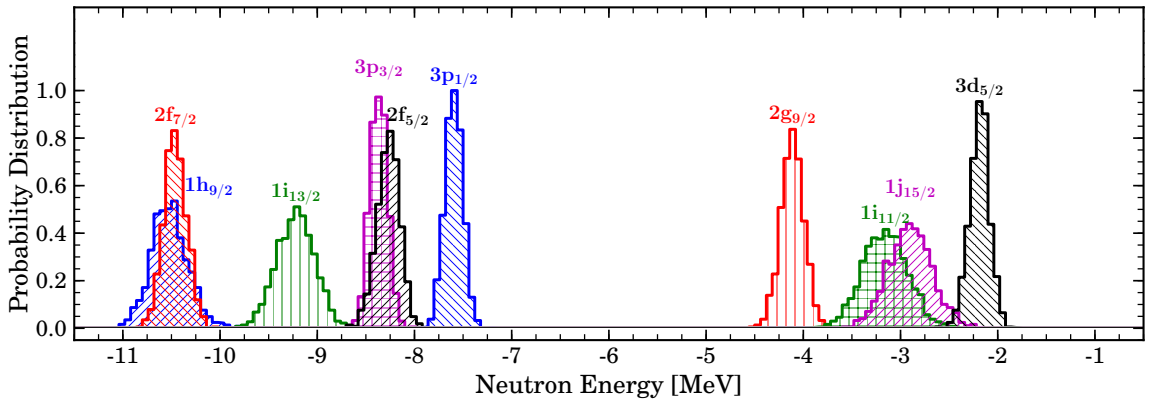


Positions of the neutron energies

together with the modelled uncertainty distributions

An Example of Stochastic Theory Predictions

• Neutron levels for ^{208}Pb. Here: A realistic mean-field WS potential



Positions of the neutron energies

together with the modelled uncertainty distributions

• In what follows we will study various uncertainty sources e.g. the ones created by intrinsic features of the Modelling and Sampling (such as parametric correlations – see below) but also weak points of the data analysis, or our incomplete knowledge of the interactions

ANNEX III

About difficulties encountered when learning about Predictive Power

What Does it Mean: 'To Have Predictive Power'?

What Does it Mean: 'To Have Predictive Power'?

- **Any result of any modelling of any phenomenon before the right experiments are performed can be called "a theoretical prediction"**

What Does it Mean: 'To Have Predictive Power'?

- **Any result of any modelling of any phenomenon before the right experiments are performed can be called "a theoretical prediction"**
- **... thus performing any model calculation can be called predicting!**

What Does it Mean: 'To Have Predictive Power'?

- **Any result of any modelling of any phenomenon before the right experiments are performed can be called "a theoretical prediction"**
- **... thus performing any model calculation can be called predicting!**
- **But if any calculation is a prediction, any theory can predict always and therefore it has always a certain prediction capacity (="power")**

What Does it Mean: 'To Have Predictive Power'?

• **Any result of any modelling of any phenomenon before the right experiments are performed can be called "a theoretical prediction"**

• **... thus performing any model calculation can be called predicting!**

• **But if any calculation is a prediction, any theory can predict always and therefore it has always a certain prediction capacity (="power")**

• **As a consequence, the very term "predictive power" applies always i.e. means no special property. In our context it will be fair to say:**

This term is void of sense - more precisely: does not tell us anything

What Does it Mean: 'To Have Predictive Power'?

• **Any result of any modelling of any phenomenon before the right experiments are performed can be called "a theoretical prediction"**

• **... thus performing any model calculation can be called predicting!**

• **But if any calculation is a prediction, any theory can predict always and therefore it has always a certain prediction capacity (="power")**

• **As a consequence, the very term "predictive power" applies always i.e. means no special property. In our context it will be fair to say:**

This term is void of sense - more precisely: does not tell us anything

• **And yet the term 'predictive power' is used continually - by many**

What Does it Mean: 'To Have Predictive Power'?

• **Any result of any modelling of any phenomenon before the right experiments are performed can be called "a theoretical prediction"**

• **... thus performing any model calculation can be called predicting!**

• **But if any calculation is a prediction, any theory can predict always and therefore it has always a certain prediction capacity (="power")**

• **As a consequence, the very term "predictive power" applies always i.e. means no special property. In our context it will be fair to say:**

This term is void of sense - more precisely: does not tell us anything

• **And yet the term 'predictive power' is used continually - by many**

• **One may introduce instead a slightly modified wording: What carries certain interest is, possibly, theory's good predictive power!**

What Does It Mean 'Obtain a Good Prediction'?

What Does It Mean 'Obtain a Good Prediction'?

- **Being good for someone may not be satisfactory for someone else**

What Does It Mean 'Obtain a Good Prediction'?

- **Being good for someone may not be satisfactory for someone else**
- **... and it becomes clear that discussions of this type unavoidably involve the elements of arbitrariness and of a subjective judgement**

What Does It Mean 'Obtain a Good Prediction'?

- **Being good for someone may not be satisfactory for someone else**
- **... and it becomes clear that discussions of this type unavoidably involve the elements of arbitrariness and of a subjective judgement**
- **Therefore directly related with the notion of "good predictions" are, sine qua non, criteria of distinction between "good" and "poor"**

What Does It Mean 'Obtain a Good Prediction'?

- **Being good for someone may not be satisfactory for someone else**
- **... and it becomes clear that discussions of this type unavoidably involve the elements of arbitrariness and of a subjective judgement**
- **Therefore directly related with the notion of "good predictions" are, sine qua non, criteria of distinction between "good" and "poor"**
- **It is not possible to talk about Predictive Power [whatever it means*)] without specifying the criteria of choice at the same time:**

The notion of Predictive Power is relative and/or subjective#)

*) *The notion of Predictive Power is still to be made more precise slightly later ...*

#) *So is the very notion of probability (several 'official' definitions and interpretations)*

After all these precautions
we are still going to use the term
“Predictive Power”
as everybody else does

After all these precautions
we are still going to use the term
“Predictive Power”
as everybody else does

but keeping in mind its shortcomings

Here we arrive at the 'dramatic consequences' [largely unknown, or deliberately ignored, or both]:

Here we arrive at the 'dramatic consequences' [largely unknown, or deliberately ignored, or both]:

- The inverse problem has no solution if the modelling does not constrain parameters [changing data does not change parameters]

Here we arrive at the 'dramatic consequences' [largely unknown, or deliberately ignored, or both]:

- The inverse problem has no solution if the modelling does not constrain parameters [changing data does not change parameters]
- ... and yet some of us choose χ^2-minimising!!

Here we arrive at the 'dramatic consequences' [largely unknown, or deliberately ignored, or both]:

- The inverse problem has no solution if the modelling does not constrain parameters [changing data does not change parameters]
  - ... and yet some of us choose χ^2-minimising!!
- Unfortunately, the χ^2 usually "works perfectly well" $\longrightarrow$

Here we arrive at the 'dramatic consequences' [largely unknown, or deliberately ignored, or both]:

- The inverse problem has no solution if the modelling does not constrain parameters [changing data does not change parameters]
- ... and yet some of us choose χ^2-minimising!!
- Unfortunately, the χ^2 usually "works perfectly well" $\longrightarrow$
- Some curves are generated,

they may even go through experimental data... ["good r.m.s."]

Here we arrive at the 'dramatic consequences' [largely unknown, or deliberately ignored, or both]:

- The inverse problem has no solution if the modelling does not constrain parameters [changing data does not change parameters]
- ... and yet some of us choose χ^2-minimising!!
- Unfortunately, the χ^2 usually "works perfectly well" $\longrightarrow$
- Some curves are generated, they may even go through experimental data... ["good r.m.s."]
- ... but these results have neither mathematical nor not much of the physical significance...

Here we arrive at the 'dramatic consequences' [largely unknown, or deliberately ignored, or both]:

- The inverse problem has no solution if the modelling does not constrain parameters [changing data does not change parameters]
- ... and yet some of us choose χ^2-minimising!!
- Unfortunately, the χ^2 usually "works perfectly well" $\longrightarrow$
- Some curves are generated, they may even go through experimental data... ["good r.m.s."]
- ... but these results have neither mathematical nor not much of the physical significance...

... and even less of prediction capacities!

Here we arrive at the 'dramatic consequences' [largely unknown, or deliberately ignored, or both]:

- The inverse problem has no solution if the modelling does not constrain parameters [changing data does not change parameters]
- ... and yet some of us choose χ^2-minimising!!
- Unfortunately, the χ^2 usually "works perfectly well" $\longrightarrow$
- Some curves are generated, they may even go through experimental data... ["good r.m.s."]
- ... but these results have neither mathematical nor not much of the physical significance...

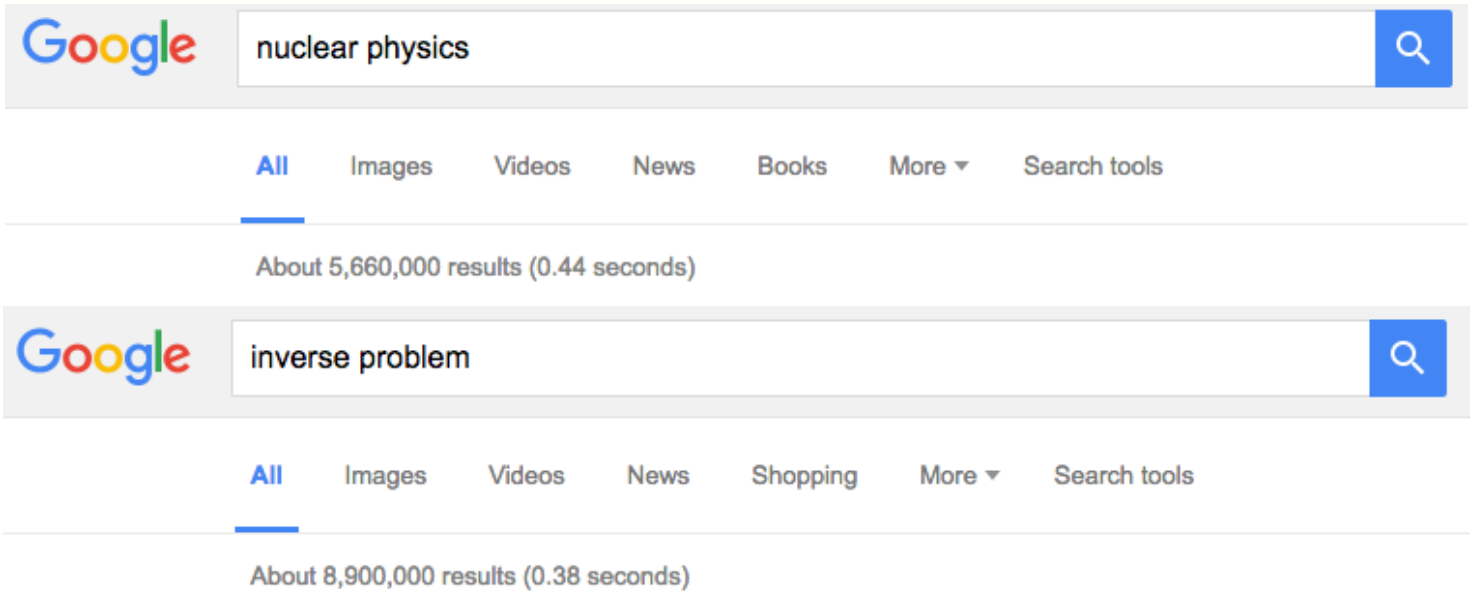
... and even less of prediction capacities! **And yet: All that is perfectly known in the textbooks as the next page shows !**

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

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

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

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



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

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

• 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" [i.e. - what is meant is: "they" obtain a 'meanigless result']

ANNEX IV

A powerful tool in parametric correlation removal: Singular Value Decomposition

A Powerful Tool: Singular-Value Decomposition

A Powerful Tool: Singular-Value Decomposition

• The problems with instabilities (i.e. ill-conditioning) can be easily illustrated using the so-called Singular-Value Decomposition of A:

$$\boldsymbol{A = U \cdot D \cdot V^T} \text{ with } \boldsymbol{U} \in \mathbb{R}^{\boldsymbol{m \times m}}, \quad \boldsymbol{V} \in \mathbb{R}^{\boldsymbol{n \times n}}, \quad \boldsymbol{D} \in \mathbb{R}^{\boldsymbol{m \times n}}$$

where diagonal matrix has a form $D = \mathrm{diag}\{\underbrace{d_1, d_2, \ \ldots \ d_{min(m,n)}}_{\text{decreasing order}}\}$

A Powerful Tool: Singular-Value Decomposition

• The problems with instabilities (i.e. ill-conditioning) can be easily illustrated using the so-called Singular-Value Decomposition of A:

$$\boxed{\boldsymbol{A = U \cdot D \cdot V^T} \text{ with } \boldsymbol{U} \in \mathbb{R}^{\boldsymbol{m \times m}},\ \ \boldsymbol{V} \in \mathbb{R}^{\boldsymbol{n \times n}},\ \ \boldsymbol{D} \in \mathbb{R}^{\boldsymbol{m \times n}}}$$

where diagonal matrix has a form $D = \mathrm{diag}\{\underbrace{d_1, d_2, \ \ldots\ d_{min(m,n)}}_{\text{decreasing order}}\}$

• Formally (but also in practice), the solution 'x' is expressed as

$$\boxed{\boldsymbol{x = A^T b;\ \ A^T = V \cdot D^T \cdot U^T}}$$

where

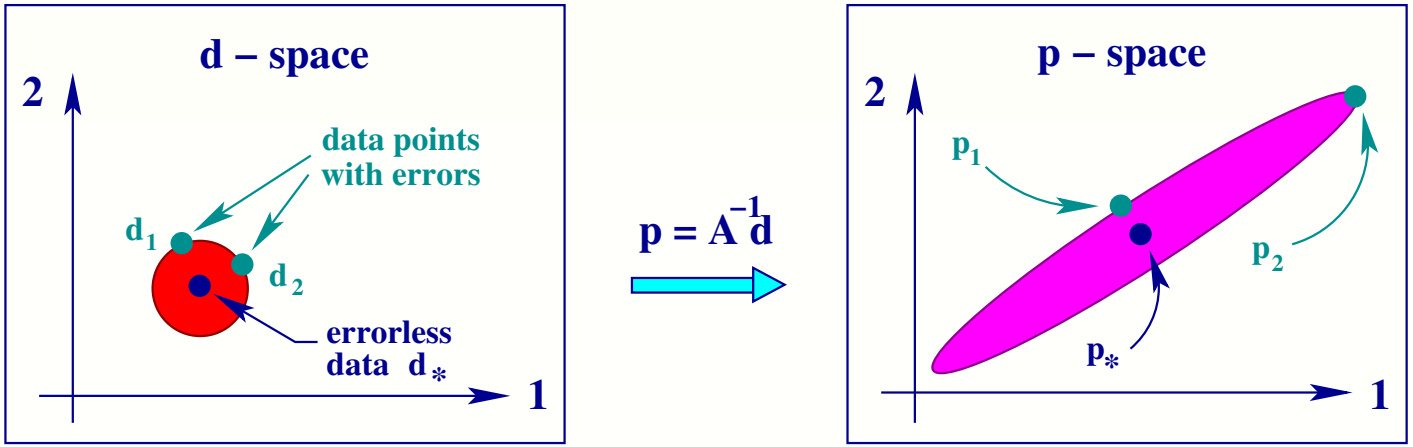
$$\boldsymbol{D^T = \mathrm{diag}\left\{\frac{1}{d_1}, \frac{1}{d_2}, \ \ldots\ \frac{1}{d_p}; 0, 0, \ \ldots\ 0\right\}}$$

Ill-Conditioned Problems: Qualitative Illustration

• An academic 2×2 problem: Suppose 'A' has eigenvalues which differ by a factor of 10 what represents correlations. One can show that solving the inverse problem will lead to result illustrated below

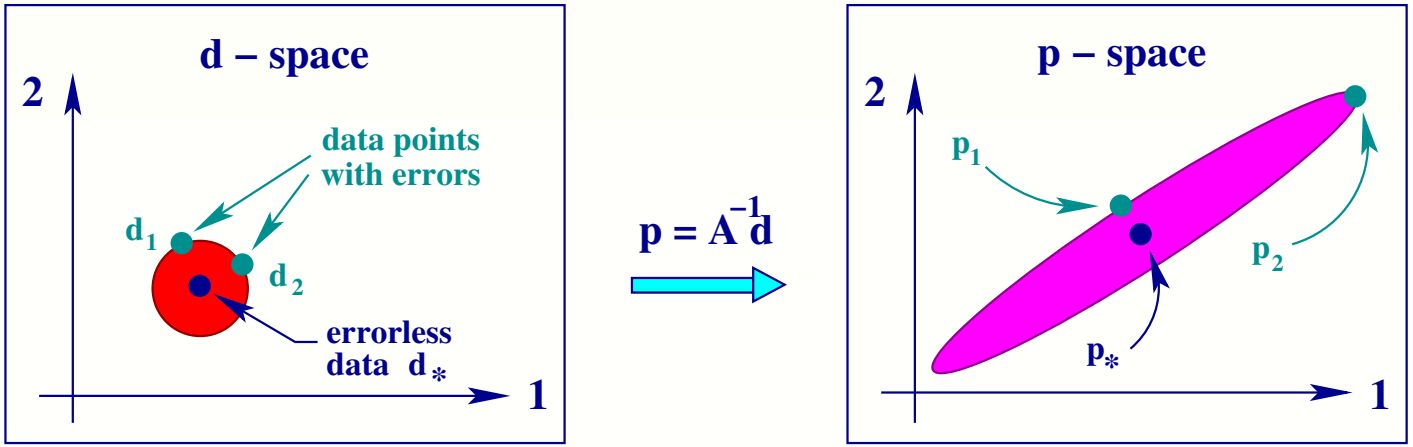
Ill-Conditioned Problems: Qualitative Illustration

• An academic 2×2 problem: Suppose 'A' has eigenvalues which differ by a factor of 10 what represents correlations. One can show that solving the inverse problem will lead to result illustrated below



Ill-Conditioned Problems: Qualitative Illustration

• An academic 2×2 problem: Suppose 'A' has eigenvalues which differ by a factor of 10 what represents correlations. One can show that solving the inverse problem will lead to result illustrated below



Left: Red circle represents points equally distant from 'noiseless' data d_*. Right: Purple oval represents the image of the circle through $p{=}A^{-1}d$. One shows that the bigger the disproportion between the eigen-values – the more 'ill-conditioned' the problem: Test with Monte-Carlo Methods→

Examples of Sampling

• We examine the predictive power capacities of the nuclear mean-field theory and its fundamental degrees of freedom: nucleon levels

• To simplify the task without loosing any conceptual liberty we limit our considerations to the 'doubly magic' spherical atomic nuclei:

^{16}O, ^{40}Ca, ^{48}Ca, ^{56}Ni, ^{90}Zr, ^{132}Sn, ^{146}Gd and ^{208}Pb

• If possible we wish to have a mean-field Hamiltonian H_{mf} capable of reproducing the single-particle level energies exactly, for purposes explained later

• The only simple Hamiltonian that we know of, which reproduces the single-particle spectra exactly, is the Woods-Saxon Hamiltonian

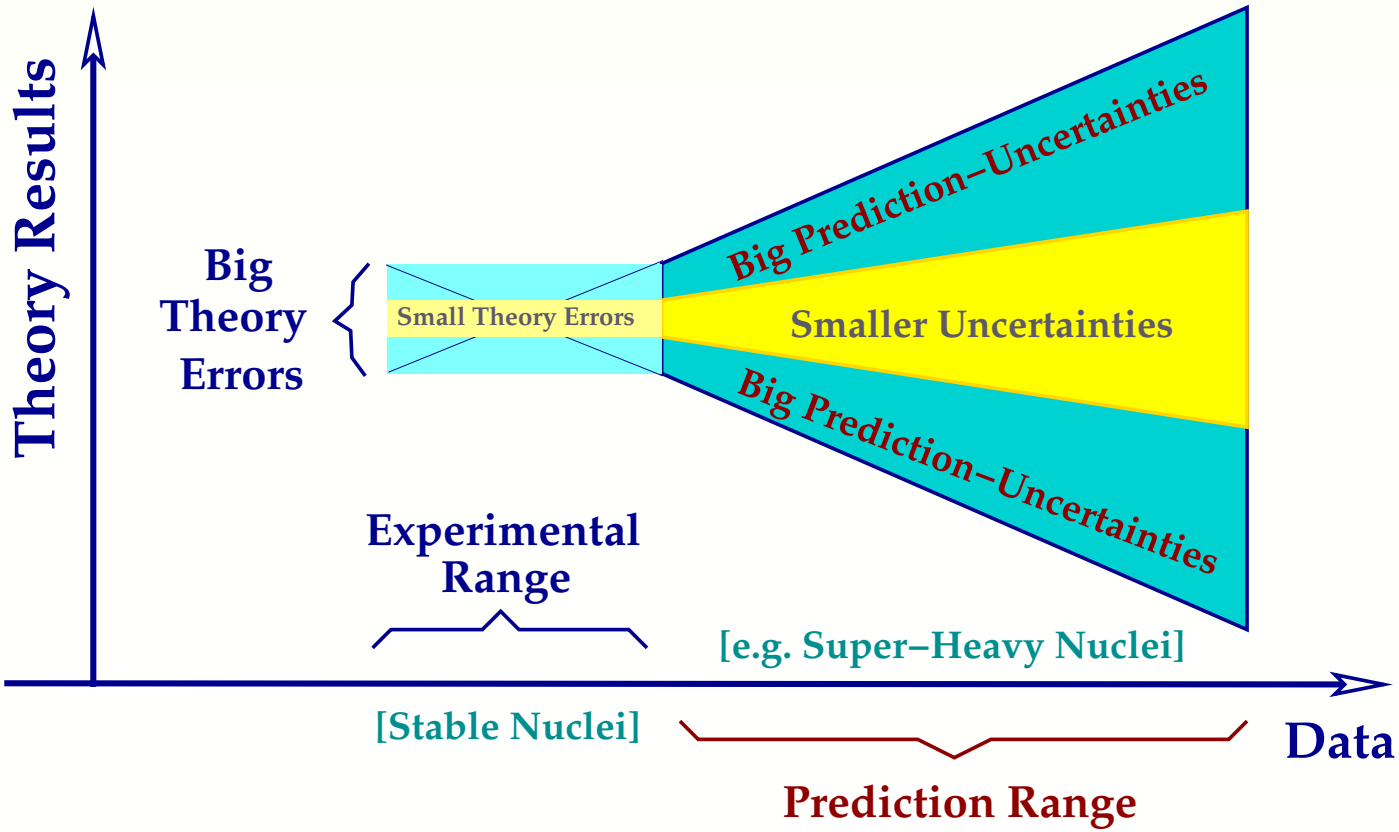
$$H_{mf}^{ws} = T + V_{cent}^{ws} + V_{so}^{ws}$$

• The Woods-Saxon mean-field has a certain elementary geometrical advantage - that is - clearly parametrised the roles of the size, depth and surface-diffuseness, according to 'broadly accepted intuition'

Uncertainties and their Propagation

• When predicting we have to be aware about Error Propagations and their increasingly important consequences for the predictions.

• Constraining theory errors may help stabilising theory predictions: The necessary but not sufficient condition of model's stability



Skyrme-HF in the EDF Formulation up to N^3LO

Skyrme-HF in the EDF Formulation up to N^3LO

- In a comprehensive study Carlsson, Dobaczewski and Kortelainen introduce Skyrme nuclear density functionals up to the sixth order (the standard Skyrme is of second order)

Skyrme-HF in the EDF Formulation up to N^3LO

- In a comprehensive study Carlsson, Dobaczewski and Kortelainen introduce Skyrme nuclear density functionals up to the sixth order (the standard Skyrme is of second order)

- Their total energy density contains all these rather than ∼15 terms

$$\mathcal{H}(\vec{r}) = \sum_{\substack{m'l',n'L'v'J' \\ ml,nLvJ,Q}} C^{m'l',n'L'v'J'}_{ml,nLvJ,Q} \times T^{m'l',n'L'v'J'}_{ml,nLvJ,Q}(\vec{r}),$$

where $C^{m'l',n'L'v'J'}_{ml,nLvJ,Q}$ are corresponding necessary coupling constants

Skyrme-HF in the EDF Formulation up to N^3LO

- In a comprehensive study Carlsson, Dobaczewski and Kortelainen introduce Skyrme nuclear density functionals up to the sixth order (the standard Skyrme is of second order)

- Their total energy density contains all these rather than ∼15 terms

$$\mathcal{H}(\vec{r}) = \sum_{\substack{m'l',n'L'v'J' \\ ml,nLvJ,Q}} C^{m'l',n'L'v'J'}_{ml,nLvJ,Q} \times T^{m'l',n'L'v'J'}_{ml,nLvJ,Q}(\vec{r}),$$

where $C^{m'l',n'L'v'J'}_{ml,nLvJ,Q}$ are corresponding necessary coupling constants

- It is instructive to think about the extentions of the EDF based approaches in terms of the increasing number of coupling constants

Skyrme-HF in the EDF Formulation up to N^3LO

- In a comprehensive study Carlsson, Dobaczewski and Kortelainen introduce Skyrme nuclear density functionals up to the sixth order (the standard Skyrme is of second order)

- Their total energy density contains all these rather than $\sim$15 terms

$$\mathcal{H}(\vec{r}) = \sum_{\substack{m'l',n'L'v'J' \\ ml,nLvJ,Q}} C^{m'l',n'L'v'J'}_{ml,nLvJ,Q} \times T^{m'l',n'L'v'J'}_{ml,nLvJ,Q}(\vec{r}),$$

where $C^{m'l',n'L'v'J'}_{ml,nLvJ,Q}$ are corresponding necessary coupling constants

- It is instructive to think about the extentions of the EDF based approaches in terms of the increasing number of coupling constants

- ... in view of all the couplings present already at the leading order formulations which suggest a totally ill-posed inverse problem $\rightarrow\rightarrow$

χ^2-Minimisation Options

• First of all, we want to find the optimal parameters that will describe the experimental single particle energies that we have considered.

• For that purpose we introduced to the program a minimisation algorithm (based on Levenberg-Marquardt algorithm) which minimises over the parameters of the Hamiltonian the distance between the experimental and the theoretical energies.

• In what follows we will highlight three important points of the construction of our code.

χ^2-Minimisation Options: Choice of Parameters

• We can choose over which and how many parameters we want to carry out the minimisation.

• For example, we may be interested on how the central parameters adapt themselves during the minimisation if we keep the spin-orbit parameters fixed, or vice-versa.

• This may be considered as a way of studying the parametric correlations. Namely, suppose we fix all the parameters and we minimise only over V_c. If then we increase the value of r_c by some factor F, and we minimise again and we see that V_c has changed also by more or less a factor F, we may start thinking that there may exist a liner correlation between them...

χ^2-Minimisation Options: Choice of Quantities

• We can take into account other quantities a part from the single particle energies in our χ^2.

• For instance, we can also add: nuclear radii, nuclear densities, Fermi energy and gap energy.

• This is a very important option because when adding a new quantity we are constraining more our problem and so we can use (if we want) all the information that we know coming from the experiment.

χ^2-Minimisation Options: Choice of Nuclei

• We can also choose from how many and which nuclei we use the information for the parametric optimisation.

• For instance, we can do the calculation considering only the information about one nucleus, or using a pair of them, or three, or all the eight at the same time... We have 255 combinations!

• Again, this serves us to constrain more the problem and to see how the parameters vary in the different cases, and so the predictions. *How well or bad the light nuclei can predict the heavy ones?*

• Moreover, if we consider all the 8 nuclei at the same time, we may hope to find a new "Universal Parametrisation" valid for all the nuclei and we can compare the results obtained with the already existing Universal Parametrisation

Programming Parametric Correlations

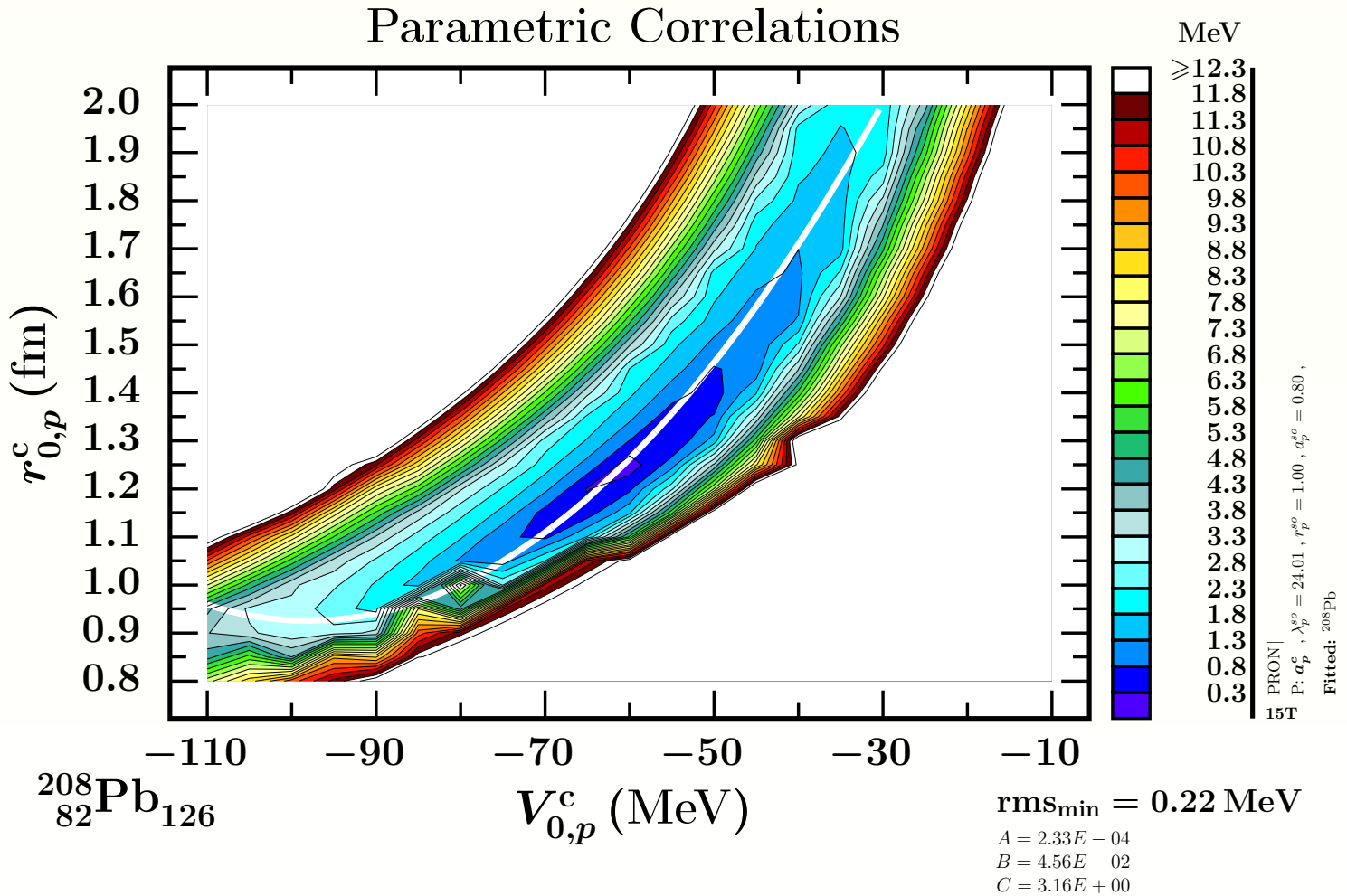
• Once we had the first contact with the results and the predictive power, we were interested in studying the parametric correlations.

• For that, we introduced another option to the program. That was the possibility of tabulating two parameters (p_1, p_2) of the Hamiltonian and run the minimisation over the other parameters (or keep them fixed, remember that we can choose at each moment over what we want to minimise).

• For each combination of (p_1, p_2) we store the $r.m.s.$ value obtained, i.e. we obtain a matrix. At the end what we produce is a 2D plot where we can see the $r.m.s.$ as a function of p_1 and p_2.

• An example may help...

Programming Parametric Correlations - Examples



Parametric correlation between V_p^c and r_p^c in ^{208}Pb with the tendency curve