Nuclear Physics Hamiltonians and the Problem of Their Predictive Power

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[1] GOOGLE SEARCH — on Sunday, May 16, 2010, at 10:30 AM

"Nuclear Physics"	3 200 000 results (∼0.18 seconds)
"Inverse Problem"	510 000 results (∼0.36 seconds)

COLLABORATORS:

Bartłomiej SZPAK, IFJ Kraków
Marie-Geneviève PORQUET, CSNSM Orsay

Bogdan FORNAL, IFJ Kraków
Hervé MOLIQUE, DRS Strasbourg
Karolina RYBAK, DRS Strasbourg

In this presentation we use some material from the article:

Nuclear Hamiltonians: The Question of their Spectral Predictive Power and the Associated Inverse Problem

JD, B. Szpak, M-G, Porquet, H. Molique, K. Rybak & B. Fornal
J. Phys. G: Nucl. Part. Phys. **37** *(2010) 064031*

FOCUS Special Issue: Open problems in nuclear structure theory

... as well as some material from the articles:

2. Nuclear Mean Field Hamiltonians and Factors Limiting their Predictive Power: Formalism

JD, K. Rybak, B. Szpak, M-G, Porquet, H. Molique & B. Fornal
Int. J. Mod. Phys. E **19** *(2010) 652*

3. Nuclear Mean Field Hamiltonians and Factors Limiting their Predictive Power: Illustrations

B. Szpak, JD, K. Rybak, M-G, Porquet, H. Molique & B. Fornal
Int. J. Mod. Phys. E **19** *(2010) 665*

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ANSWER: Yes, we always do when one of our friends
winns a bigger amount of money in a poker game...

This and the following presentation are about:

How to help our 100 theorists to arrive at close-lying results

Part I

Nuclear Hamiltonians from the Predictive-Power Perspective

About this Particular Project: What? and Why?

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Conclusion 2: The desired truth remains unknown to us $\longrightarrow$ lack of knowledge $\longrightarrow$ ignorance imposed[#)] by nature

[#)]**... and thus well excused - because not resulting from our lazyness**

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Find <u>relative</u> probability of what we think the right answer is!

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Conclusion: We need to introduce probabilities of ignorance!

Combining the Theoretical and the Experimental Errors

A Few Comments about the Nature of Errors

- Theories are incomplete whereas experiments plagued with errors:

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

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- Errors propagate to the theory predictions through parameter fits

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

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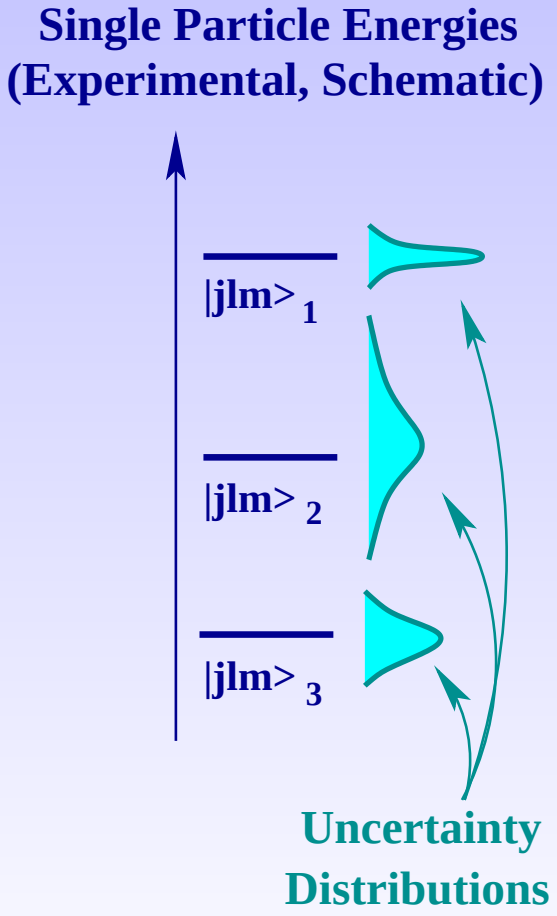
- The final theory predictions will depend on the convolution

$$\mathbf{P^{pred.}(p) = \{P^{th}(e) \; * \; P^{exp}(\varepsilon)\}}$$

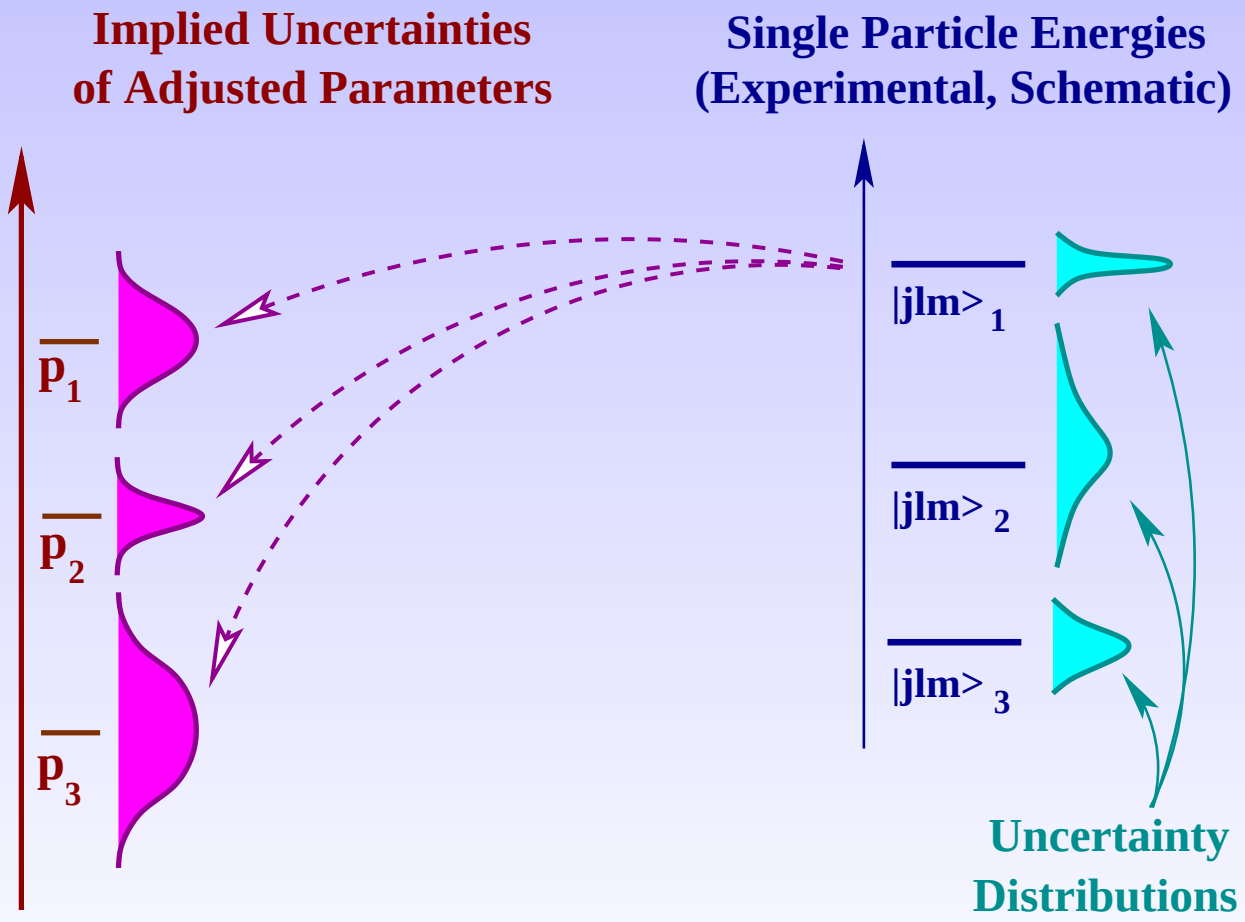
Single-Particle Levels as Probability Distributions

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



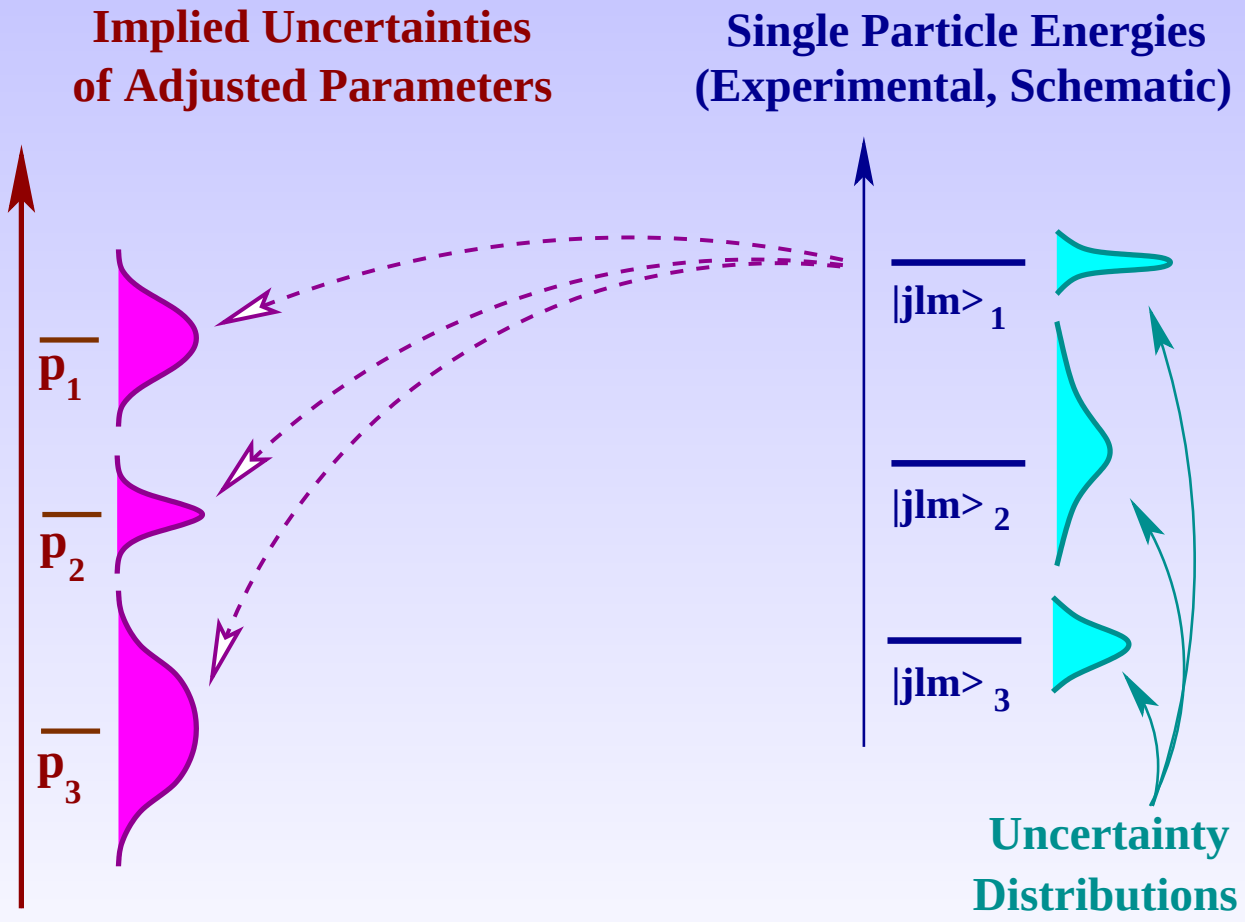
Single-Particle Levels as Probability Distributions

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



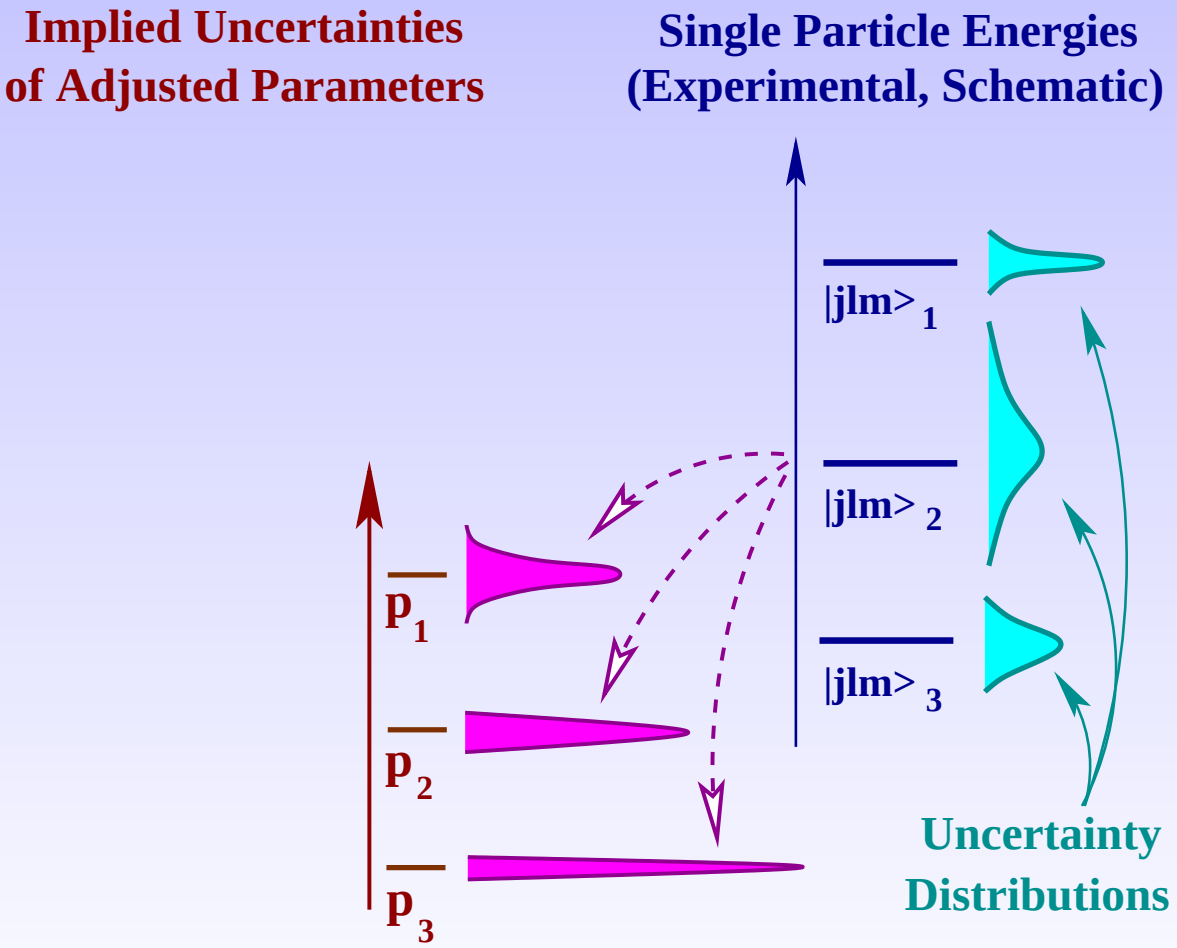
Single-Particle Levels as Probability Distributions

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



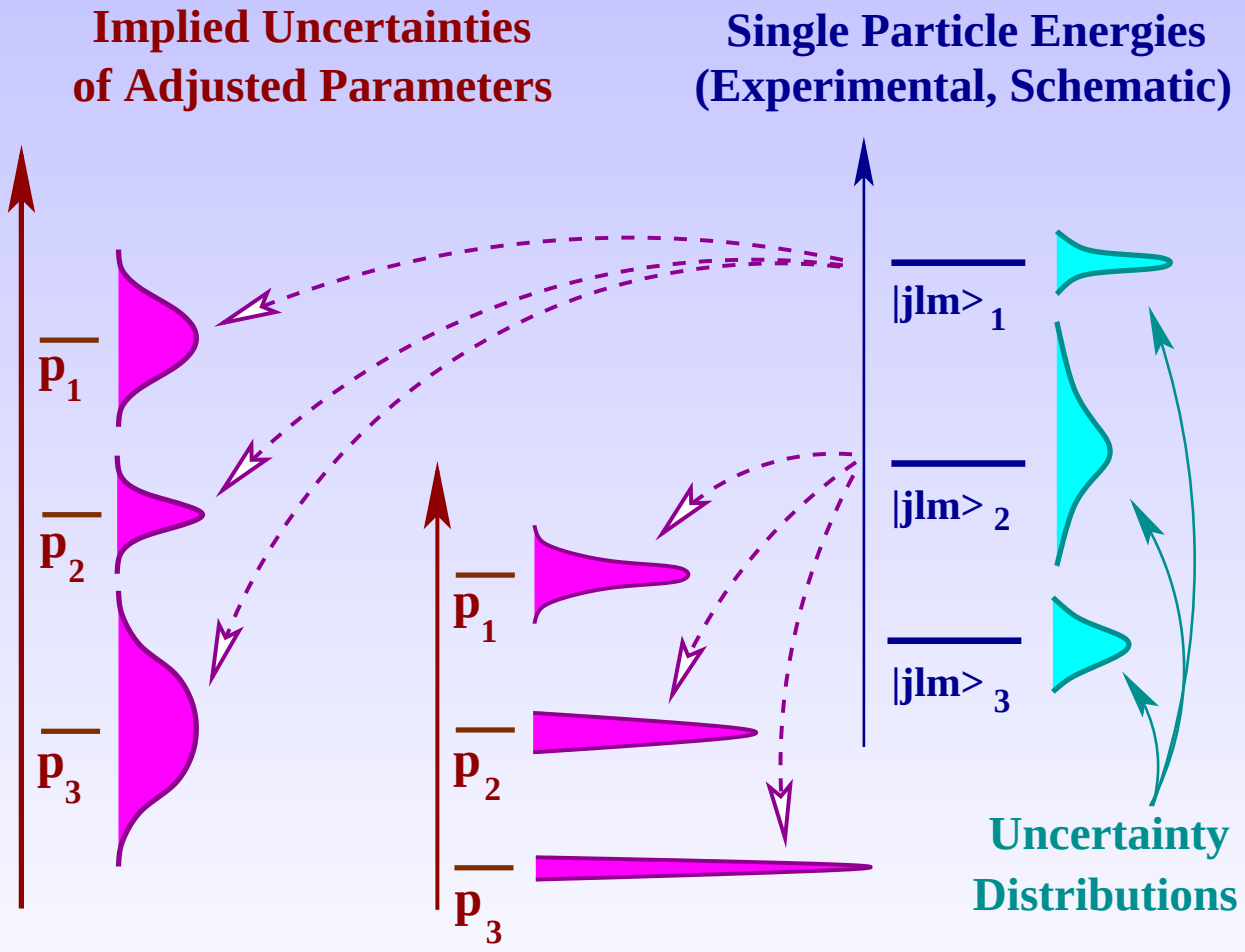
Single-Particle Levels as Probability Distributions

... while at the same time big uncertainties on other levels have a small impact: as in life, all are equal but some more than the others



Single-Particle Levels as Probability Distributions

Conclusion: the quality of adjustement depends strongly on the quality of the data implying the existence of theoretical error bars



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permit

Inverse Problem and Predictive Power: ^{132}Sn

Neutron levels around N=82					
Level	States in ^{133}Sn				
	e_1^{exc}	shift 1$^{(a)}$	shift 2$^{(b)}$	$\bar{\varepsilon}$	B. E.
$\nu f_{7/2}$	0.0000	0.2	0.6(4)	0.6(4)	-1.9(4)
$\nu p_{3/2}$	(0.8537)	-	-	-	-
$\nu h_{9/2}$	1.5609	0.1	0.6(5)	2.2(5)	-0.3(5)
$\nu p_{1/2}$	(1.6557)	-	-	-	-
Level	States in ^{131}Sn				
	e_1^{exc}	shift 1$^{(a)}$	shift 2$^{(b)}$	$\bar{\varepsilon}$	B. E.
$\nu d_{3/2}$	0.0000	0.25	0.6(4)	0.6(4)	-7.9(4)
$\nu h_{11/2}$	0.0651	0.3	0.6(3)	0.7(3)	-8.0(3)
$\nu s_{1/2}$	0.3317	0.25	0.6(4)	0.9(4)	-8.2(4)
$\nu d_{5/2}$	1.6545	-	0.6(4)	2.3(4)	-9.6(4)
$\nu g_{7/2}$	2.4341	-	0.6(4)	3.0(4)	-10.3(4)

$^{(a)}$ *Shifts in energy from level fragmentation measured in neighbouring nuclei.*
$^{(b)}$ *The values obtained through analogy by extrapolating from the data on ^{208}Pb.*
The numbers in parentheses give errors in the last digit.

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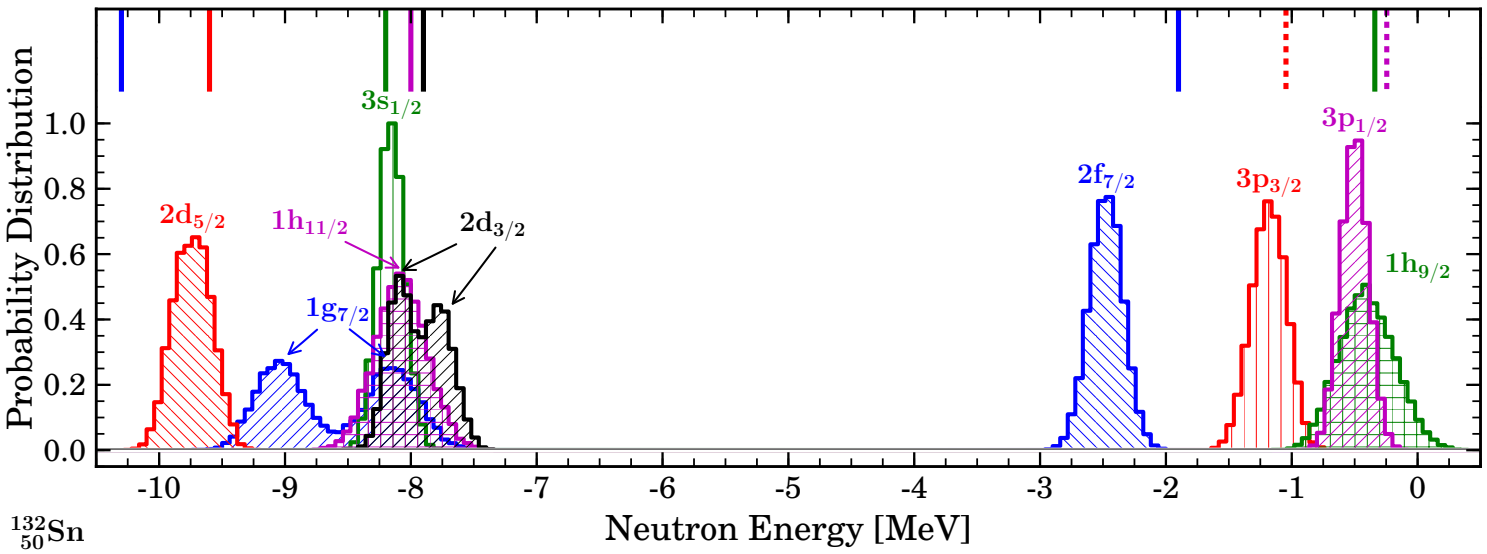

Results of the extrapolation from the ^{208}Pb to the ^{132}Sn nucleus for the neutrons, bars - cf. preceding table. Monte-Carlo simulation with N=20 000 Gaussian-distributed parameter sets, based on ^{208}Pb results; noise width σ=0.1MeV. With each of the so obtained N=20 000 sets of parameters the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

Applied Mathematics: About Inference & Inverse Problems

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THE PREDICTIVE POWER

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• Statistically sound $\Leftrightarrow$ Instead of saying: $e_{g_{9/2}} = -8.8$ MeV we better provide also the probability function $P = P(e_{g_{9/2}})$

Simple Mathematics of the Nonlinear Inverse Problem

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- Consider an example of a spherical mean-field Hamiltonian:

$$\boxed{\mathbf{H_{mf}} = \mathbf{H_{mf}}(\hat{\mathbf{r}}, \hat{\mathbf{p}}, \hat{\mathbf{s}}; \{\mathbf{p}\}); \quad \{\mathbf{p}\} \longrightarrow \text{parameters}}$$

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- In looking for 'an as adequate approach as possible in a search for coupling constants' we need some guidelines. Our choice:

The mean-field Hamiltonian should first of all describe optimally the mean field degrees of freedom

$$\boxed{\{\varphi_\nu, \mathbf{e}_\nu\} \ \text{ in } \ \mathbf{H_{mf}}\varphi_\nu(\mathbf{r}, \{\mathbf{p}\}) = \mathbf{e}_\nu(\mathbf{p})\,\varphi_\nu(\mathbf{r}, \{\mathbf{p}\})}$$

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• In an Appendix we explain at length why not the nuclear masses...

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- Introduce linearisation procedure [after simplification $e_j^{th}(p) \rightarrow f_j$]

$$f_j(p) \approx f_j(p_0) + \sum_{i=1}^{n}\left(\frac{\partial f_j}{\partial p_i}\right)\Big|_{p=p_0}(p_i - p_{0,i})$$

$$J_{jk} \equiv \sqrt{W_j}\left(\frac{\partial f_j}{\partial p_k}\right)\Big|_{p=p_0} \quad \text{and} \quad b_j = \sqrt{W_j}\,[e_j^{exp} - f_j(p_0)]$$

$$\boxed{\chi^2(\mathbf{p}) = \frac{1}{\mathbf{m}-\mathbf{n}}\sum_{\mathbf{j}=1}^{\mathbf{m}}\left[\sum_{\mathbf{i}=1}^{\mathbf{n}} \mathbf{J_{ji}}\cdot(\mathbf{p_i} - \mathbf{p_{0,i}}) - \mathbf{b_j}\right]^2}$$

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$$\boxed{\{\mathbf{p}\} \leftrightarrow \mathbf{x} \leftrightarrow \text{'causes'} \text{ and } \{\mathbf{e}\} \leftrightarrow \mathbf{b} \leftrightarrow \text{'effects'} \leftrightarrow \mathbf{A} \cdot \mathbf{x} = \mathbf{b}}$$

From the measured effects represented by 'b' we extract information about the causes 'x' by inverting the matrix: $\mathbf{A} \longrightarrow \mathbf{x} = \mathbf{A}^{-1} \cdot \mathbf{b}$

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- Some mathematical details: $J \equiv A \in \mathbb{R}^{m \times n}$; $x \in \mathbb{R}^n$, and $b \in \mathbb{R}^m$

A Powerful Tool: Singular-Value Decomposition

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

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

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

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

where

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

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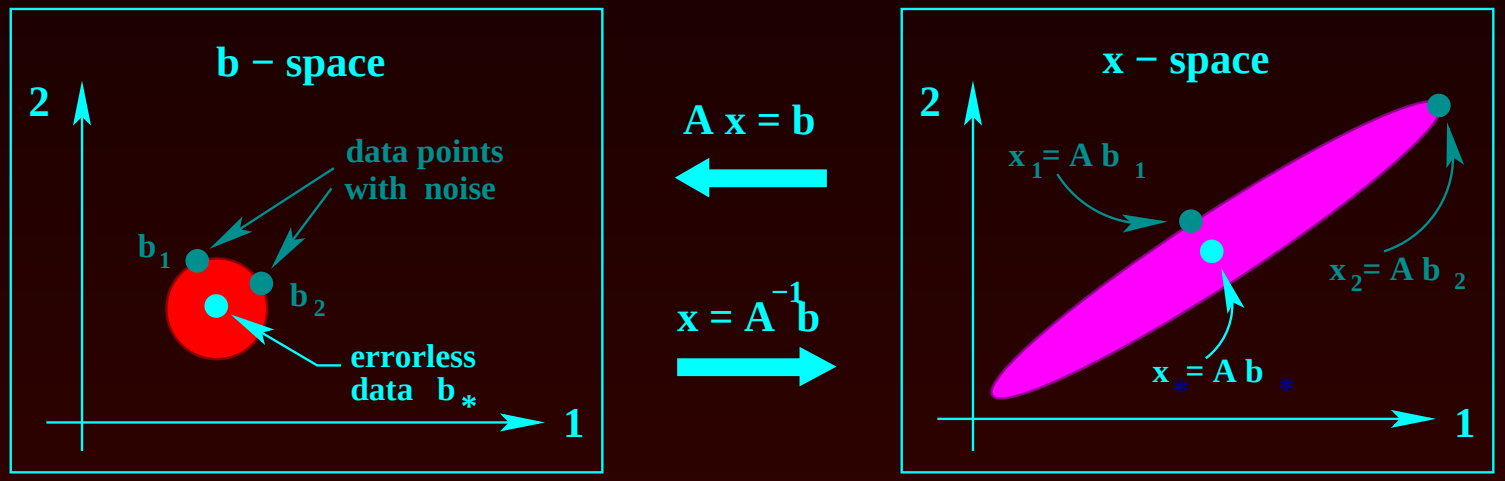
- Introduce errorless data (b_*) and uncertain (noisy) data: b_1 & b_2



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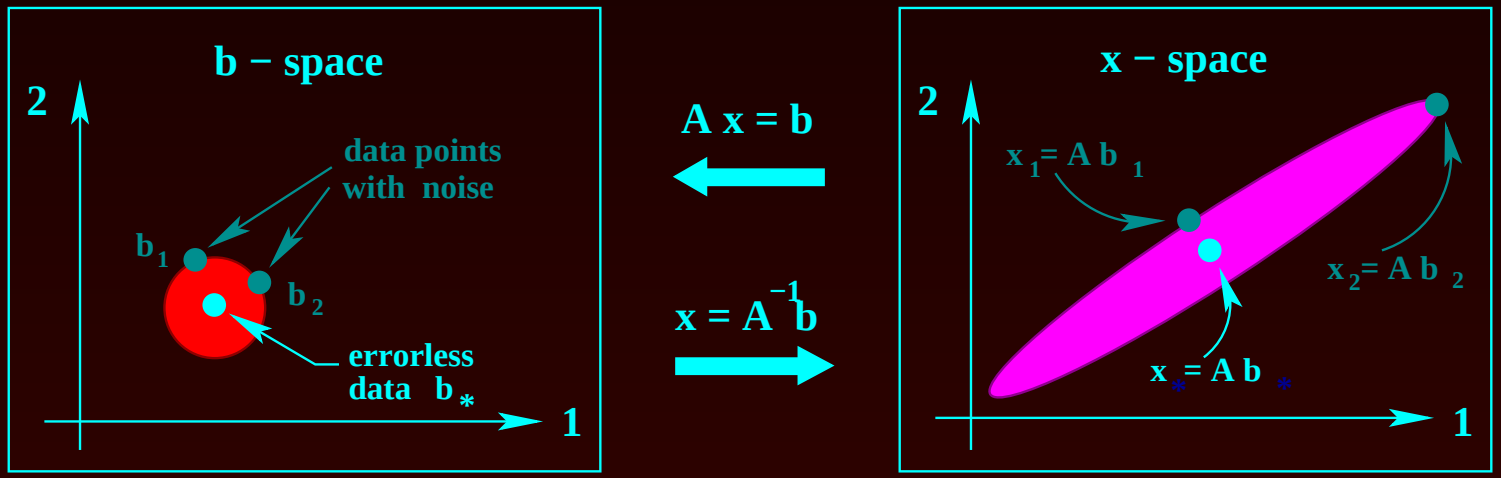

Left: Red circle represents points equally distant from 'noisless' data b_*. Right: Purple oval represents the image of the circle through $Ax=b$. One may show that instability is directly dependent on the condition number

$$\boxed{cond(A) \equiv \frac{d_1}{d_r}}$$

- the bigger the condition number the more 'ill-conditioned' the problem

Fitting, Implied Errors and Confidence Intervals

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$J_{ik} = \sum_{\ell=1}^{r} U_{i\ell}\, d_\ell\, V^T_{\ell k}$ one shows that $(J^T J)^{-1} = V \frac{1}{d^2} V^T$

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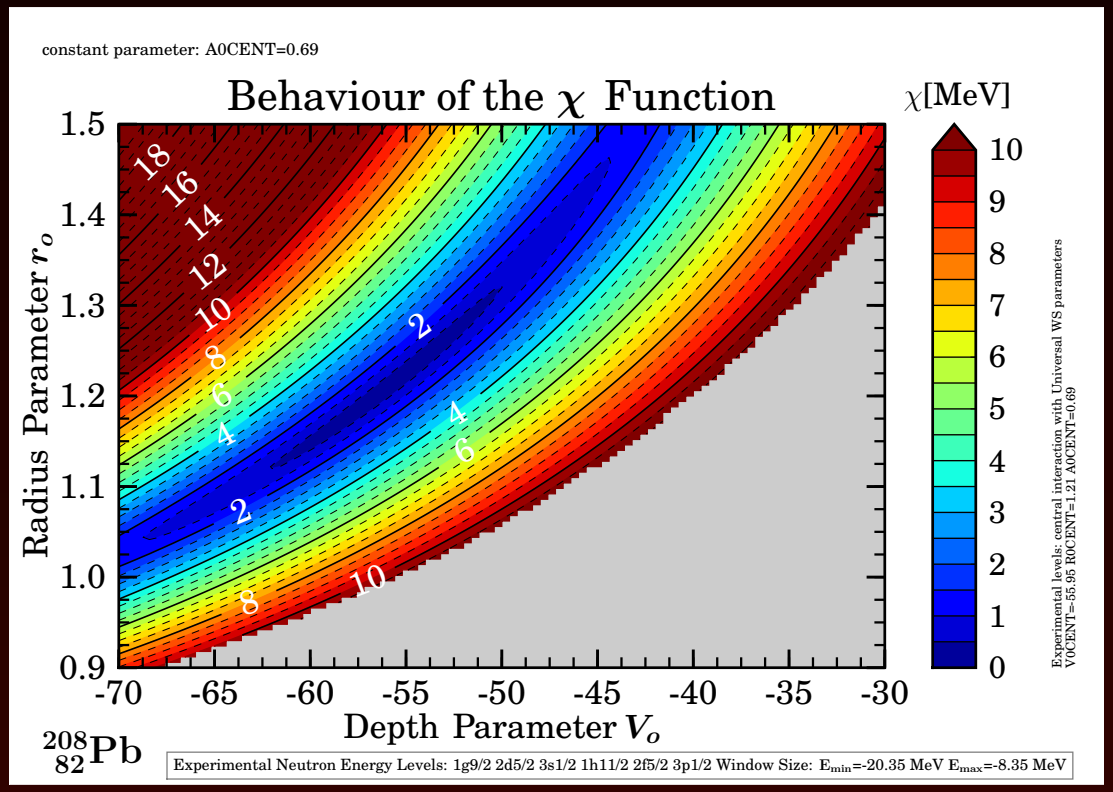
- **If one or more $d_k \longrightarrow 0$ then $(J^T J)^{-1}$ tends to infinity and generally, the <u>confidence intervals of all parameters diverge</u>**

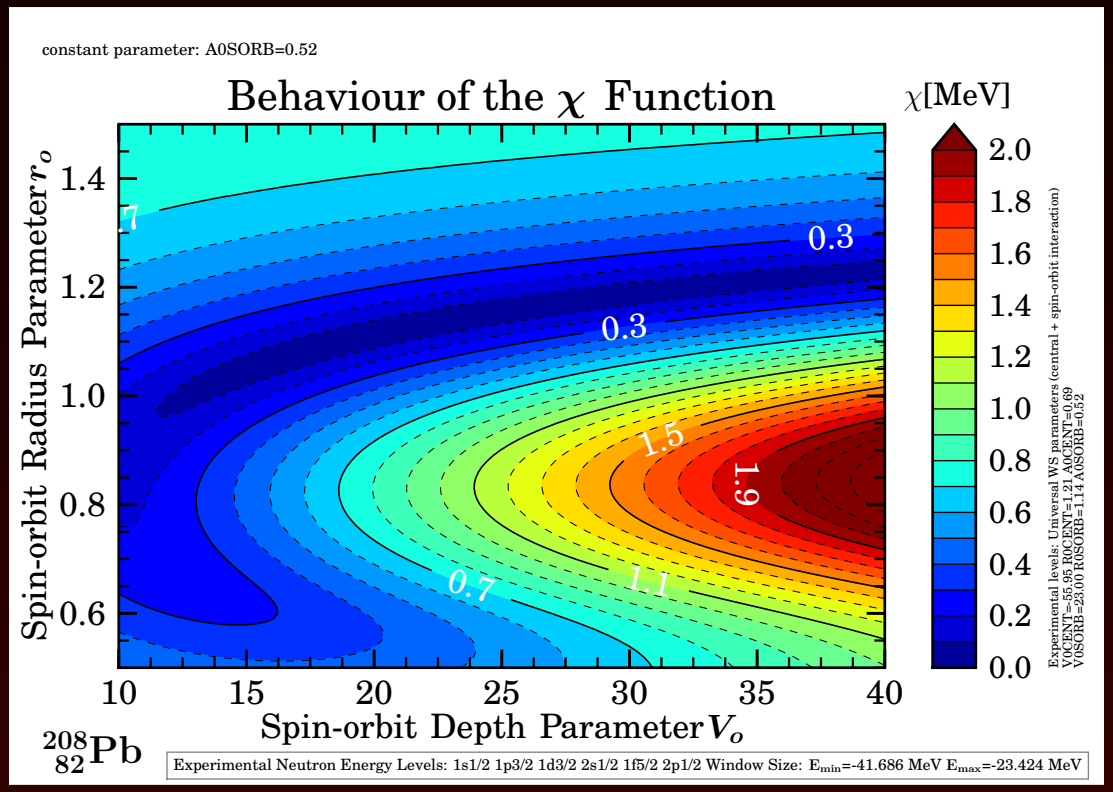
Undesired Parametric Correlations: Illustrative Examples

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.

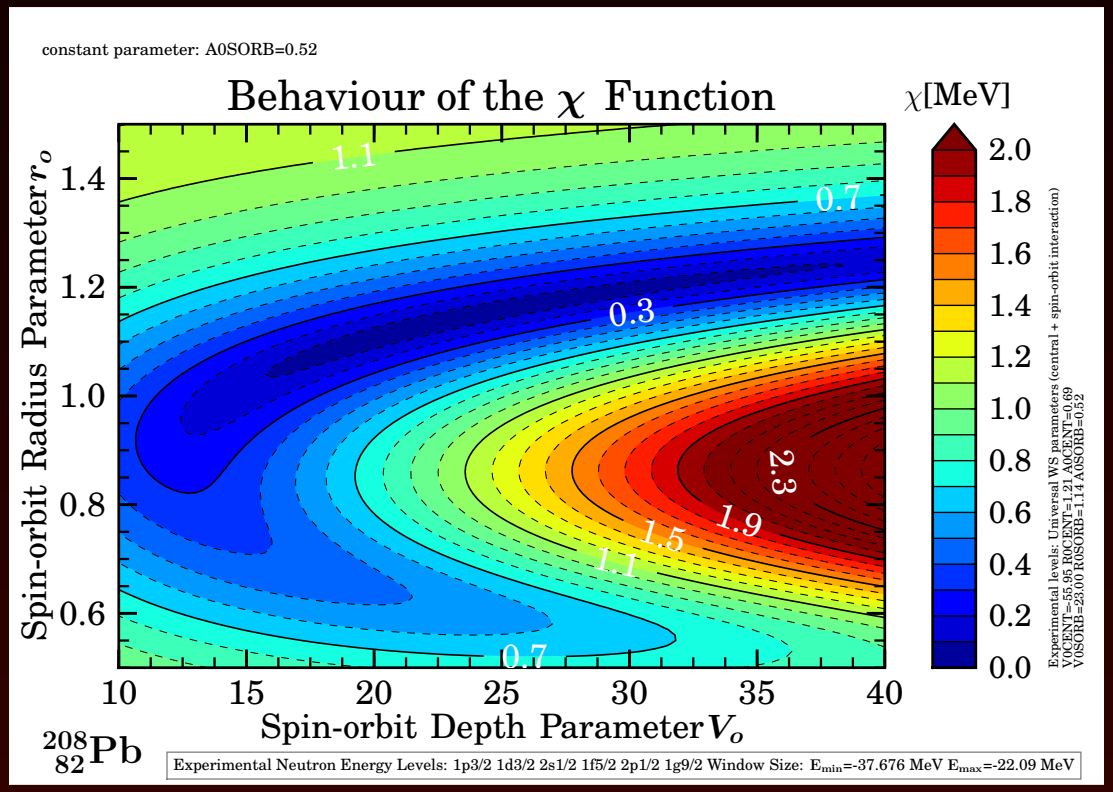
Parametric Correlations and Their Consequences



We plot the χ^2 in function of the S-O strength (horizontal) and the S-O radius (vertical) axis. We start with six very lowest levels. Note: 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 the energy of the six levels helps localising the spin-orbit strength only very slowly!

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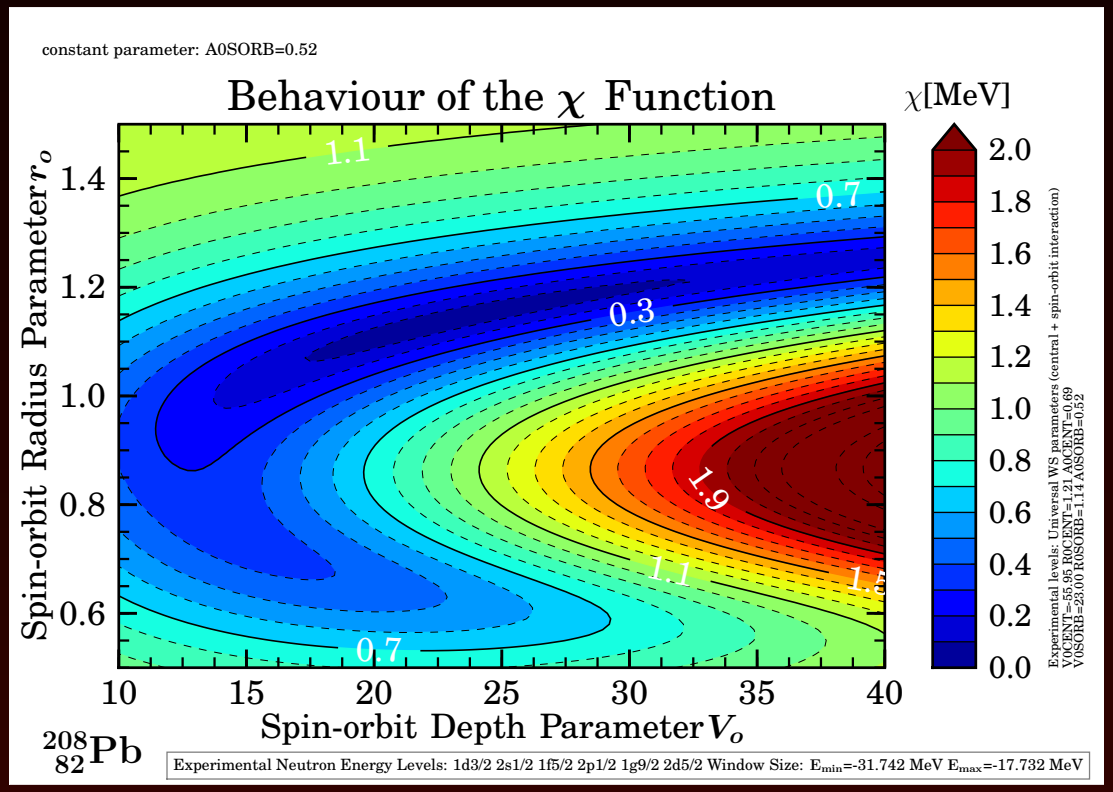

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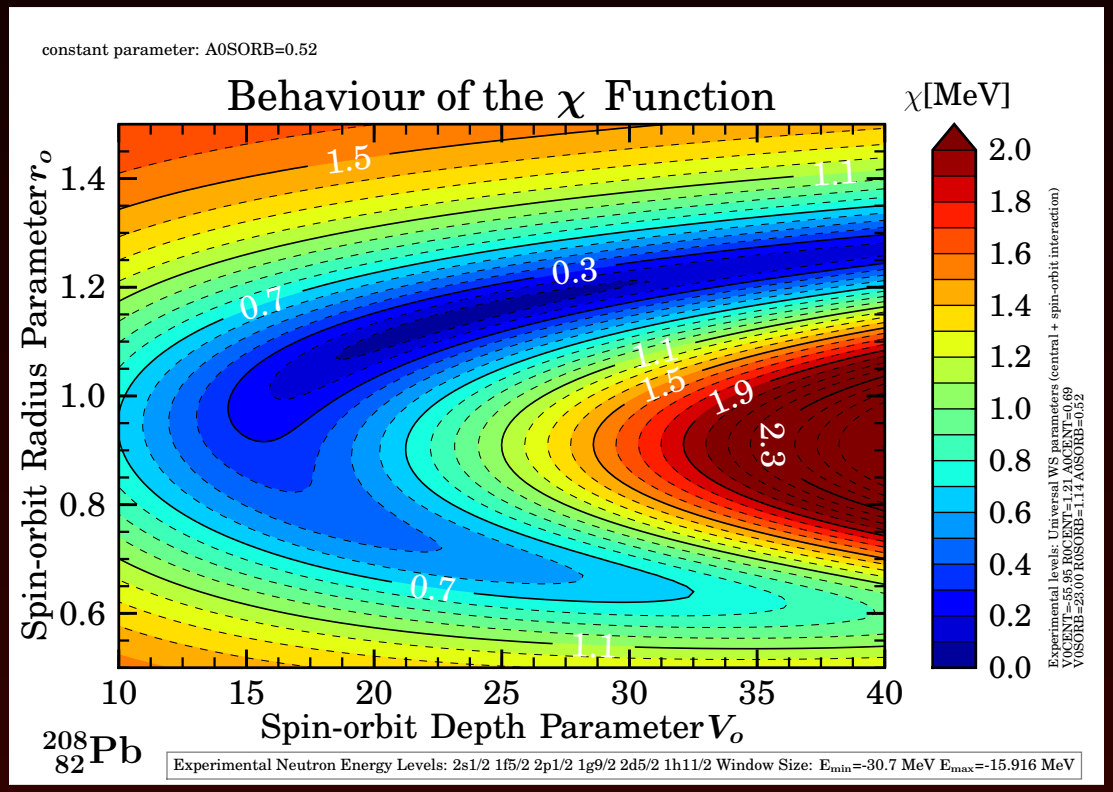

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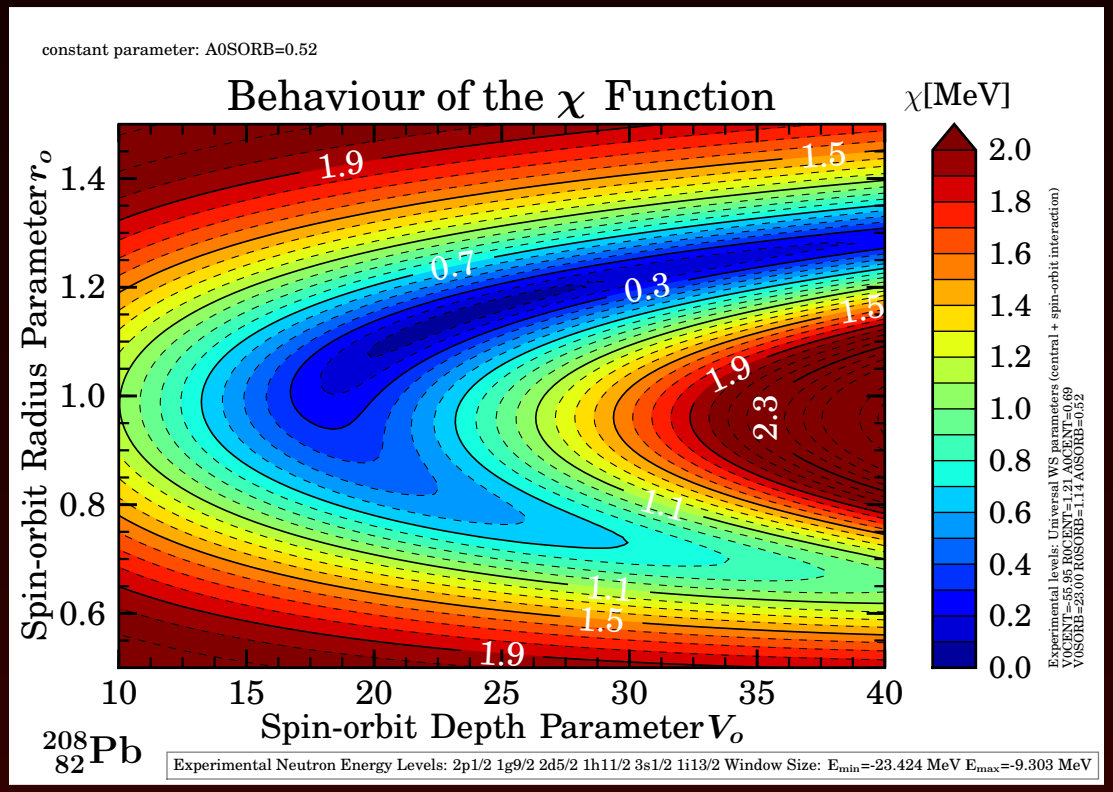

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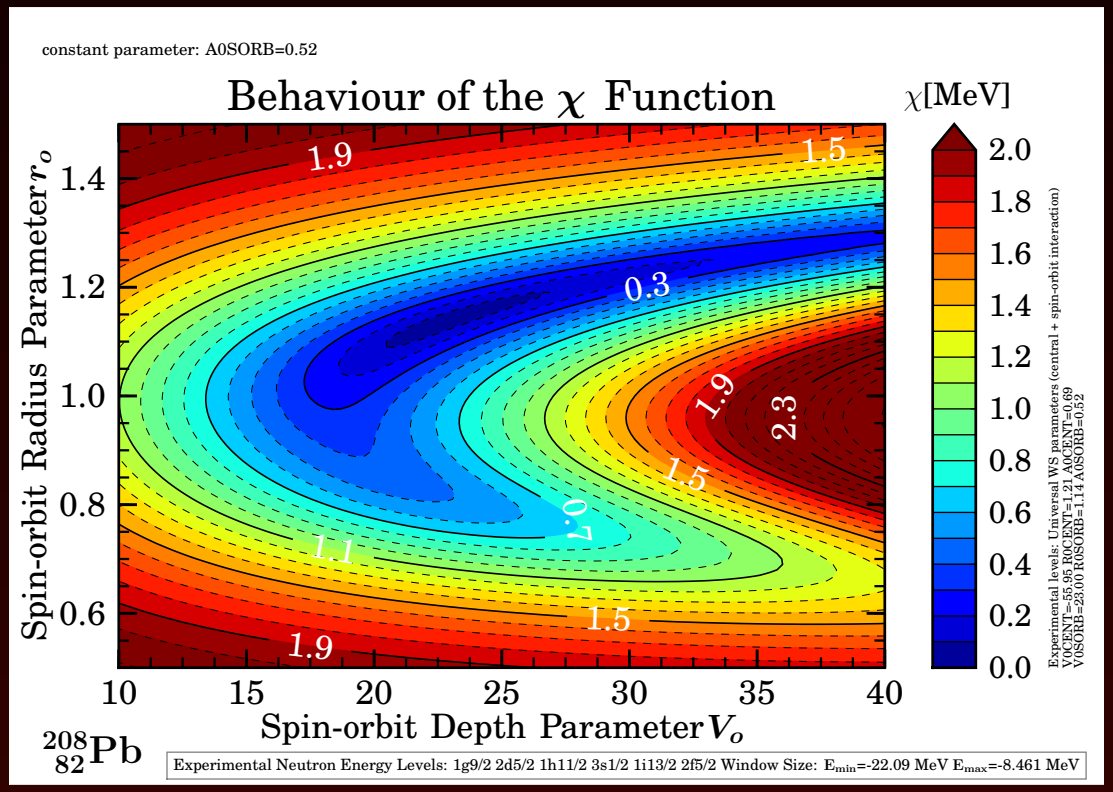

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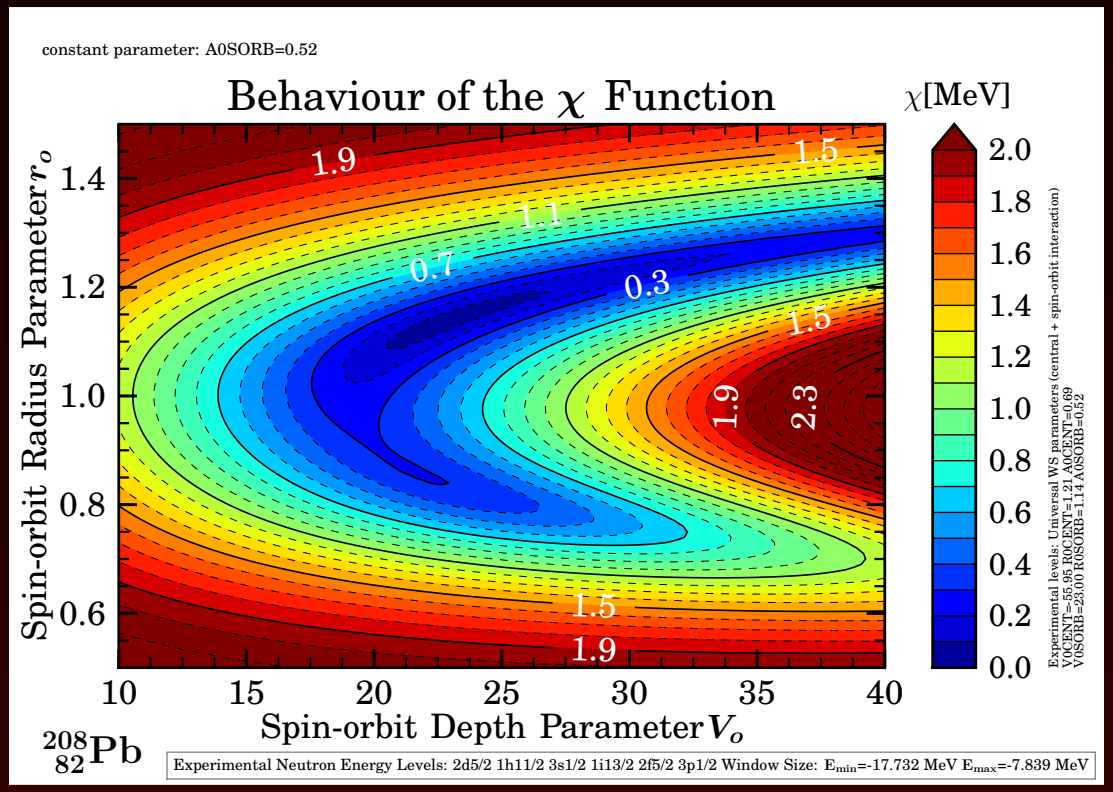

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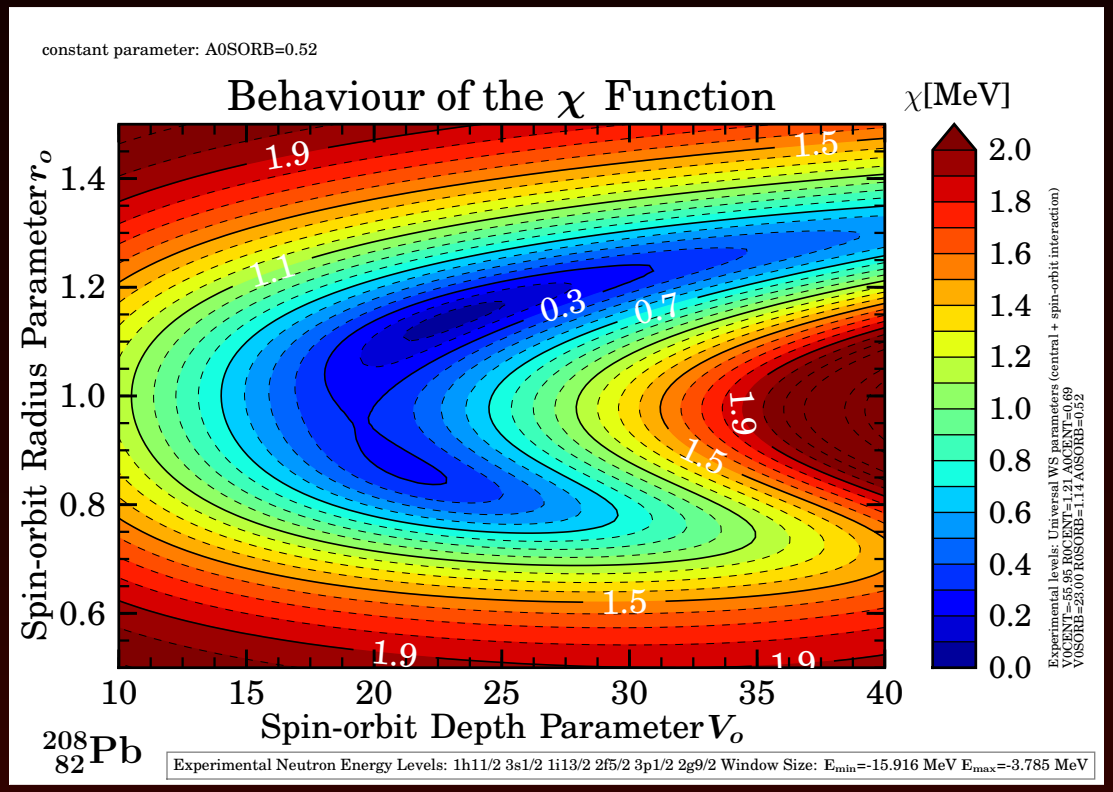

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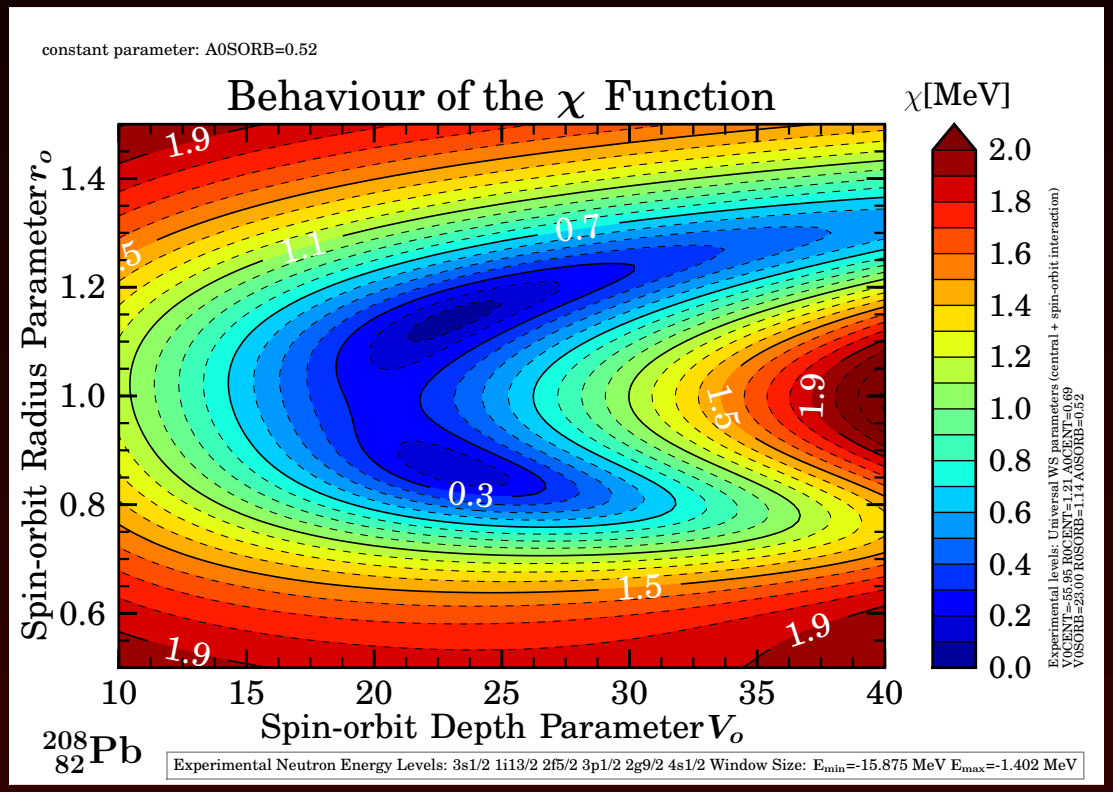

... and here we discover the existence of <u>two solutions</u> - we call them compact and non-compact.

What Can We Conclude from the This Set of Tests?

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

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

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

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On the Way to the Land-of-Meaningful-Probabilities

our brave saylors will see a lot of sharks and rocks

ILLUSTRATIONS

The Following Messages

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About Contemporary Skyrme-Type Functionals

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

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

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- **It is instructive to think about the extentions of the EDF based approaches in terms of increasing number of coupling constants and the preceding illustrations...**

About Contemporary Skyrme-Type Functionals

Numbers of terms of different orders in the EDF up to N^3LO. Numbers of terms depending on the time-even and time-odd densities are given separately. The last two columns give numbers of terms when the Galilean or gauge invariance is assumed, respectively. To take into account both isospin channels, the numbers of terms should be multiplied by a factor of two.

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

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

Theory Predictions and Their Statistical Significance

Consider a mean-field Hamiltonian: RMF, HF, Phenomenological ...

$$\boxed{\mathbf{H_{mf} = H_{mf}(\hat{r}, \hat{p}, \hat{s}; \{p\})}; \quad \{\mathbf{p}\} \longrightarrow \text{parameters}}$$

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After laborious constructions of H_{mf}, we often 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 chapter *'Modeling of Data'*, the authors of *'Numerical Recipes"* (p. 651), observe with sarcasme:

"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 ment is: "they" get a 'statistical nonsense']

A Realistic Toy Model - Noise-Simulation Example

- Let us calculate $\{e_\mu\}$-levels for a given W-S parameter set, here:

Woods-Saxon parameters for the neutrons in ^{208}Pb reproduce the experimental levels with the r.m.s. deviation of 0.164 MeV and maximum error of 0.353 MeV.

V_o^c	r_o^c	a_o^c	λ	r_o^{so}	a^{so}
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• We will obtain the response of all the levels to a 'linear noise' - vary a level position within a window and refit the H-parameters $\{p\}$

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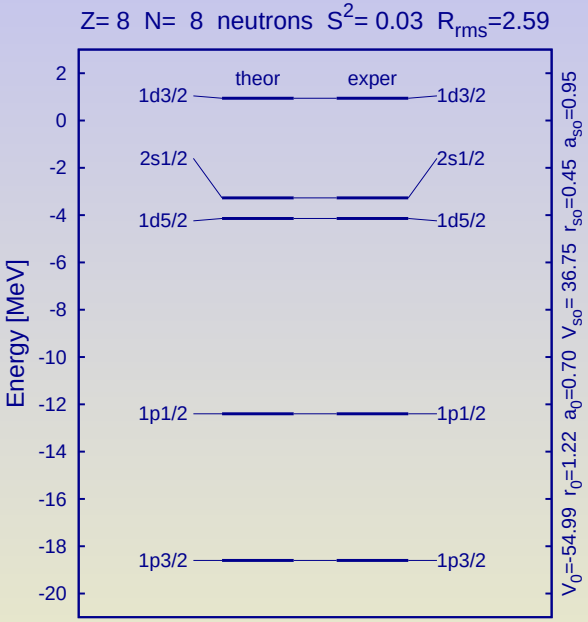
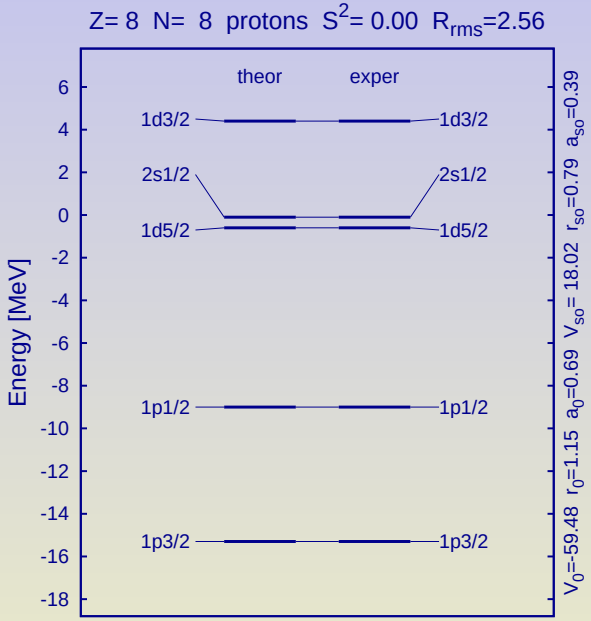
- We fit the single-particle experimental levels in ^{16}O using Woods-Saxon potential (six parameters for protons and neutrons each)





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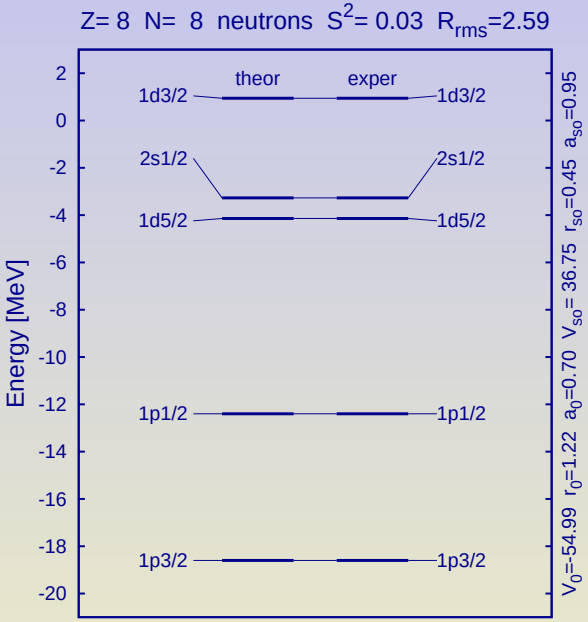

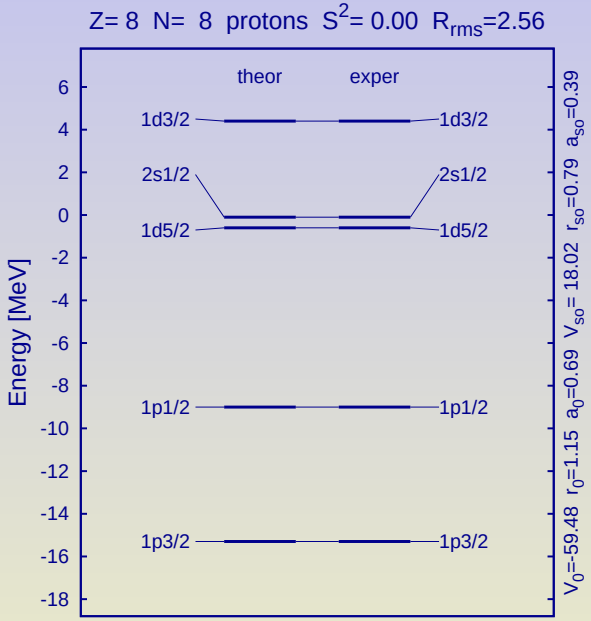

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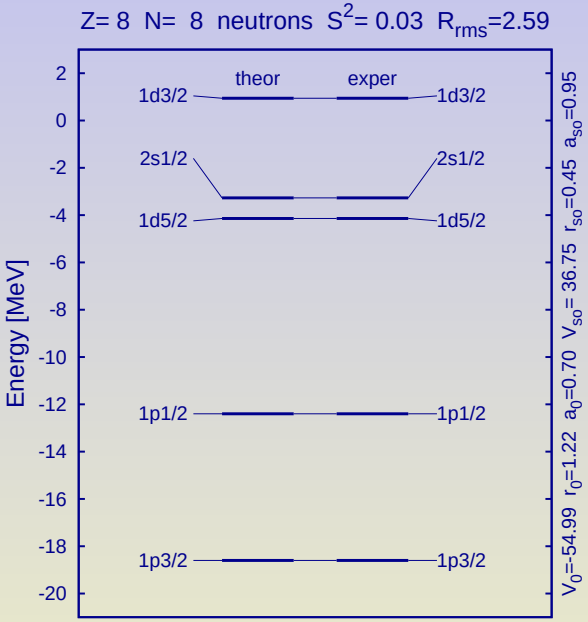

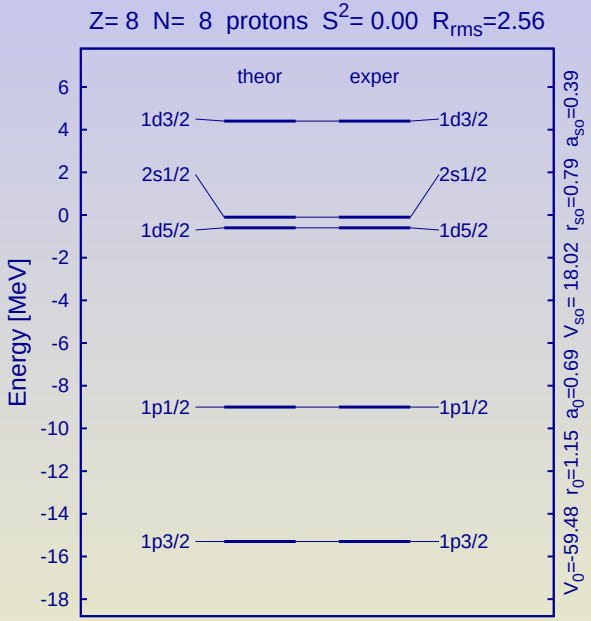

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• On the other hand: <u>If</u> we trust the model - we may hope that also the remaining levels are close to the experimental results to come

Unprecedented Precision of the Fits: 10^{-1} keV!

→ The standard Woods-Saxon Hamiltonian has been used:

No.	E_{calc}	E_{exp}	Level	Err.(th-exp)
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3.	-0.600	-0.600	$1d_{5/2}$	0.0000
4.	-0.100	-0.100	$2s_{1/2}$	0.0000
5.	4.400	4.400	$1d_{3/2}$	0.0001

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→ Couple of questions may come to one's mind...:

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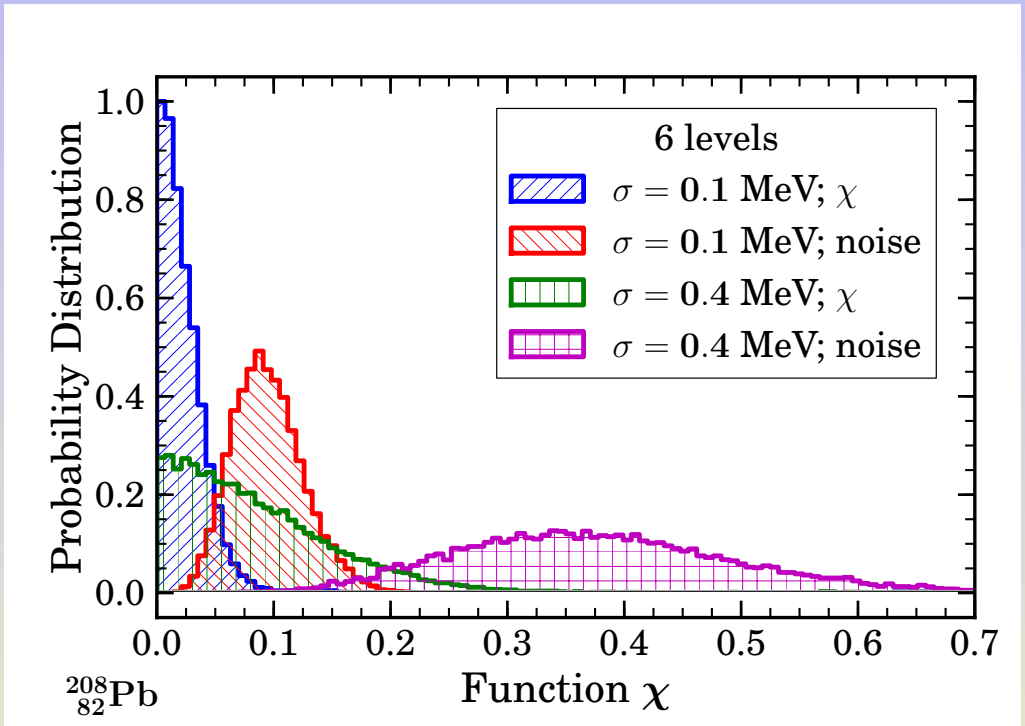
- *What is the mathematical/physical significance of the result?*

Unprecedented Precision ... Known as 'Overfitting'



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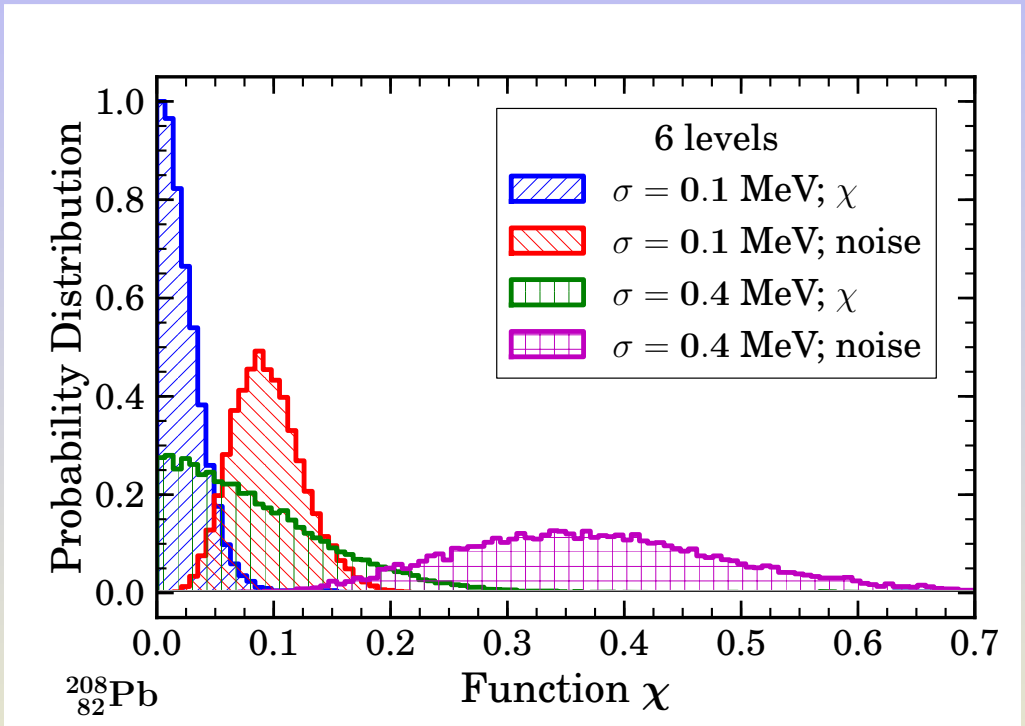

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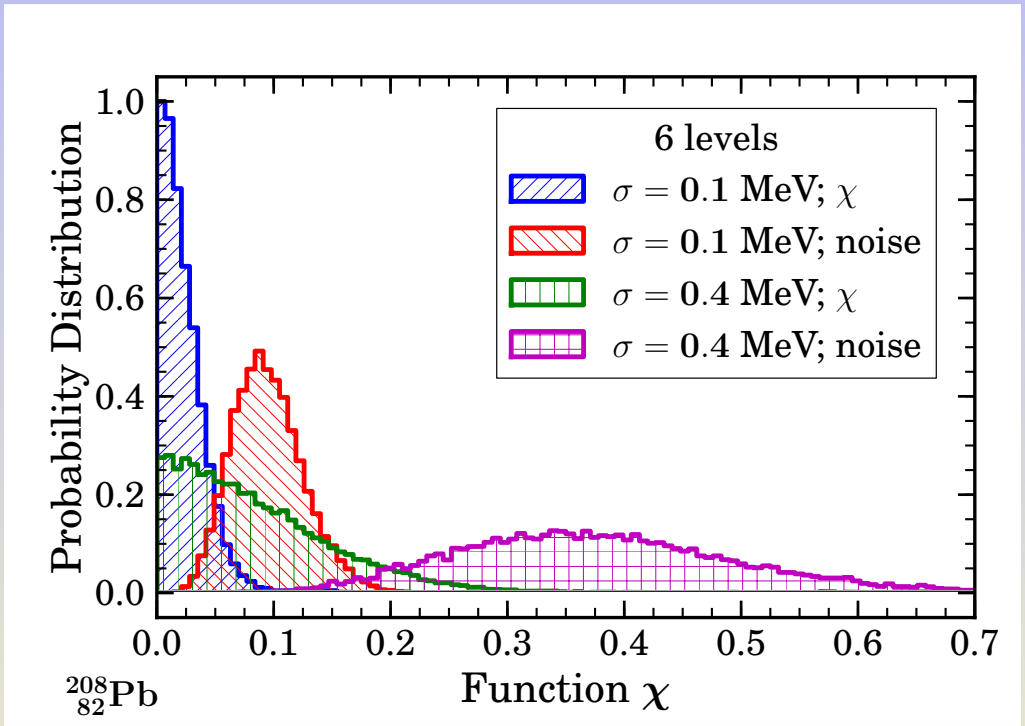

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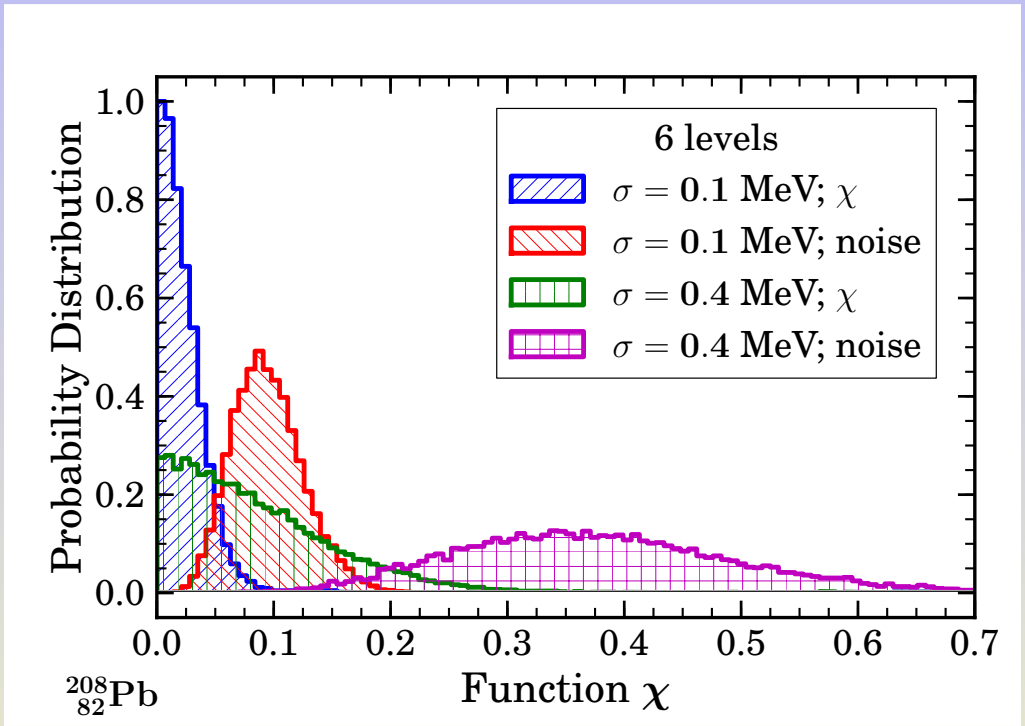

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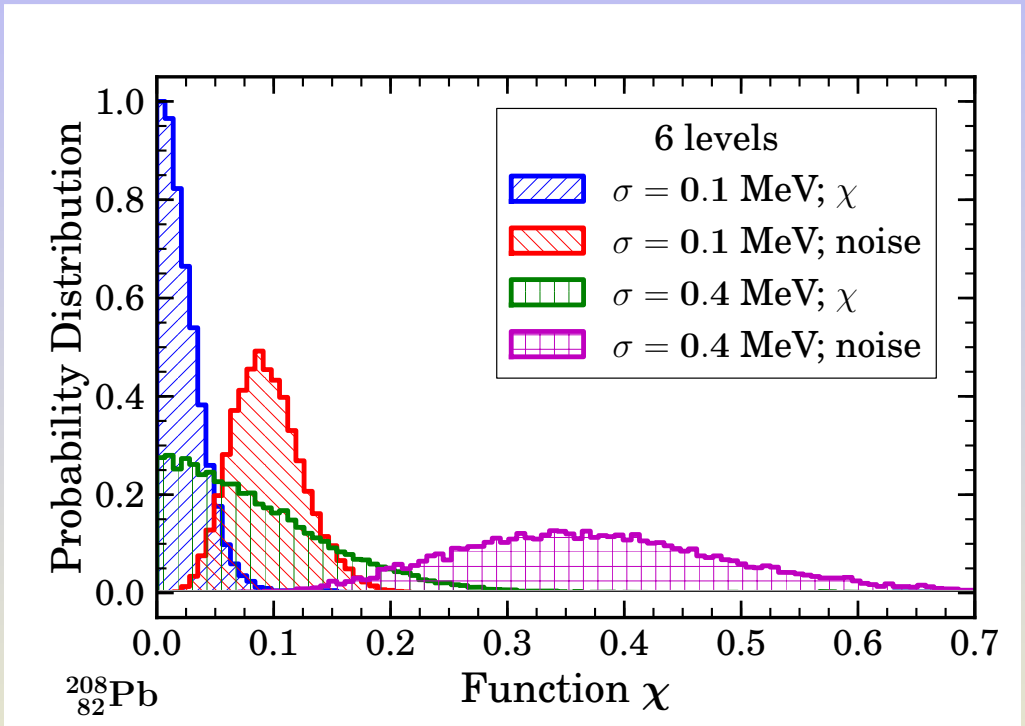

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• We improve the model by reducing the number of parameters

Part II

Overparametrized Nuclear Hamiltonians: Why? How to Deal with the Problem?

Decrease Parametric Freedom: 'Be More Microscopic'

• We suggest to replace a too neat W-S spin-orbit parametrisation by using the density gradient

$$\mathbf{V_{ws}^{so}} \sim \frac{\mathbf{1}}{\mathbf{r}}\frac{\mathbf{d}}{\mathbf{dr}}\left\{\frac{\boldsymbol{\lambda}}{\mathbf{1+\exp[(r-R_o)/a_o]}}\right\} \quad \leftrightarrow \quad \mathbf{V_{ws}^{so}} \sim \frac{\boldsymbol{\lambda}'}{\mathbf{r}}\frac{\mathbf{d}\boldsymbol{\rho}}{\mathbf{dr}}$$

• The nucleonic density can be seen as describing the interaction source: in systems with short range interactions, on the average, the higher the density (gradient) - the more chance to S-O interact.

• Similarly, in the relativistic approach

$$\mathbf{V_{rel}^{so}} \sim \frac{\mathbf{1}}{\mathbf{r}}\frac{\mathbf{d}}{\mathbf{dr}}[\mathbf{S(r)-V(r)}]$$

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A New Toy-Model, Half-Microscopic Hamiltonian

• Consider a given nucleus with the density ρ and a series of neighbouring nuclei with extra occupied orbitals $j_1 \leftrightarrow \rho_{j_1}$, $j_2 \leftrightarrow \rho_{j_2}$, etc. We expect that the density-dependent spin-orbit potentials

$$\mathbf{V^{so}} \sim \frac{\mathbf{d}\rho}{\mathbf{dr}}, \quad \frac{\mathbf{d}\rho_{\mathbf{j_1}}}{\mathbf{dr}}, \quad \frac{\mathbf{d}\rho_{\mathbf{j_2}}}{\mathbf{dr}} \quad \ldots$$

account much better for these extra orbitals than just a flat WS potential introduced long ago for numerical simplicity

• Therefore we will test the following Hartree-Fock like hypothesis

$$\boxed{V_\pi^{so} = \frac{\lambda_{\pi\pi}}{r}\frac{d\rho_\pi}{dr} + \frac{\lambda_{\pi\nu}}{r}\frac{d\rho_\nu}{dr}} \quad \text{and} \quad \boxed{V_\nu^{so} = \frac{\lambda_{\nu\pi}}{r}\frac{d\rho_\pi}{dr} + \frac{\lambda_{\nu\nu}}{r}\frac{d\rho_\nu}{dr}}$$

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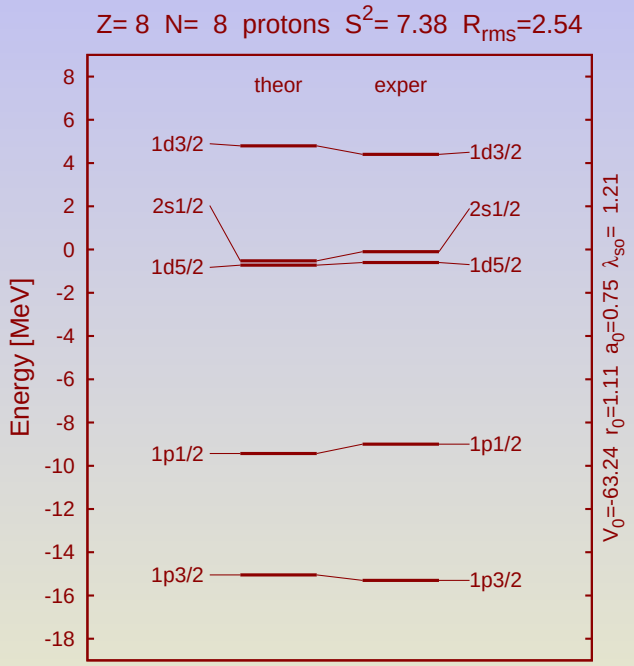
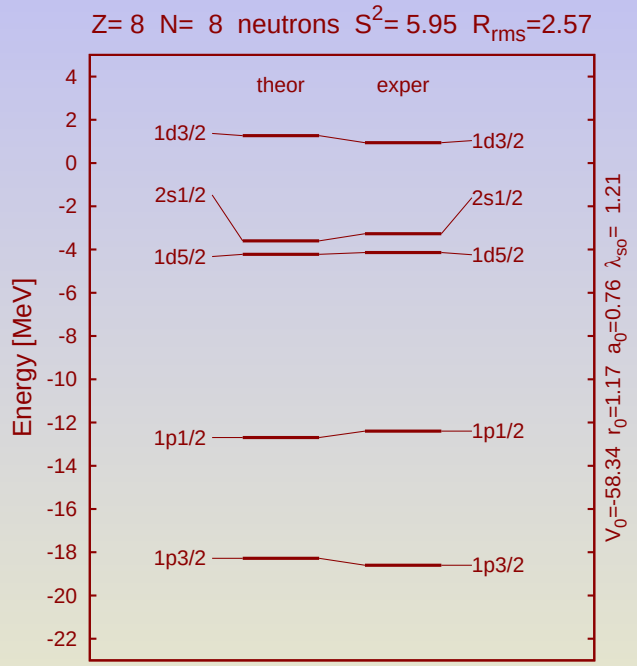
Comparing with Experimental Results: Example ^{16}O

Single particle proton and neutron states in ^{16}O





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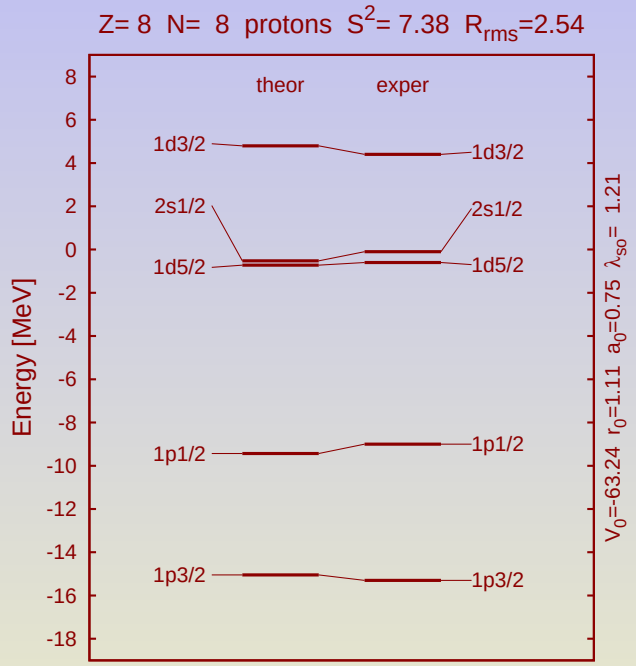

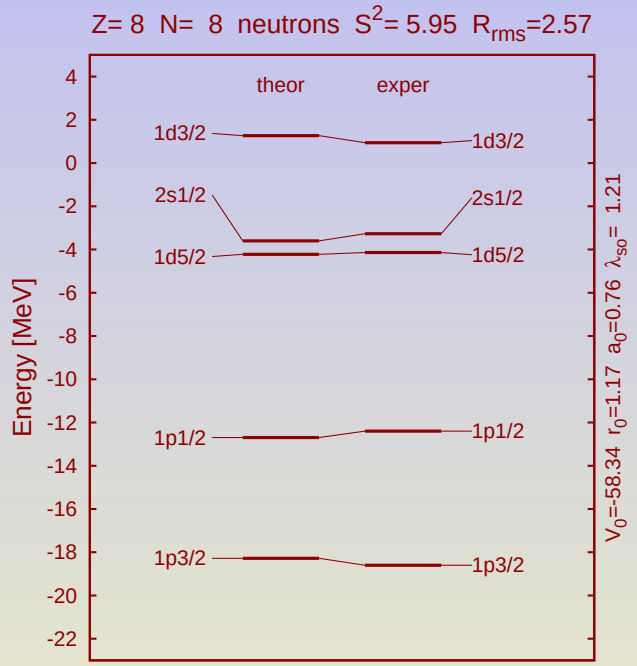

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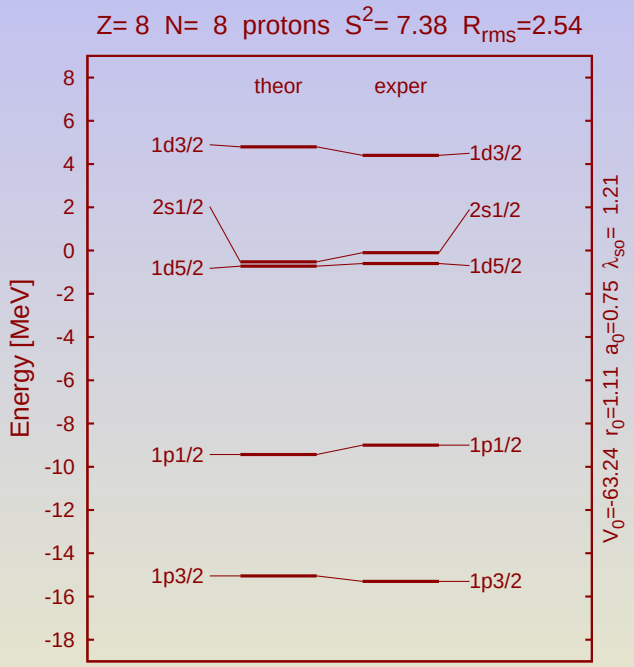

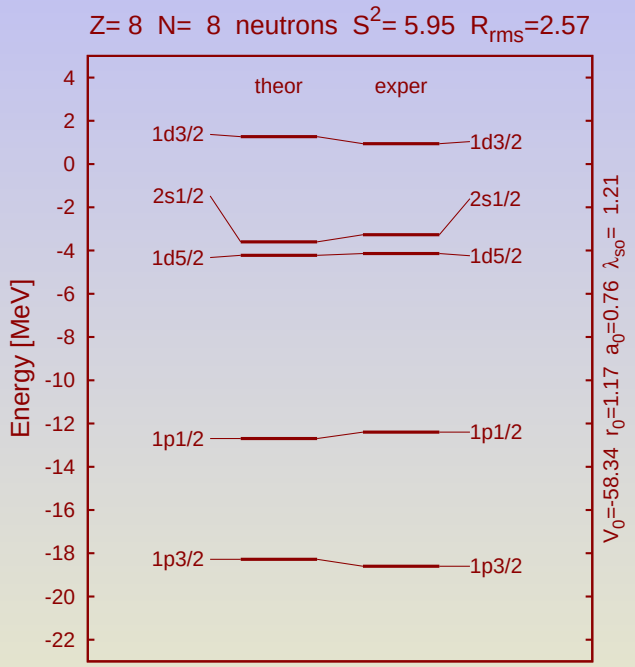

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The maximum error $\sim$ *200 keV*

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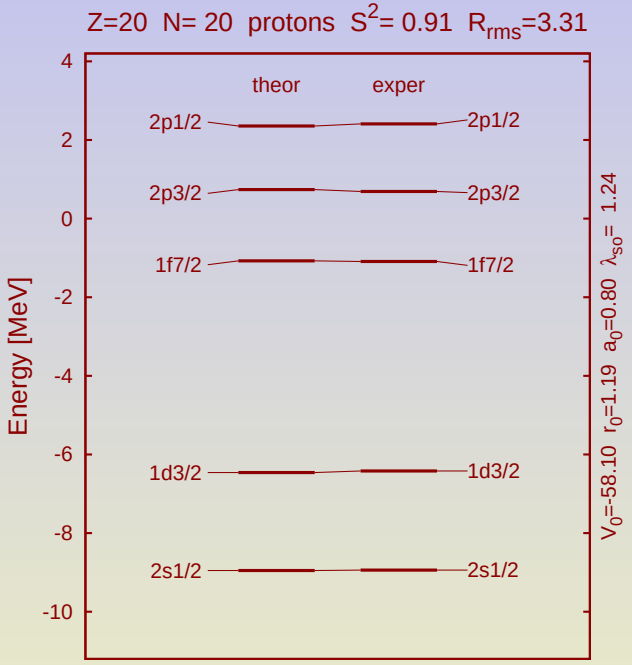

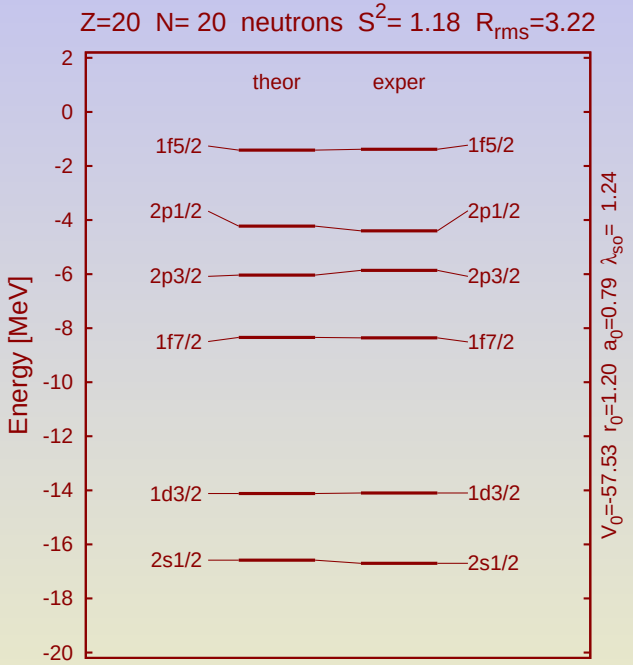

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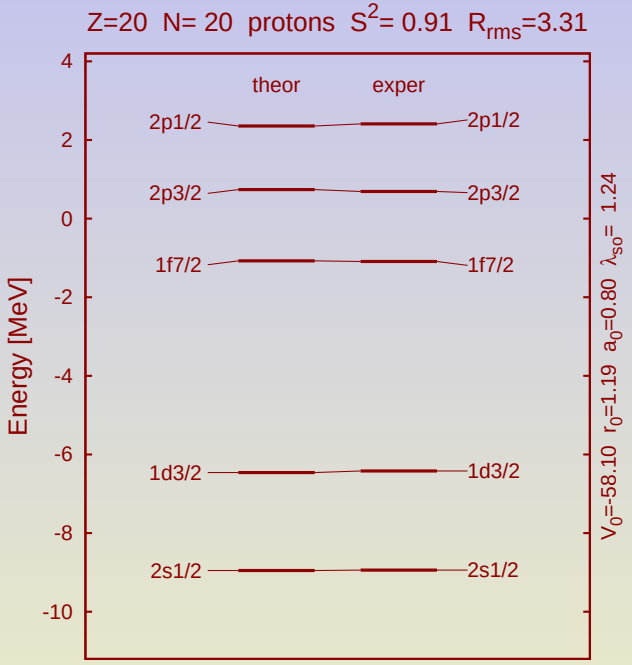

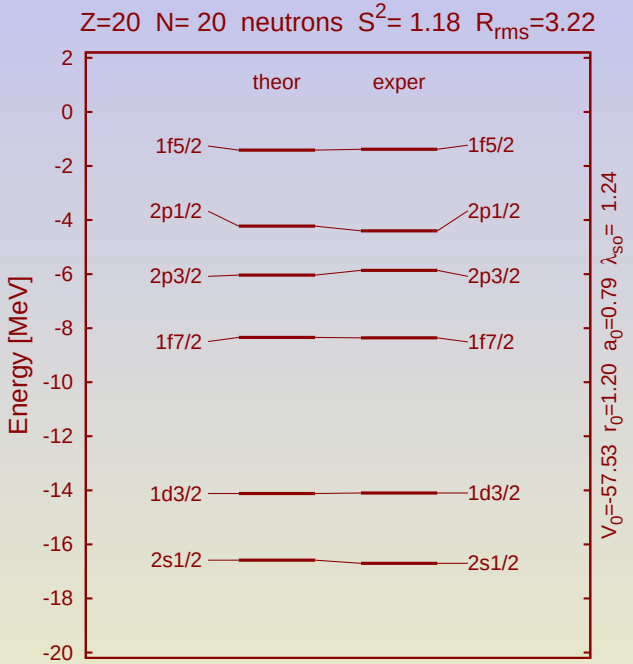

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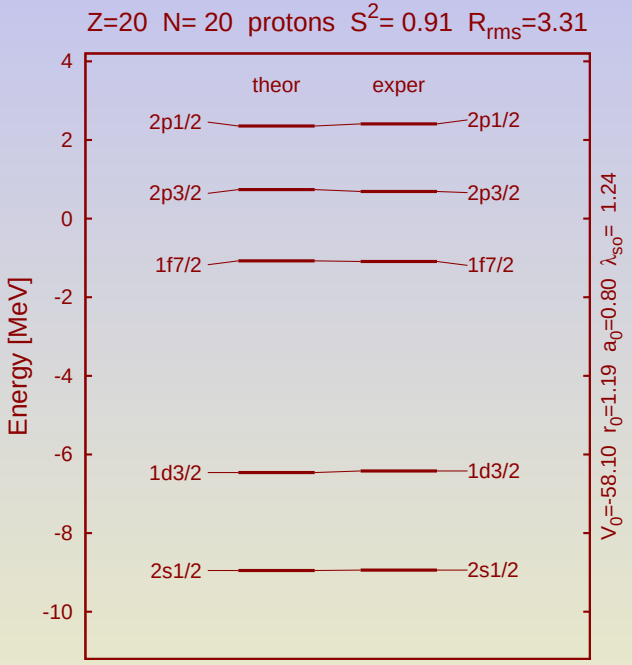

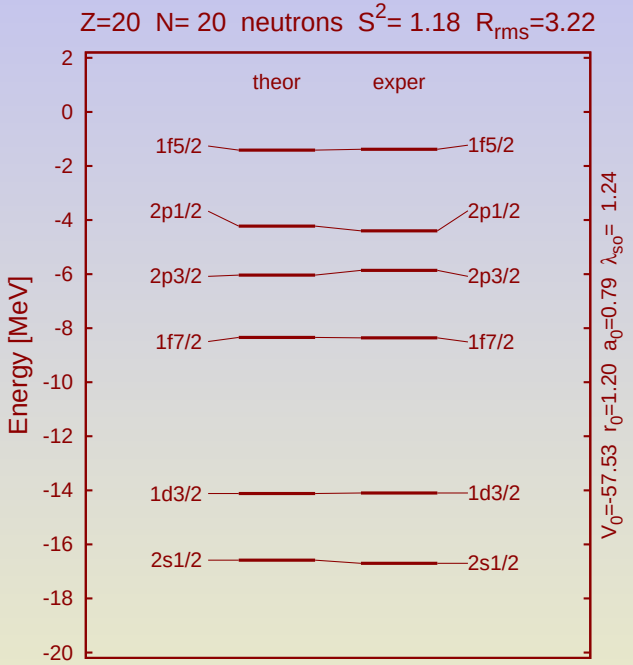

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We have V_o^π, V_o^ν, r_o^π, r_o^ν and $a_o^\pi = a_o^\nu$ parameters. In the case of ^{208}Pb we have $13_\nu + 11_\pi$ data points.

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Removing the Overfit: Increase Physical Significance

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   - Most importantly, Fits show that the density fluctuations are needed for the gradients in the realistic spin-orbit terms!

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• Needless to say - we aim at the microscopic level (theories), in particular HF - but today there will still be some simple semi-quantitative illustrations $\rightarrow$ presented by another speaker