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 ($\sim$0.18 seconds)
"Inverse Problem"	510 000 results ($\sim$0.36 seconds)

COLLABORATORS:

Arthur DROMARD, UdS/IPHC-CNRS Strasbourg
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Marie-Geneviève PORQUET, CSNSM Orsay

Bogdan FORNAL, IFJ Kraków
Hervé MOLIQUE, UdS/IPHC-CNRS Strasbourg
Karolina RYBAK, UdS/IPHC-CNRS 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
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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: 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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Conclusion: We need to introduce probabilities of ignorance!

Combining Theoretical and Experimental Errors

A Few Comments about the Nature of Errors

- Theories are incomplete whereas experiments plagued with errors:

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

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- Errors propagate to the theory predictions through parameter fits

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- Conclusion: All the predictions have the probability distributions!

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but also by their probability distributions:

$$\boxed{P_1 = P_1(f_1), \;\; P_2 = P_2(f_2), \; \ldots \; P_p = P_1(f_p)}$$

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• Questions of statistical significance of the theory modeling the most basic questions asked in other domains of research are seldom - if ever - posed $\longrightarrow$ This will be our subject today

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

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

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!*

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• 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']

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- An example: the data for $\nu d_{3/2}$ states $(3/2^+)$:

$$\begin{array}{lll} E_1 = 2042\ keV & \text{with} & S_1 = 0.78 \\ E_2 = 2871\ keV & \text{with} & S_1 = 0.08 \\ E_3 = 3083\ keV & \text{with} & S_1 = 0.16 \\ E_4 = 3290\ keV & \text{with} & S_1 = 0.22 \\ E_2 = 3681\ keV & \text{with} & \underline{S_1 = 0.16} \end{array}$$

$$\boxed{\langle \mathbf{E} \rangle = \left(\textstyle\sum_\mathbf{i} \mathbf{E_i} \times \mathbf{S_i}\right)/\left(\textstyle\sum_\mathbf{i} \mathbf{S_i}\right)} \quad \longrightarrow\longrightarrow\longrightarrow\longrightarrow \quad \langle E \rangle = 2592\ keV$$

$$\boxed{E_{d_{3/2}} = -S_n + \langle E \rangle = (-7194.5 + 2592)\ keV = -4602.5\ keV}$$

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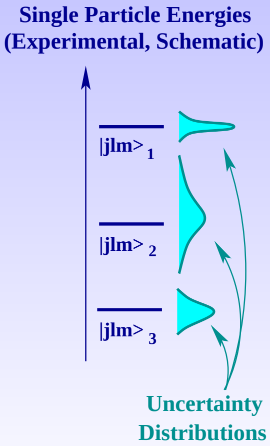
5. Paradoxally, the so-called experimental single-particle levels are highly complicated, model-dependent objects - this leads to errors!

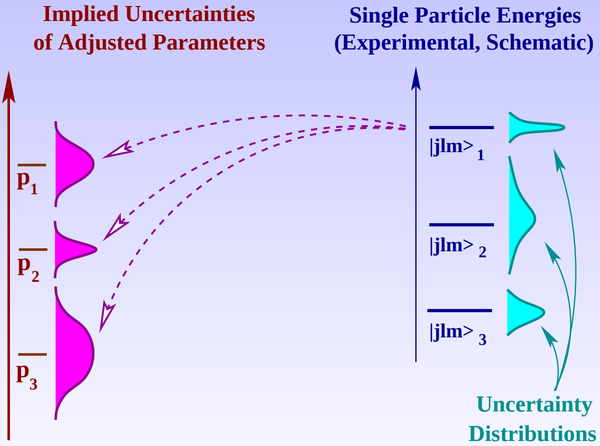
Single-Particle Levels as Probability Distributions

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

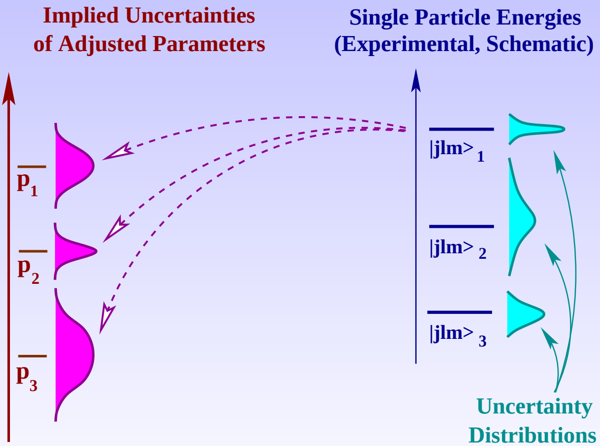


Single-Particle Levels as Probability Distributions

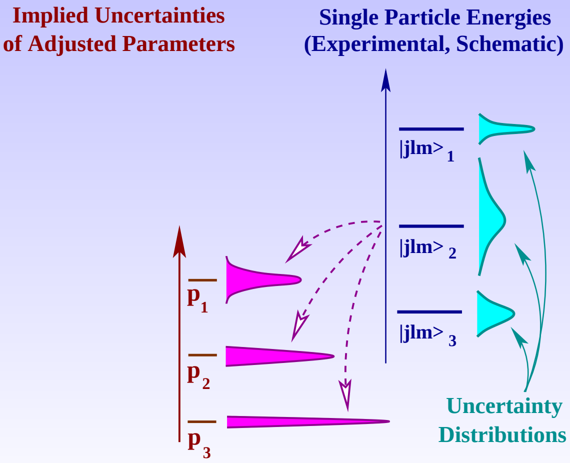
Uncertainties propagate to sought parameters $\{p_1, p_2, \ldots\} \equiv \{p\}$ in $\hat{H}(\hat{r}, \hat{p}; \{p\})\,\psi_n = e_n(p)\,\psi_n$: Parameters $\rightarrow$ Probability Distributions



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

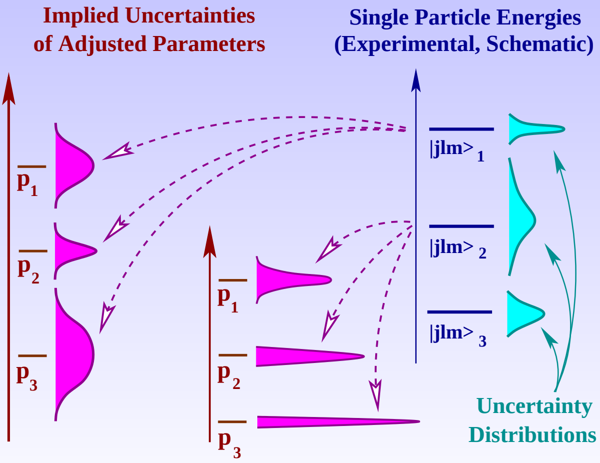


... while at the same time big uncertainties on other levels have a small impact: as in life, all are equal but some more than the others



Single-Particle Levels as Probability Distributions

Conclusion: the quality of adjustement depends strongly on the quality of the data implying the existence of <u>theoretical error bars</u>



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• At this point - what begins - are the issues of lacking precision in very posing of the problem, arbitrariness and semantical confusion, the implied questions, troubles, possibly mathematical non-sense...

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• ...and one may try using similar, a slightly modified wording: What carries certain interest is, possibly, theory’s good predictive power!

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*) *This notion is still to be defined for you here ...*

#) *So is the very notion of probability (12 ‘official’ definitions and 16 interpretations)*

There will be no way to present the full richness of the problem today

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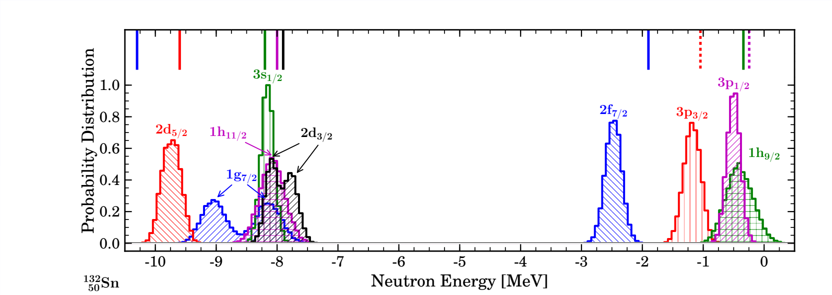
... and continue with presenting as much as Time
(and the Chairman)
permit

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.

Inverse Problem and Predictive Power: ^{132}Sn



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. Observe 'pathologies': $1g_{7/2}$ and $1f_{7/2}$ cf. following figures.

Single-Particle Levels - Noise-Simulation Example

• Consider a single particle spectrum $\{e^o_\nu\} \leftrightarrow H\varphi^o_\nu = e^o_\nu\,\varphi^o_\nu$ obtained with the 'optimal' set of parameters $\{p\}_o$ as in the preceding Table;

• Define the "pseudo-experimental" levels $\{e^{exp}_\nu\} \equiv \{e^o_\nu\}$. Applying the minimisation procedure will now reproduce those $\{e^o_\nu\}$ exactly;

• Chose one level, say $e^o_\kappa \in \{e^o_\nu\}$, and arbitrarily modify its position:

$$e^o_\kappa \to e_\kappa \equiv (e^o_\kappa - e) \;\; \text{with, say} \;\; e \in [-2, +2] \text{ MeV};$$

then refit the χ^2-test $\to$ all other levels will move to new positions

• Collect these new positions: they are functions $e_\nu = e_\nu(e_\kappa)$, below referred to as 'error response functions' $\to$ see illustrations

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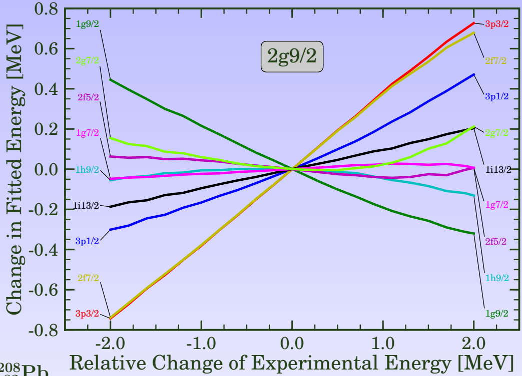
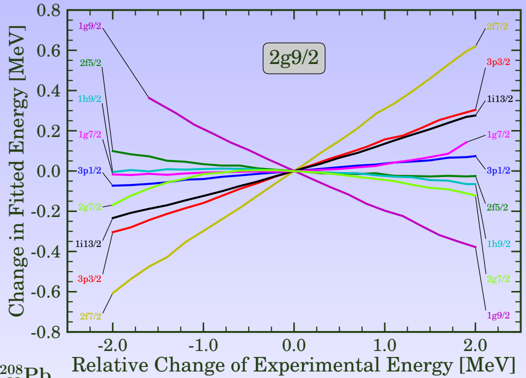
Example: Error Response Functions to $2g_{9/2}$-Orbital



$^{208}_{82}$Pb

To determine precisely the parameters through fitting the energies of $3p_{3/2}$, $2f_{7/2}$ etc. the right position of $2g_{9/2}$ must be analyzed particularly carefully (associated spectroscopic factors precise, particle vibration subtracted, pairing effect subtracted)

Example: Alternative Representation for $2g_{9/2}$-Orbital



$^{208}_{82}$Pb

<u>Attention:</u> The figure may look similar but it contains a totally opposite information:

All the curves represent the $2g_{9/2}$-level - this is how the fitting will modify $2g_{9/2}$ if we vary the indicated levels

Conclusions from the Error Response-Function Tests

• Observe rather precise indications as to *'which levels influence which'* what allows to discuss the experimental strategies precisely

• The low-ℓ orbitals (such as $3p_{1/2}$, $3p_{3/2}$) have relatively small impact on the error-response functions ...

• ... while some pairs of orbitals couple very strongly

• The highest-ℓ orbitals do not couple in the strongest way

• ... all that in a particular case presented; analysis of this type may require a case-by-case mode of operating...

Part II

Inverse Problem of Applied Mathematics

Applied Mathematics: About Inference & Inverse Problems

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THE PREDICTIVE POWER

- 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

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

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

Introduction: χ^2-Problem and Its Linearisation

- Parameter adjustement usually corresponds to a minimisation of:

$$\boxed{\chi^2(p) = \frac{1}{m-n}\sum_{j=1}^{m} W_j\,[e_j^{exp} - e_j^{th}(p)]^2 \;\rightarrow\; \frac{\partial \chi^2}{\partial p_k} = 0,\; k = 1\ldots n}$$

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

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

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

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

χ^2-Problem Using Applied-Mathematics' Jargon

- **One may easily show that within the linearized representation**

$$\boxed{\frac{\partial\chi^2}{\partial \mathbf{p_i}} = 0 \quad \longrightarrow \quad (\mathbf{J^T J}) \cdot (\mathbf{p} - \mathbf{p_0}) = \mathbf{J^T\, b}}$$

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- In *Applied Mathematics* we usually change wording and notation:

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

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

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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

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

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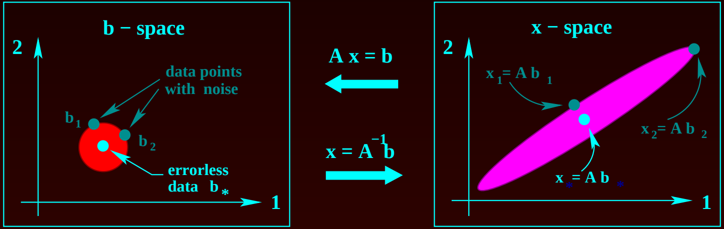
- Introduce errorless data (b_*) and uncertain (noisy) data: b_1 & b_2



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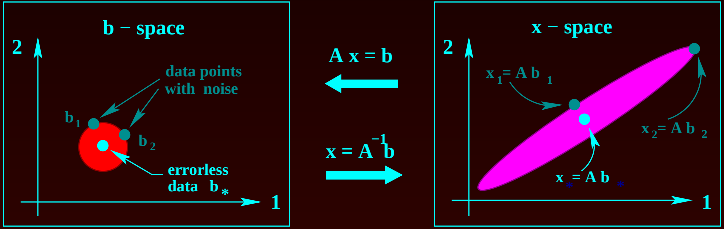

Left: Red circle represents points equally distant from 'noisless' data b_*. *Right: Purple oval represents the image of the circle through* $Ax=b$. *One may show that instability is directly dependent on the condition number*

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

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

- Let us come back to the underlying χ^2 minimum condition:

$$\frac{\partial \chi^2}{\partial \mathbf{p_j}} \quad \longrightarrow \quad (\mathbf{J^T J})(\mathbf{p} - \mathbf{p_0}) = \mathbf{J^T b}$$

Fitting, Implied Errors and Confidence Intervals

- Let us come back to the underlying χ^2 minimum condition:

$$\frac{\partial \chi^2}{\partial \mathbf{p_j}} \quad \longrightarrow \quad \mathbf{(J^T J)(p - p_0) = J^T b}$$

- Using the Singular-Value Decomposition written down explicitly

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

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- Independently one derives the expression for the correlation matrix

$$\boxed{\langle(\mathbf{p_i} - \langle \mathbf{p_i}\rangle) \cdot (\mathbf{p_j} - \langle \mathbf{p_j}\rangle)\rangle = \chi^2(\mathbf{p})\, \mathbf{t}^2_{\alpha/2,m-n}\, (\mathbf{J^T J})^{-1}_{ij}}$$

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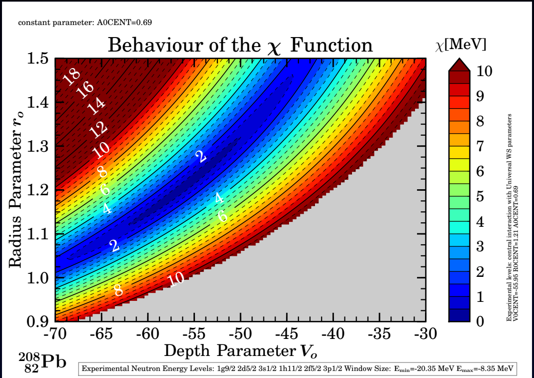
- **If one or more $d_k \rightarrow 0$ then $(J^T J)^{-1}$ tends to infinity and generally, the confidence intervals of all parameters diverge**

Part III

Totally Undesired Parameteric Correlations

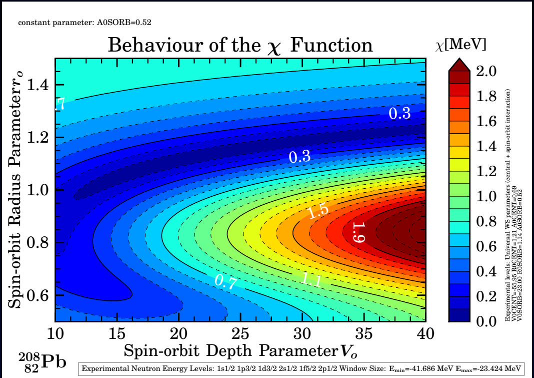
Undesired Parametric Correlations: Illustrative Examples

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.

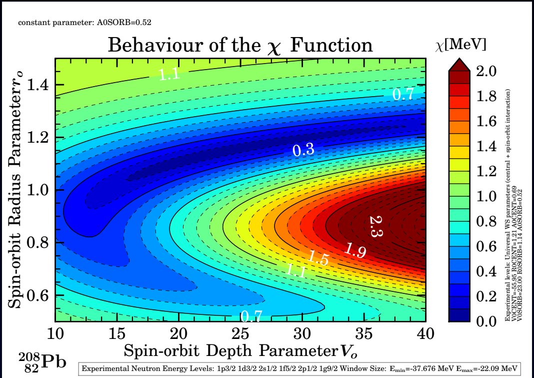
Parametric Correlations and Their Consequences



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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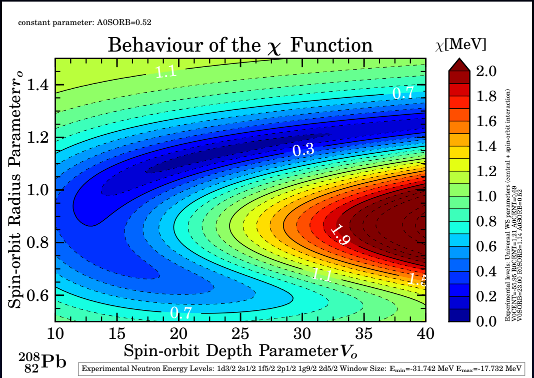

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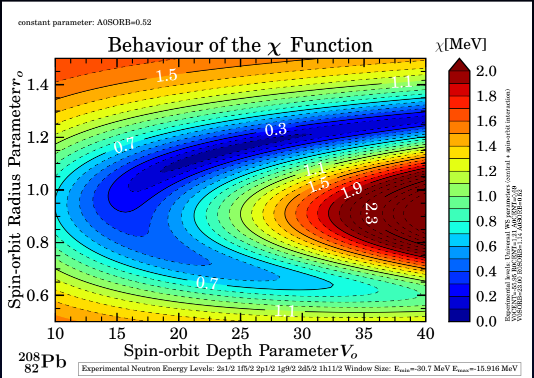

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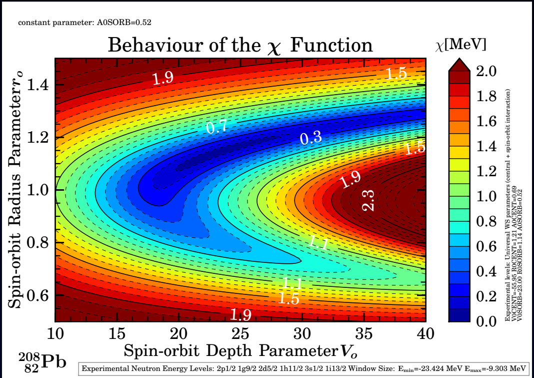

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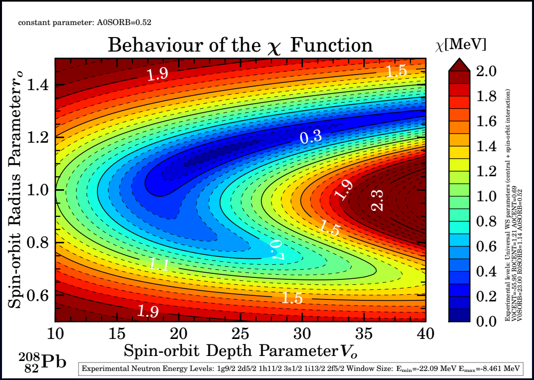

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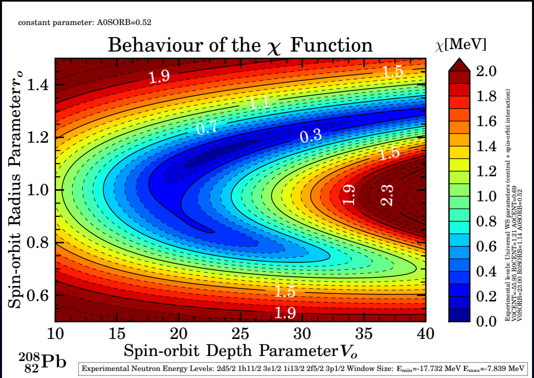

Increasing the energy of the six levels helps localising the spin-orbit strength only very slowly... whereas gradually another solution ...

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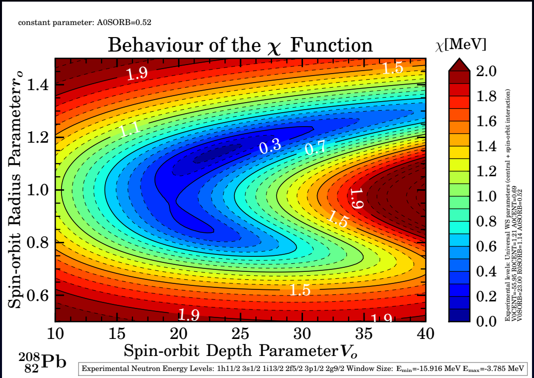
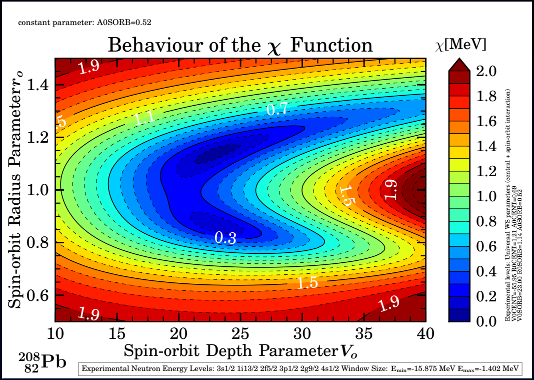


Increasing the energy of the six levels helps localising the spin-orbit strength only very slowly... Attention: Second solution is coming !

Limited Experimental Input: How Little is Sufficient?



... and here we discover the existence of *<u>two solutions</u>* *- 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}**

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

A Kind of Summary and a Historical Analogy

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Part IV

Predicitive Power in Terms of Soluble Models

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- **What useful could we learn from such a 'naive' formulation?**

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- **We construct histograms of occurrence of each parameter; After normalisation $\longrightarrow$ probability distributions of a, b, c & d**

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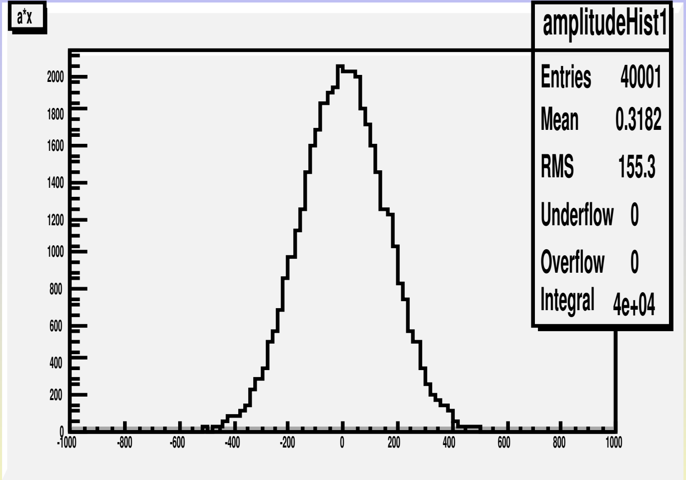
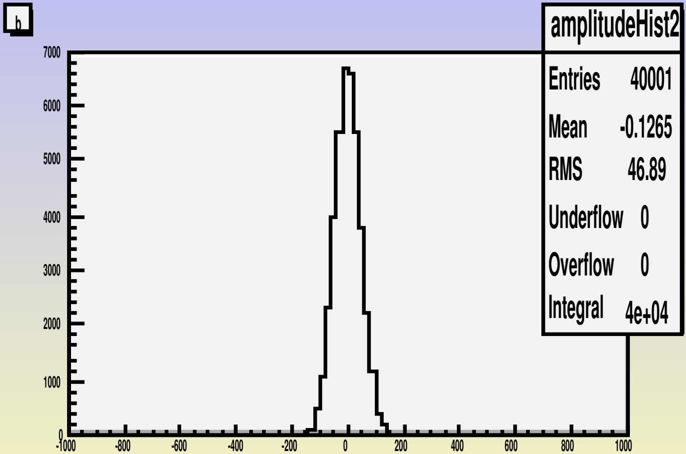


Probability Distribution of the *a*-parameter of the ‘theory’



Probability Distribution of the *b*-parameter of the ‘theory’

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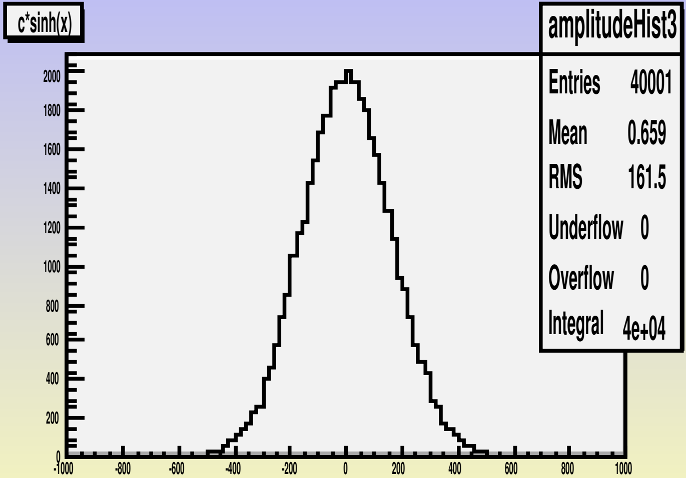
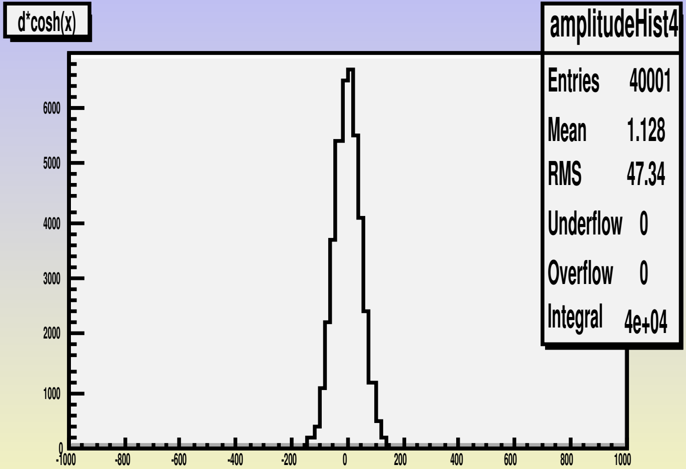
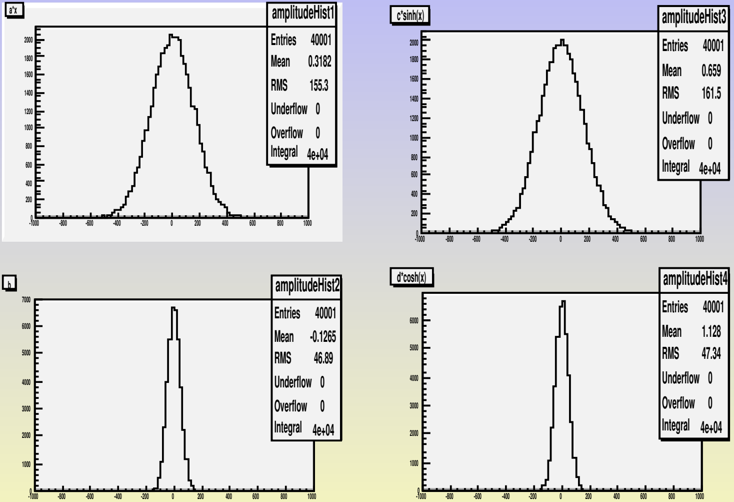


Probability Distribution of the *c*-parameter of the 'theory'



Probability Distribution of the *d*-parameter of the 'theory'

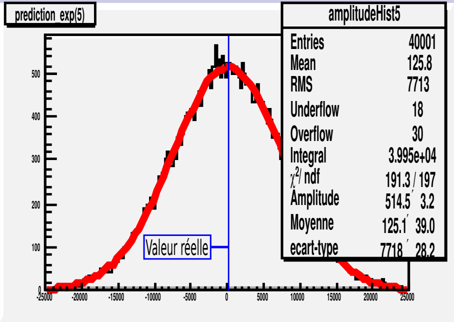


Observe different behaviour of the positive and negative parities

Predictive Power in Terms of Soluble Models

- **Extraneous Predictive Power $\leftrightarrow$ Extrapolations by theory:**

$$\boxed{\mathbf{exp(5) = ?}}$$



Probability Distribution of the 'exact theory' prediction for $\exp(5) = 148.4$

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$$\boxed{\boxed{\textbf{What is the fundamental origin of the `theory' failure?}}}$$

The Inverse Problem Related to the Theory

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$$\boxed{\mathbf{a = 0,\ b = 0,\ c = 1,\ d = 1 \quad \longrightarrow \quad a = f(b)\ \ and\ \ c = g(d)}}$$

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- When there are correlations $[p_i = f(p_j)]$ at least one $d \to 0$

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- **The real problem: How about small but $\neq 0$ singular values?**

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- There is no divergence in the solution for the parameters

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Hidden Charms... But What if $d \neq 0$, Yet Small?

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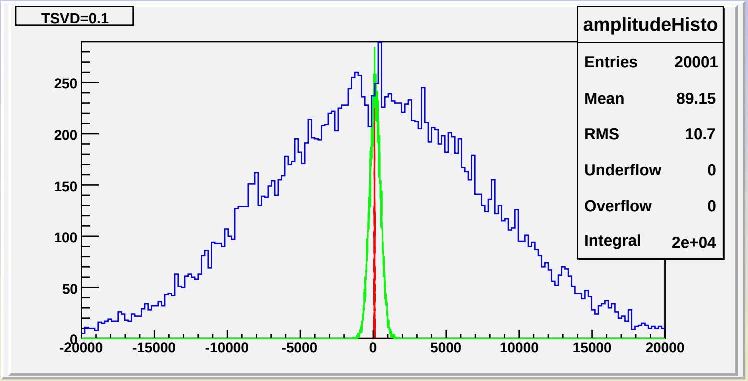
- **Before we start looking for a compromise $\to$ an illustration**

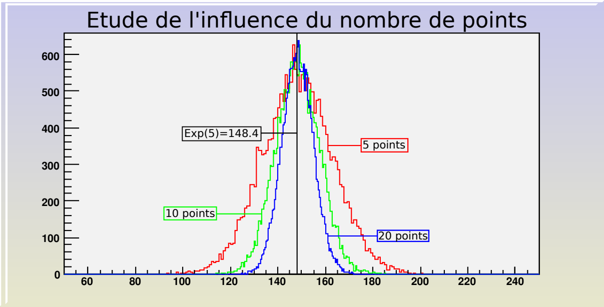
- **TSVD: $\Rightarrow$ efficiently counteracts the problem of instability**



Blue: no TSVD truncation, Green = cut off = 0.01, Red = cut off 0.1

Sampling: Increasing the Number of Experimental Points

- **Divergence depend on the 'Hamiltonian' <u>and</u> on data points**



Increasing the no. of data points increases the constraint on the model and as a consequence - stabilises the final solution

The Following Messages

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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

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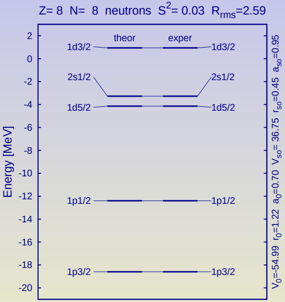
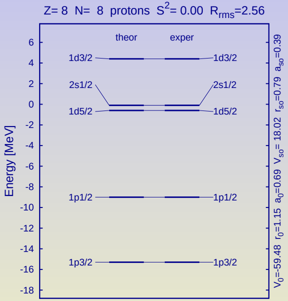
• We will obtain the response of all the levels to a 'linear noise' - vary a level position within a window and refit the H-parameters $\{p\}$

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





'Chi-by-the-eye' Results May Look Attractive...

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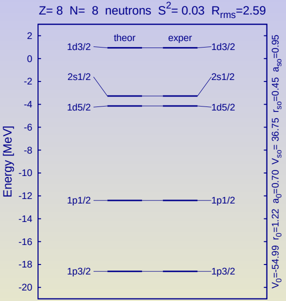

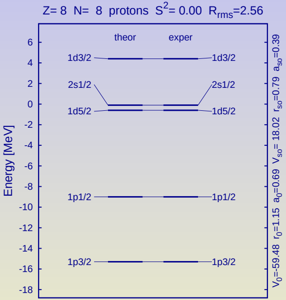

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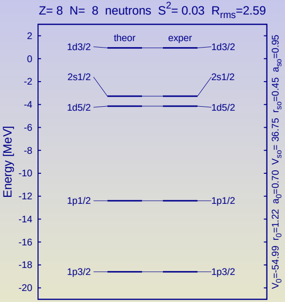

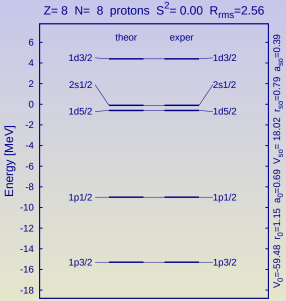

• This result may look surprising: the quality of the fit is such that *graphical illustrations are insufficient to show it* !!!

• On the other hand: If 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)
1.	-15.300	-15.300	$1p_{3/2}$	-0.0001
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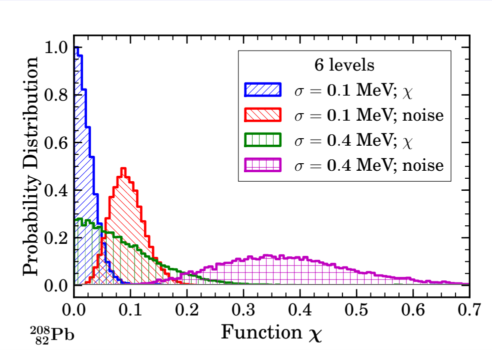
- *What is the mathematical/physical significance of the result?*

Unprecedented Precision ... Known as 'Overfitting'



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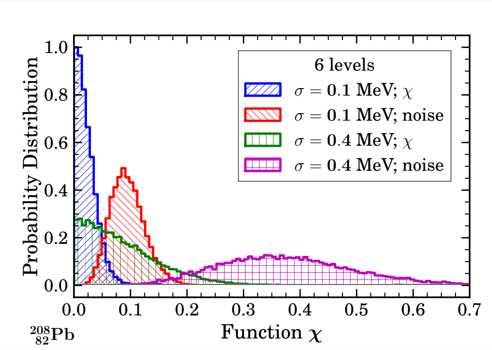

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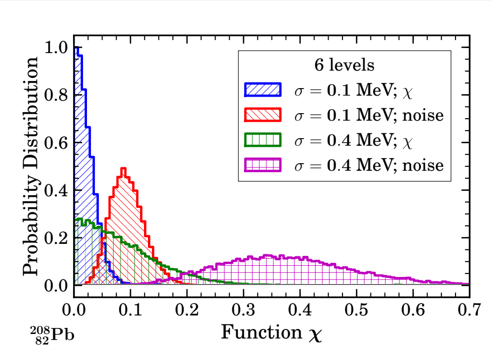

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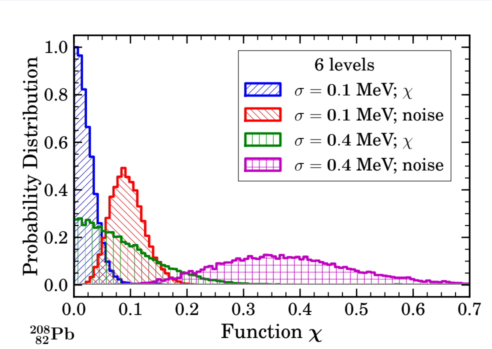

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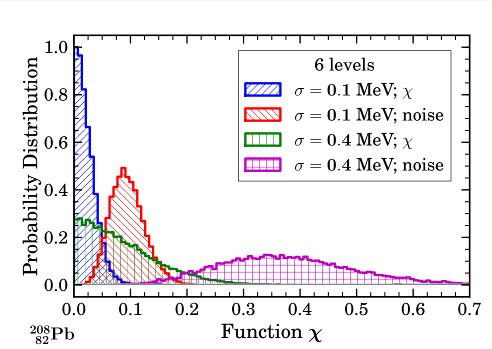

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- Under the mathematical conditions discussed there are $N = \infty^6$ exact fits possible. Is it totally trivial?

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• We improve the model by reducing the number of parameters

Part V

Nuclear Hamiltonians: Sampling vs. Microscopic Structure

Decrease Parametric Freedom: 'Be More Microscopic'

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

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

• 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

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

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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

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

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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• On the other hand we will modify the HF idea of self-consistency from the usual variational context to the spectroscopic context:

$$\mathbf{H}(\rho)\psi_\mathbf{n} = \mathbf{e_n}\,\psi_\mathbf{n} \;\rightarrow\; \rho = \sum \psi^*\psi \;\rightarrow\; \mathbf{H}(\rho)\psi_\mathbf{n} = \mathbf{e_n}\,\psi_\mathbf{n}\ldots$$

We will iterate to obtain the self-consistency that in this context we call 'auto-reproduction' - it is not a result of energy minimisation!

• **In other words: If at $\mathbf{i^{th}}$ iteration the spectrum is $\{\mathbf{e_n^i}\}$ and at $\mathbf{i+1^{st}} \rightarrow \{\mathbf{e_n^{i+1}}\}$, we stop iterating when**

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Self-consistent Formulation: Minimum Coupling

• For the first tests we apply what we call a minimum coupling hypothesis

$$\boxed{\boldsymbol{\lambda_{\pi\pi} = \lambda_{\pi\nu} = \lambda_{\nu\pi} = \lambda_{\nu\nu} \stackrel{\mathrm{df}}{=} \lambda}}$$

• We adjust parameters of the central potential together with $|\lambda|$

• **In other words: We will reduce the number of spin-orbit parameters from 6 (3 per particle kind: λ, r_o^{so} and a^{so}) to one!**

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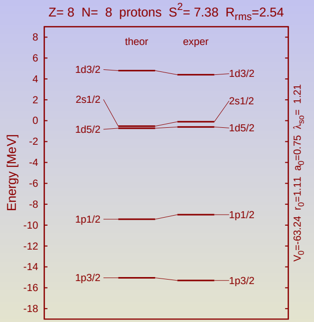
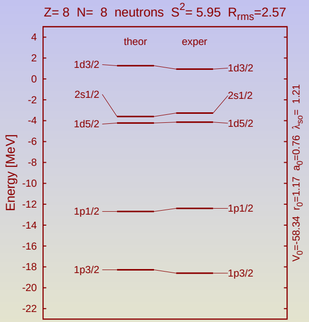
Comparing with Experimental Results: Example ^{16}O

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





These results corresponds to just one λ-parameter fit instead of 6.

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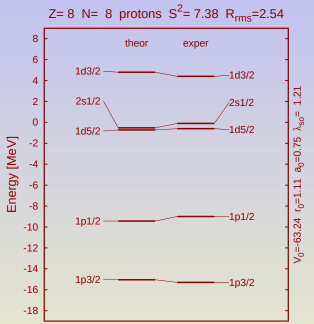

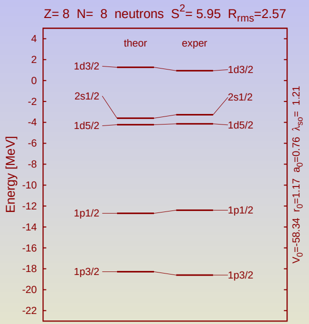

These results corresponds to just <u>*one λ-parameter fit instead of 6.*</u>

Recall: spin-orbit strength parameter $\lambda = \lambda_{\nu\nu} = \lambda_{\nu\pi} = \lambda_{\pi\nu} = \lambda_{\pi\pi}$.

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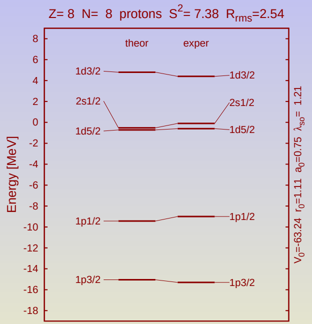

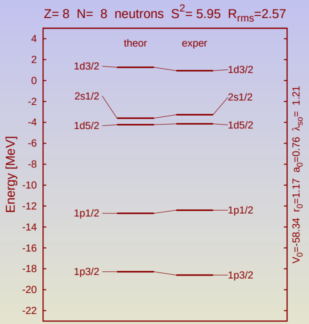

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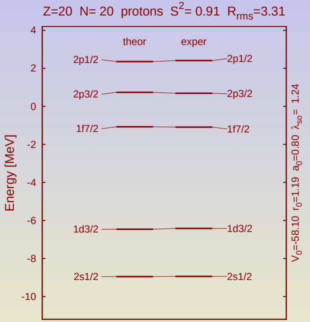
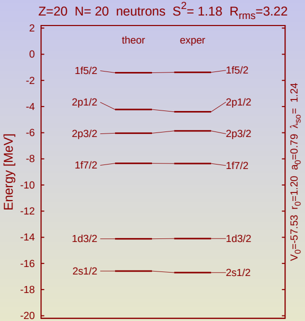
The maximum error $\sim$ 200 keV

Similarly the single particle proton and neutron states in ^{40}Ca





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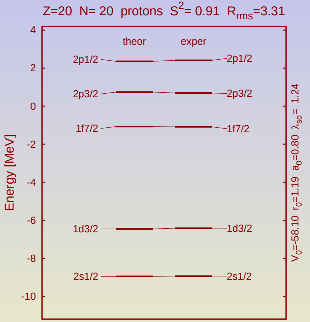

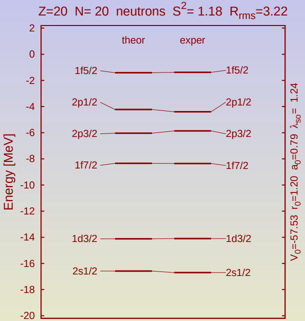

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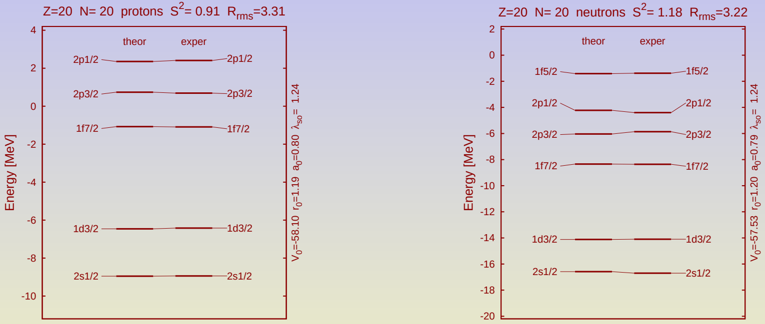

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We have V_o^π, V_o^ν, r_o^π, r_o^ν and $a_o^\pi = a_o^\nu$ parameters. In the case of ^{208}Pb we have $13_\nu + 11_\pi$ data points.

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   - 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 we have presented some simple semi-quantitative illustrations