

About Predictive Power of Nuclear Theories: Strengthening Links with Experiment

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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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QUESTION: Should we congratulate the happy one?

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

This presentation is about:

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

Part I

New Strategies in Constructing Theories: Predictive-Power Perspective

The New Strategies in Constructing Theories

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Conclusion 2: The desired truth remains unknown to us
→ lack of knowledge → ignorance imposed^{#)} by nature

^{#)}... and thus well excused - because not resulting from our laziness

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Conclusion: We need to introduce probabilities of ignorance!

Comments: Mathematical Sense of Uncertainties

- Theories are incomplete whereas experiments plagued with errors:

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

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

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- Conclusion: All the predictions have the probability distributions!

Observe a Paradox:

It is NOT that we need to do something extra:

Our theories already
Contain Information about Uncertainties

It will be sufficient to start NOT ignoring it!!!

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but also by their probability distributions:

$$P_1 = P_1(\mathbf{f}_1), \quad P_2 = P_2(\mathbf{f}_2), \quad \dots \quad P_p = P_p(\mathbf{f}_p)$$

An Example of Theory Predictions [Uncertainty Distributions]

Inverse Problem and Predictive Power: ^{132}Sn

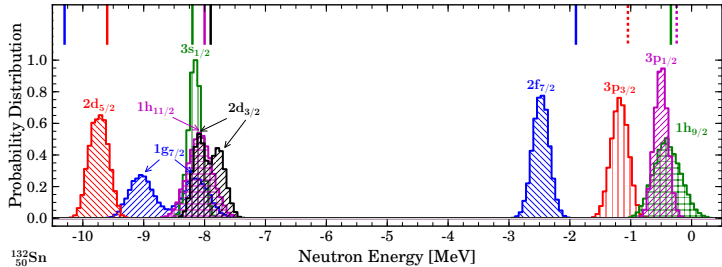
Neutron levels around $N=82$					
Level	States in ^{133}Sn				
	e_1^{exc}	shift 1 ^(a)	shift 2 ^(b)	$\bar{\epsilon}$	B. E.
$\nu f_{7/2}$	0.0000	0.2	0.6(4)	0.6(4)	-1.9(4)
$\nu p_{3/2}$	(0.8537)	-	-	-	-
$\nu h_{9/2}$	1.5609	0.1	0.6(5)	2.2(5)	-0.3(5)
$\nu p_{1/2}$	(1.6557)	-	-	-	-
Level	States in ^{131}Sn				
	e_1^{exc}	shift 1 ^(a)	shift 2 ^(b)	$\bar{\epsilon}$	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 $\sigma=0.1\text{MeV}$. 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': $1g_{7/2}$ and $2d_{3/2}$ cf. following figures.

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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)

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... Are Hardly Experimental Anymore ...

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

$$E_1 = 2042 \text{ keV} \quad \text{with} \quad S_1 = 0.78$$

$$E_2 = 2871 \text{ keV} \quad \text{with} \quad S_1 = 0.08$$

$$E_3 = 3083 \text{ keV} \quad \text{with} \quad S_1 = 0.16$$

$$E_4 = 3290 \text{ keV} \quad \text{with} \quad S_1 = 0.22$$

$$E_2 = 3681 \text{ keV} \quad \text{with} \quad \underline{S_1 = 0.16}$$

$$\langle \mathbf{E} \rangle = (\sum_i \mathbf{E}_i \times \mathbf{S}_i) / (\sum_i \mathbf{S}_i) \quad \rightarrow \rightarrow \rightarrow \rightarrow \quad \langle E \rangle = 2592 \text{ keV}$$

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

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4. Levels depend, among others, on the spectroscopic factors, defined in the presence of simplifying assumptions in reaction theory; the latter may facilitate the self-control through the sum rule tests
5. Paradoxally, the so-called experimental single-particle levels are highly complicated, model-dependent objects - this leads to errors!

Since the Experimental Single-Particle Levels

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**Since the Experimental Single-Particle Levels
Are Hardly Really Experimental**

**it follows that their errors are
much, much larger
than the instrumental ~ 1 keV**

Single-Particle Levels - Noise-Simulation Example

- Consider a single particle spectrum $\{e_\nu^o\} \leftrightarrow H\varphi_\nu^o = e_\nu^o \varphi_\nu^o$ obtained with the 'optimal' set of parameters $\{p\}_o$ as in the preceding Table;
- Define the "pseudo-experimental" levels $\{e_\nu^{exp}\} \equiv \{e_\nu^o\}$. Applying the minimisation procedure will now reproduce those $\{e_\nu^o\}$ exactly;
- Chose one level, say $e_\kappa^o \in \{e_\nu^o\}$, and arbitrarily modify its position:

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

then refit the χ^2 -test \rightarrow 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' \rightarrow see illustrations

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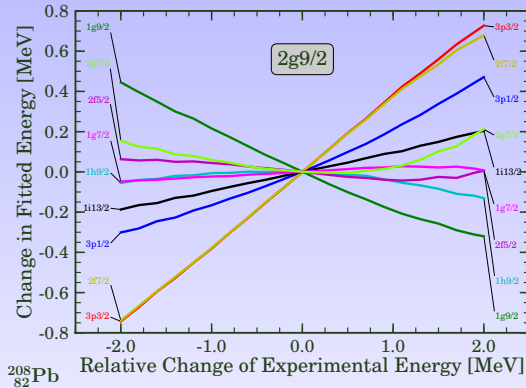
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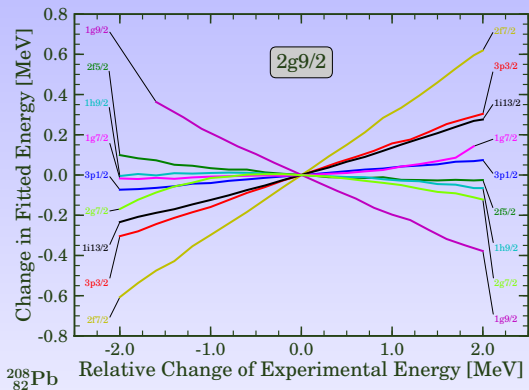
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Example: Error Response Functions to $2g_{9/2}$ -Orbital



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



Attention: 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

Single-Particle Levels - Monte-Carlo Simulations

- Consider a single particle spectrum $\{e_\nu^o\} \leftrightarrow H\varphi_\nu^o = e_\nu^o \varphi_\nu^o$ obtained with the 'optimal' set of parameters $\{p\}_o$ as in the preceding tests;
- For a given level e.g. $i_{13/2}$, define a Gaussian distribution with σ^2 -width corresponding to the information we have about this level;
- Vary the energy of the $i_{13/2}$ -level and repeat the χ^2 minimisation:

$$e_{13/2}^o \rightarrow e_{13/2} \equiv (e_{13/2}^o - e) \quad \text{with, say} \quad e \in [-3\sigma, +3\sigma] \text{ MeV};$$

after that \rightarrow all other levels will move to the new positions: $e_\kappa \rightarrow e'_\kappa$

- Define the new coupling-probability $P_\kappa(e'_\kappa)$ as equal $P_{13/2}(e_{13/2})$; They are functions of $e'_\kappa(e_{13/2})$, and they can be interpreted as the relative-coupling probability distributions

Single-Particle Levels - Monte-Carlo Simulations

- Consider a single particle spectrum $\{e_\nu^o\} \leftrightarrow H\varphi_\nu^o = e_\nu^o \varphi_\nu^o$ obtained with the 'optimal' set of parameters $\{p\}_o$ as in the preceding tests;
- For a given level e.g. $i_{13/2}$, define a Gaussian distribution with σ^2 -width corresponding to the information we have about this level;
- Vary the energy of the $i_{13/2}$ -level and repeat the χ^2 minimisation:

$$e_{13/2}^o \rightarrow e_{13/2} \equiv (e_{13/2}^o - e) \quad \text{with, say} \quad e \in [-3\sigma, +3\sigma] \text{ MeV};$$

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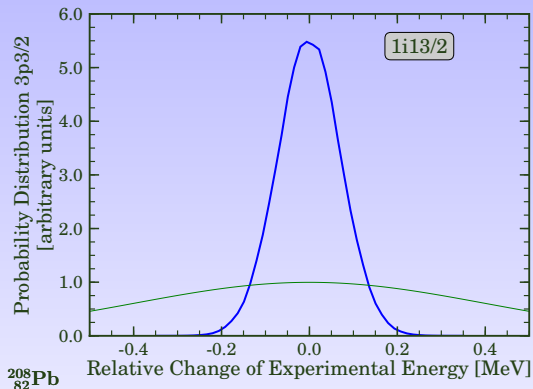
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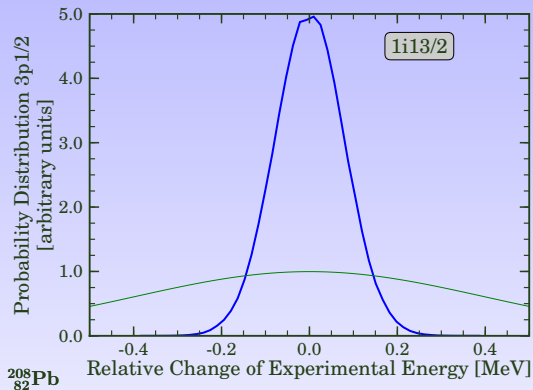
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Relative-Coupling Probability Distributions for $1i_{13/2}$



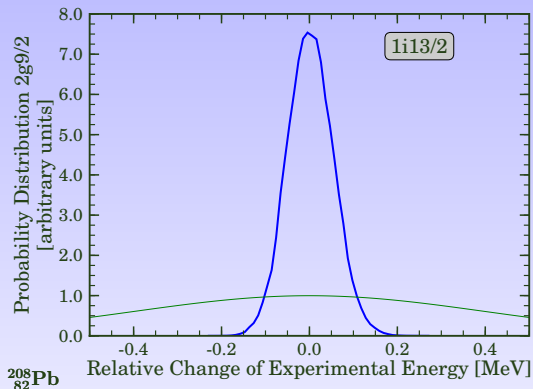
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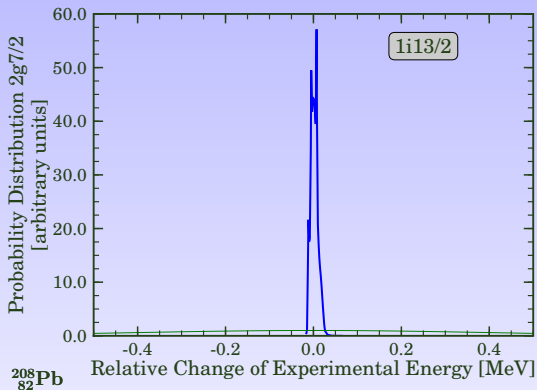
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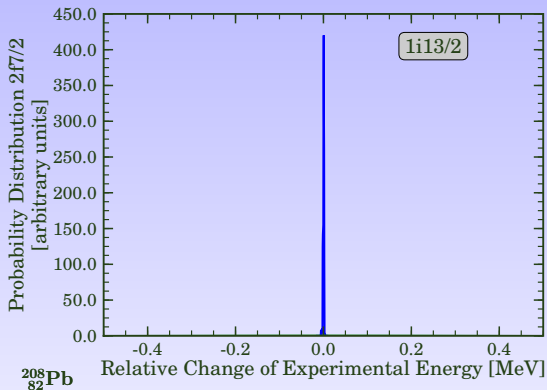
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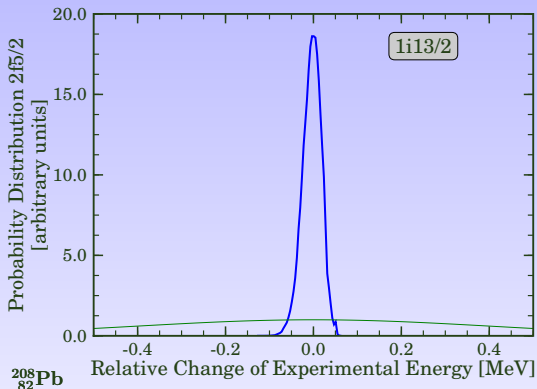
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Conclusions from Discussed Simulations

- 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 necessarily couple 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

Theory Predictions - Their Statistical Significance

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

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

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 meant is: “they” get a ‘statistical nonsense’]

Applied Mathematics: Inference & Inverse Problems

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THE PREDICTIVE POWER

- Statistically sound \Leftrightarrow Instead of saying: $e_{g_{9/2}} = -8.8 \text{ MeV}$ we better provide also the probability function $P = P(e_{g_{9/2}})$, as narrow as possible to allow for the precise energy-indication

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

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

Introduction: χ^2 -Problem and Its Linearisation

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

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

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

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

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- "An unusual" feature: $J \leftrightarrow m \times n$ rectangular matrix ($m \neq n$).

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

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- Formally (but also in practice), the solution 'e' is expressed as

$$\mathbf{e} = \mathbf{A}^T \mathbf{p}; \quad \mathbf{A}^T = \mathbf{V} \cdot \mathbf{D}^T \cdot \mathbf{U}^T$$

where

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

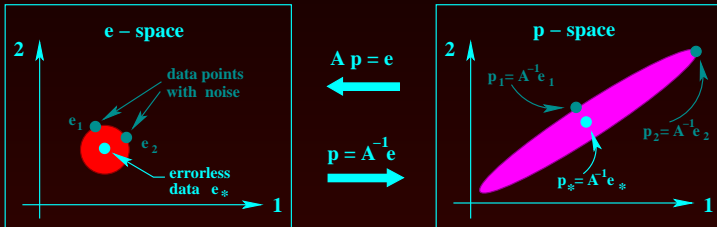
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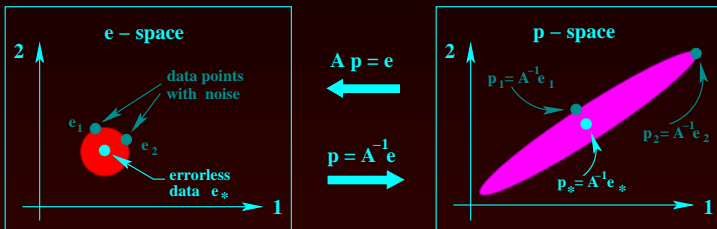
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Left: Red circle represents points equally distant from 'noisless' data e_* .
Right: Purple oval represents the image of the circle through $p=A^{-1}e$. One may show that instability is directly dependent on the condition number

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

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

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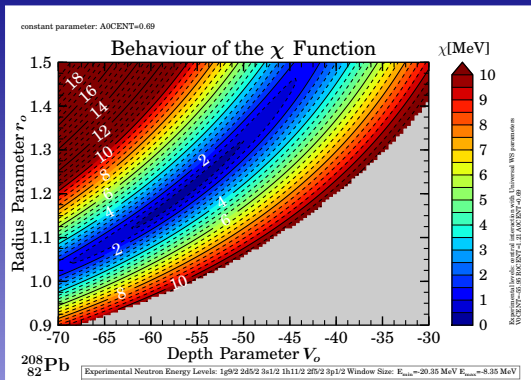
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- If one or more $\mathbf{d}_k \rightarrow 0$ then $(\mathbf{J}^T \mathbf{J})^{-1}$ tends to infinity and generally, the confidence intervals of a l parameters diverge**

Part III

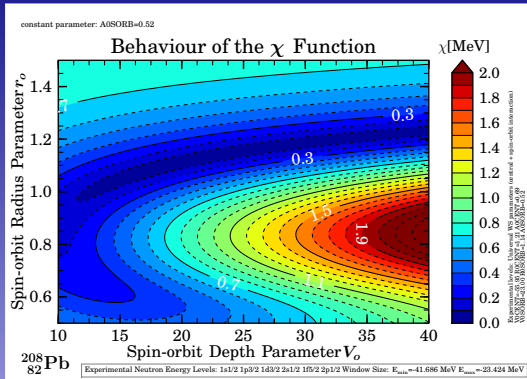
About Undesired Parameteric Correlations

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



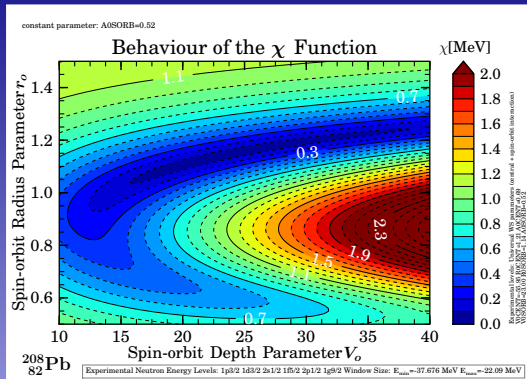
A map of χ^2 from the fit based on six levels close to the Fermi level.

Parametric Correlations and Their Consequences



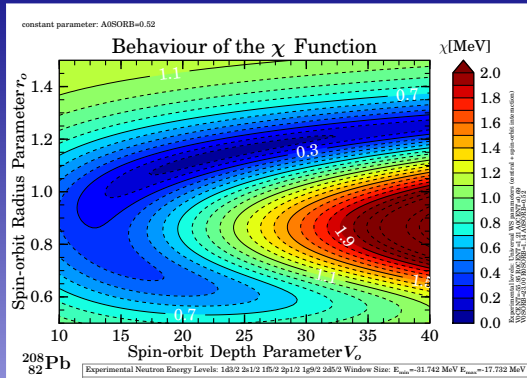
We will gradually increase the energy of the six-level window to approach the nucleon binding region and thus simulate the present-day experimental situation

Limited Experimental Input: How Little is Sufficient?



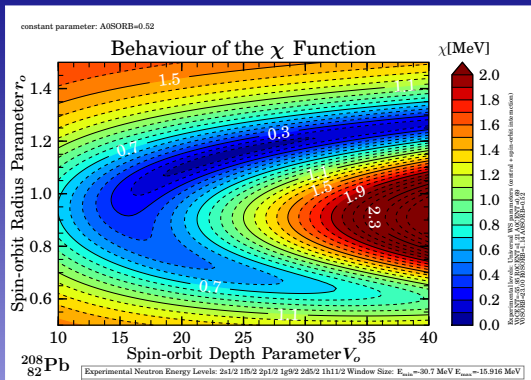
Increasing the energy of the six levels helps localising the spin-orbit strength only very slowly!

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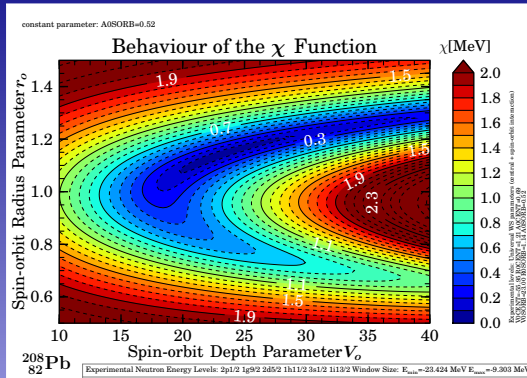
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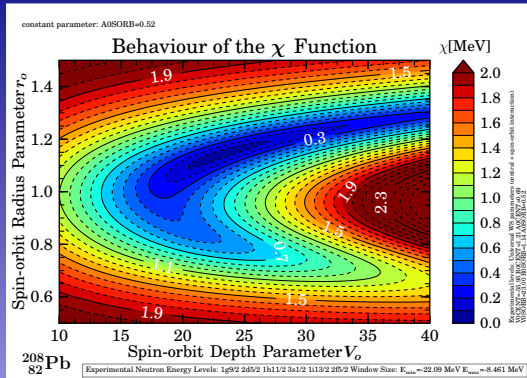
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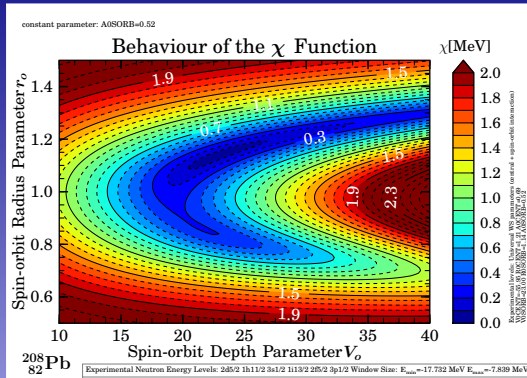
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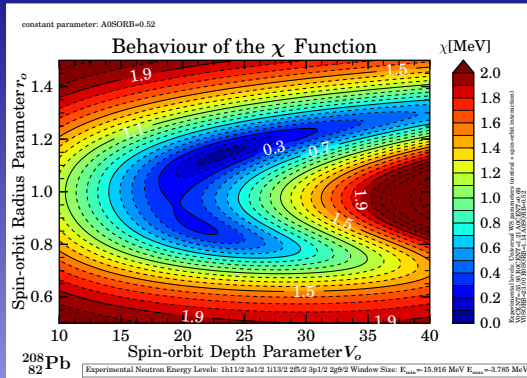
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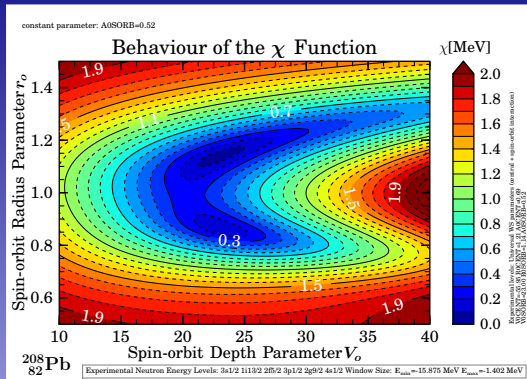
Increasing the energy of the six levels helps localising the spin-orbit strength only very slowly... whereas gradually another solution ...

Limited Experimental Input: How Little is Sufficient?



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 two solutions - we call them *compact* and *non-compact*.

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

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"Do they always have a right answer in Paris?"

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"Do they always have a right answer in Paris?"

"Never", said William,

A Kind of Summary and a Historical Analogy

If the confidence intervals diverge we loose unique answers,
but on the other hand we are confident of our errors

*A similar problem has been encountered,
according to Umberto Eco, about 1327 ("Il nome della rosa")*

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Part IV

Predictive Power in Terms of Soluble Models

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

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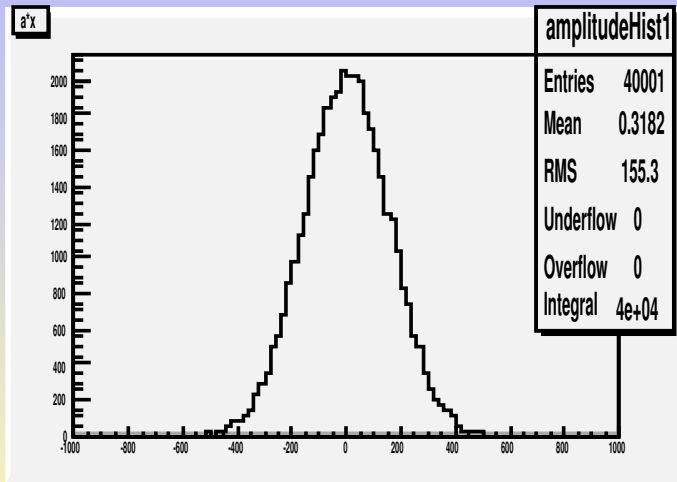
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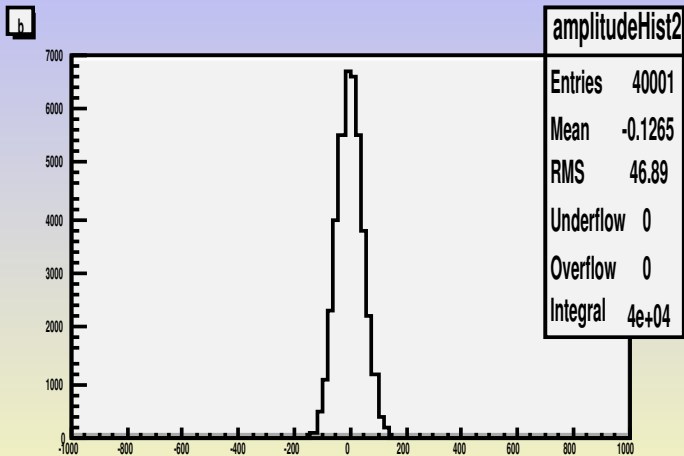
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- We construct histograms of occurrence of each parameter;
After normalisation \rightarrow probability distributions of a, b, c & d

Predictive Power in Terms of Soluble Models



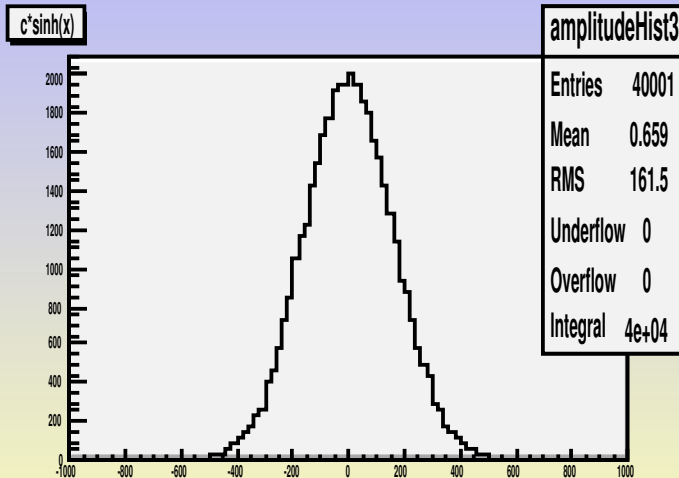
Probability Distribution of the a -parameter of the 'theory'

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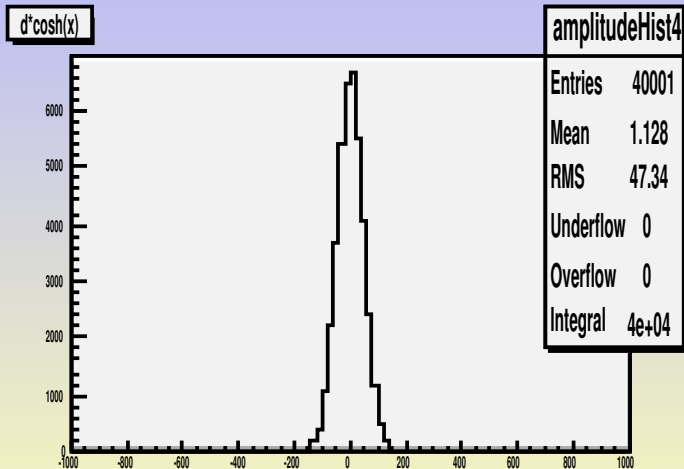
Probability Distribution of the b -parameter of the 'theory'

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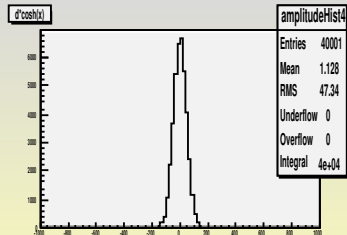
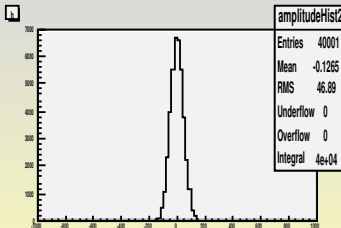
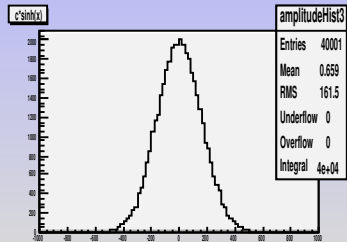
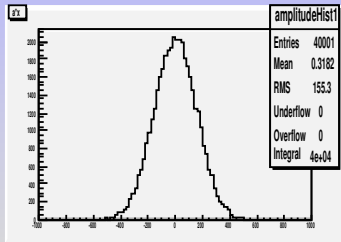
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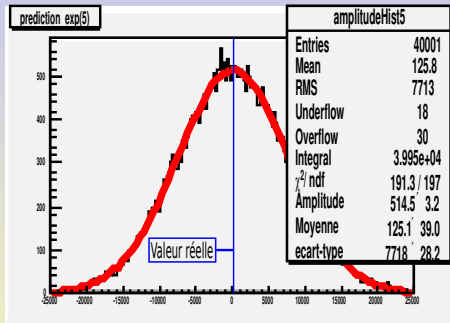


Observe different behaviour of the positive and negative parities

Predictive Power in Terms of Soluble Models

- Extraneous Predictive Power \leftrightarrow Extrapolations by theory:

$$\exp(5) = ?$$



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

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What is the fundamental origin of the 'theory' failure?

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- Our 'theory' is dangerously near the parametric correlations

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

$$(p - p_0) = \underbrace{[(J^T J)^{-1} J^T]}_{d \rightarrow 0 \text{ singularity}} b; \quad p\text{-parameters}; \quad b\text{-data}$$

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At the end : Predictive Power Disappears

Truncated Singular Value Decomposition (TSVD)

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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

$$(p - p_0) = \underbrace{[(J J^T)^{-1} J^T]}_{\text{NO singularity}} b; \quad \underline{\underline{\text{Problem is well posed}}}$$

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

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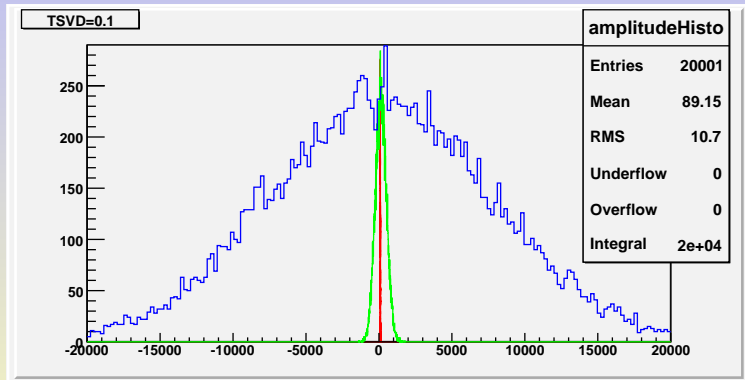
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- Before we start looking for a compromise \rightarrow an illustration

Effect of Truncating Non-Zero Singular Values

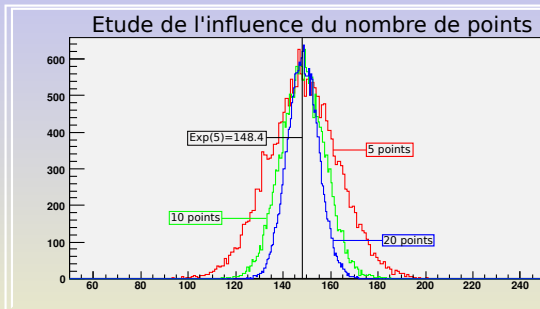
- **TSVD:** \Rightarrow efficiently counteracts the problem of instability



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' and 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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are intended**

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- It is instructive to think about the extensions 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 $N^3\text{LO}$. 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
$N^3\text{LO}$	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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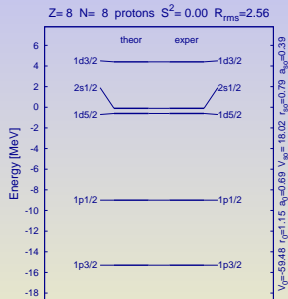
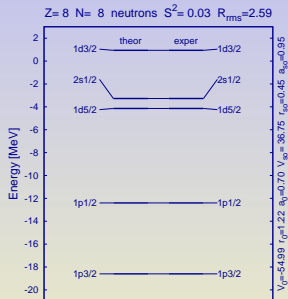
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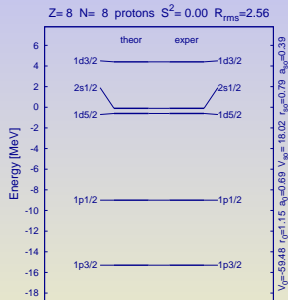
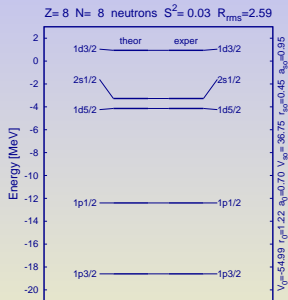
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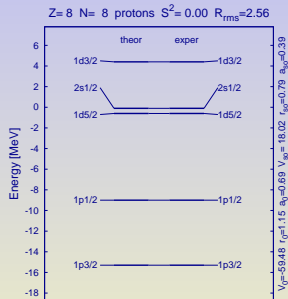
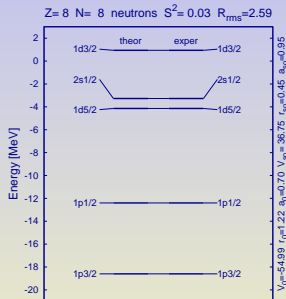
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- On the other hand: If we trust the model - we may hope that also the remaining levels are close to the experimental results to come

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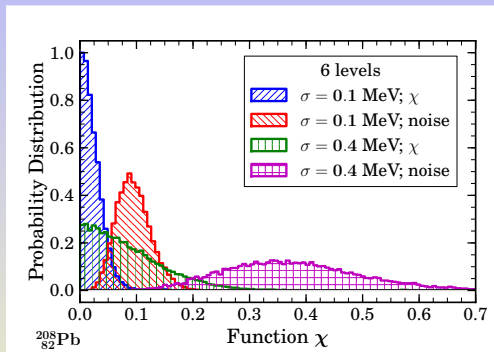
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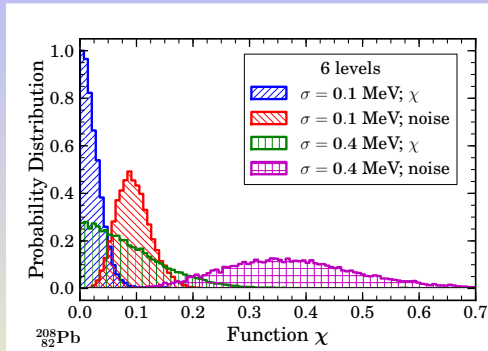
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- *What is the mathematical/physical significance of the result?*

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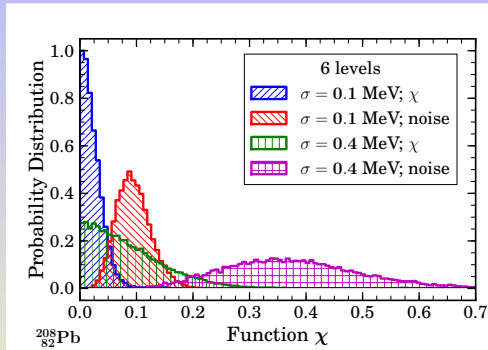


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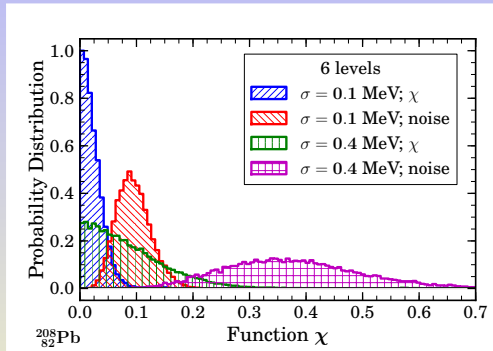
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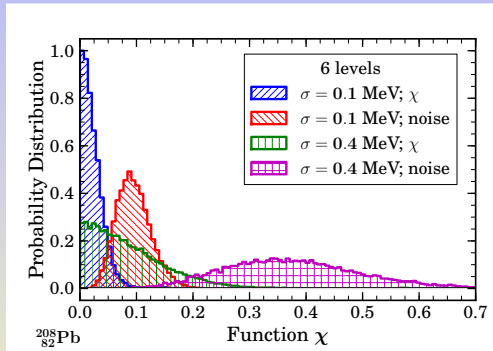
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- Under the mathematical conditions discussed there are $N = \infty^6$ exact fits possible. Is it totally trivial?

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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

$$\mathbf{V}_{\text{WS}}^{\text{so}} \sim \frac{1}{r} \frac{d}{dr} \left\{ \frac{\lambda}{1 + \exp[(r - R_0)/a_0]} \right\} \leftrightarrow \mathbf{V}_{\text{WS}}^{\text{so}} \sim \frac{\lambda'}{r} \frac{d\rho}{dr}$$

- 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

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

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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

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

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

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$$\mathbf{H}(\rho)\psi_n = \mathbf{e}_n \psi_n \rightarrow \rho = \sum \psi^* \psi \rightarrow \mathbf{H}(\rho)\psi_n = \mathbf{e}_n \psi_n \dots$$

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

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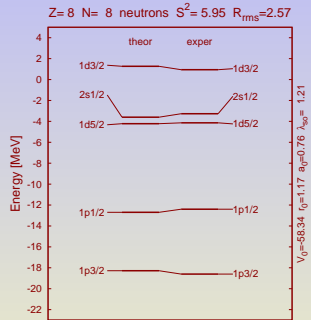
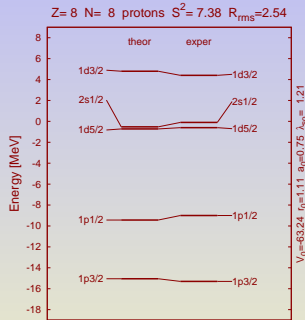
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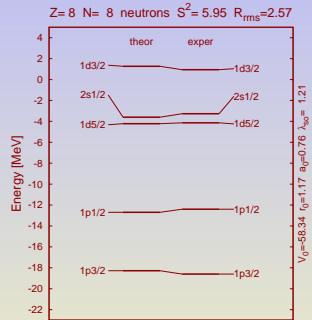
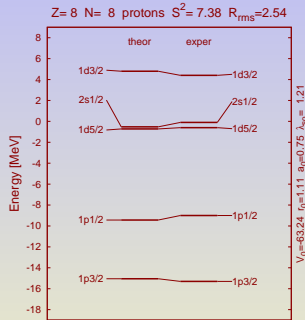
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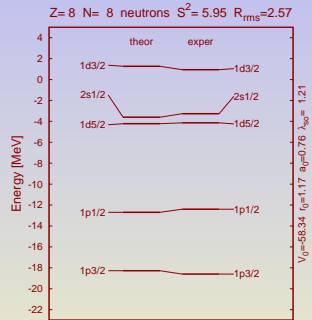
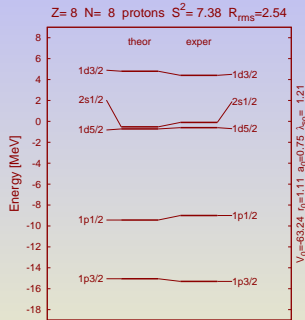
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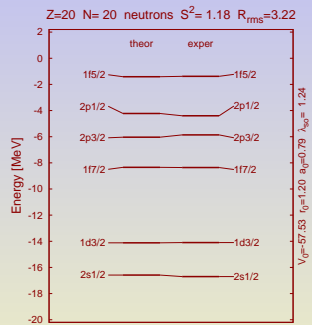
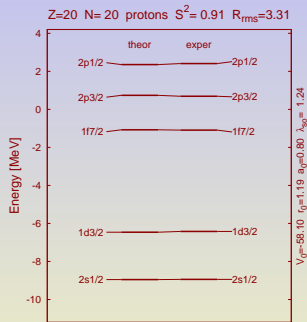
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The maximum error ~ 200 keV

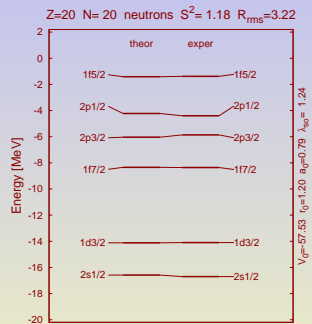
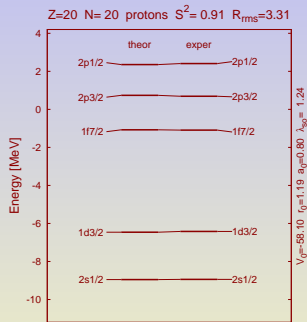
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Similarly the single particle proton and neutron states in ^{40}Ca



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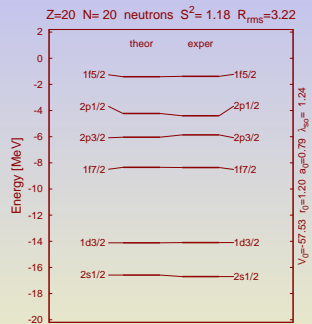
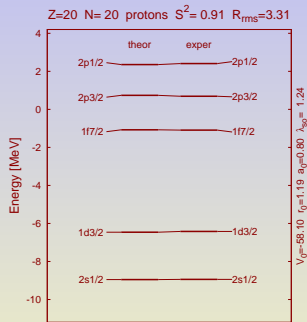
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We have V_o^π , V_o^ν , r_o^π , r_o^ν and $a_o^\pi = a_o^\nu$ parameters. In the case of ^{208}Pb we have $13_\nu + 11_\pi$ data points.

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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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- The audience is warned not to be misled by the **simplicity of the illustrations** based on the toy model (here: spherical Woods-Saxon) vs. **generality and importance of the Inverse-Problem Theory** which applies to all realistic Hamiltonians
- Needless to say - we aim at the microscopic level (theories), in particular HF - but today we have presented some simple semi-quantitative illustrations