Regularisation Methods to Stabilise Nuclear Inverse Problem via Physics-Based Improvements

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Shapes and Symmetries in Nuclei: from Experiment to Theory

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The Method Employed:

Inverse Problem Theory

[A Branch of Applied Mathematics]

Inverse Problem in Quantum Theories

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

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

Taylor Expansion of $\chi^2(p)$: An Analogue to the Inverse Problem

- Parameter adjustment is obtained via the χ^2-minimisation

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

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$$e_j^{th}(p^{[\mathrm{it}+1]}) \approx e_j^{th}(p^{[\mathrm{it}]}) + \sum_{k=1}^{n_m} \left(\frac{\partial e_j^{th}}{\partial p_k} \right)\Bigg|_{p=p^{[it]}} \left(p_k^{[\mathrm{it}+1]} - p_k^{[\mathrm{it}]} \right)$$

Short-hand notation: $J_{jk}^{[\mathrm{it}]} \overset{df}{=} \left(\frac{\partial e_j^{th}}{\partial p_k} \right)\Bigg|_{p=p^{[\mathrm{it}]}}$ and $b_j^{[\mathrm{it}]} = \left[e_j^{exp} - e_j^{th}(p^{[\mathrm{it}]}) \right]$

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- Inserting into $\chi^2(p)$ gives the linearised iterative representation

$$\chi^2(p^{[\text{it}+1]}) = \sum_{j=1}^{n_d} \left[\sum_{k=1}^{n_m} J_{jk}^{[\text{it}]} \cdot (p_k^{[\text{it}+1]} - p_k^{[\text{it}]}) - b_j^{[\text{it}]} \right]^2$$

- One may easily show that within the new, linearised representation

$$\boxed{\frac{\partial \chi^2}{\partial p_i} = 0 \quad \rightarrow \quad (J^T J) \cdot p = J^T b \quad \leftrightarrow \quad J^T J \stackrel{df}{=} \mathcal{A}}$$

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

$$\{p\} \rightarrow \mathcal{P} : \text{'Causes' and } \{J^T b\} \rightarrow \mathcal{D} : \text{'Effects'} \Rightarrow \mathcal{A} \cdot \mathcal{P} = \mathcal{D}$$

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- From the measured 'Effects', called Data, represented by $\mathcal{D}$, we extract information about the optimal parameters, $\mathcal{P}$, by inverting the matrix $\mathcal{A}$:

$$\underbrace{\mathcal{A} \cdot \mathcal{P} = \mathcal{D}}_{\text{Direct Problem}} \quad \to \quad \underbrace{\mathcal{P} = \mathcal{A}^{-1} \cdot \mathcal{D}}_{\text{Inverse Problem}}$$

Possibly Loosing Correlation Between Data and Parameters

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

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

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

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

Parametric Correlations May Contribute to the Ill-Posedeness of the Inverse Problem

Partial Conclusions

Parametric Correlations May Contribute to the Ill-Posedeness of the Inverse Problem

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... especially if the inverse problem is ‘just about’ ill posed!

About Parametric Correlations within the Inverse Problem:

a. How to determine their presence?

b. How to counteract their negative consequences which are likely to destroy the predictive power?

Selection of the Model Mean-Field Hamiltonian for This Project

Woods-Saxon Hamiltonian: Central Potential

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

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

It has unique features among most of the mean field potentials, namely,

each parameter is related to an independent class of experiments:

- V_c - depth parameter; from specific transfer reactions
- r_c - radius parameter; from e.g. electron scattering
- a_c - diffuseness parameter; from hadron scattering

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

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

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

with a fixed parameter set for thousands of nuclei ⇒ Thus the name ‘**universal**’

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

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

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

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

‘WS Universal’: Among Popular Realistic Models

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• They use WS-Universal Hamiltonian for nuclear structure calculations

Back to Parametric Correlations

Detecting Parametric Correlations

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- **Parametric correlations can be also detected by projecting the $\chi^2(p)$ onto a (p_j, p_k)-plane:**

$$\min_{i \neq j,k} \chi^2(p_1, p_2, \ \ldots p_m)$$

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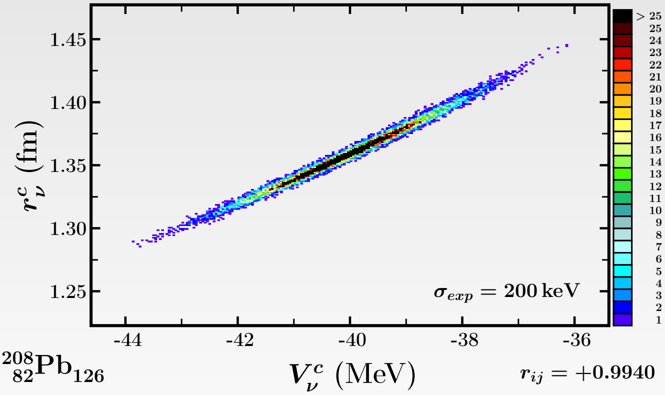

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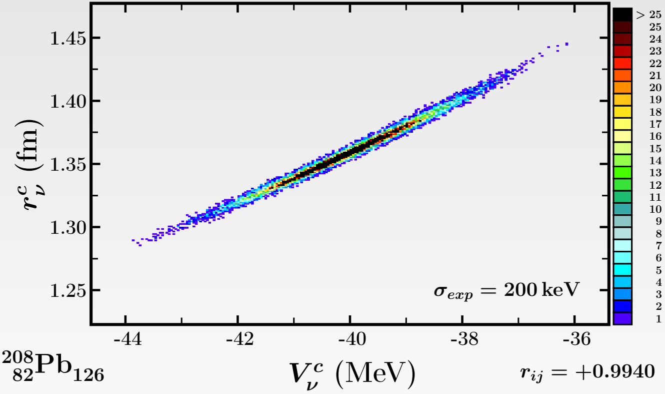
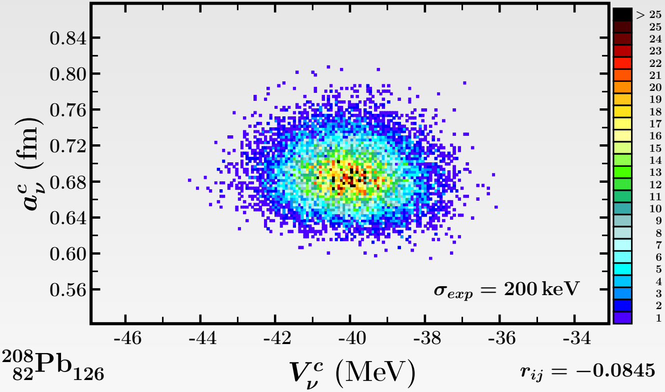


- **These results show that the central potential depth and central potential radius are correlated: $V_c \times r_c^2 \approx$ const.** **A possible ad hoc choice: $r_c \to r_c^{exp}$**

Parametric Correlations within WS-Central Potential: II

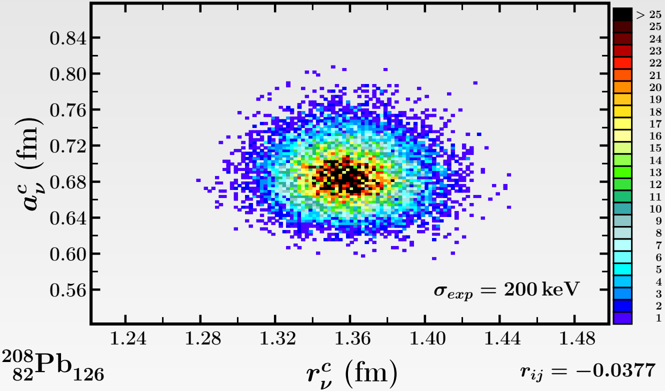
- **Using Monte Carlo Simulations and imposing $\sigma_{exp} = 200$ keV on the experimental neutron single particle energy levels of ^{208}Pb**



- **An approximate circular symmetry of this diagram shows ($r_{ij} \approx 0$) that the central potential depth and the central potential diffuseness are not correlated - therefore no danger to the predictive power!**

Parametric Correlations within WS-Central Potential: III

- **Using Monte Carlo Simulations and imposing $\sigma_{exp} = 200$ keV on the experimental neutron single particle energy levels of ^{208}Pb we find:**



- **Once again, the circular symmetry of this diagram shows ($r_{ij} \approx 0$) that the central potential radius and central potential diffuseness are not correlated - thus no danger to the predictive power**

Conclusion:

The central potential has only one correlation

$$\boxed{V_0^c = V_0^c(r_0^c)}$$

easy to remove

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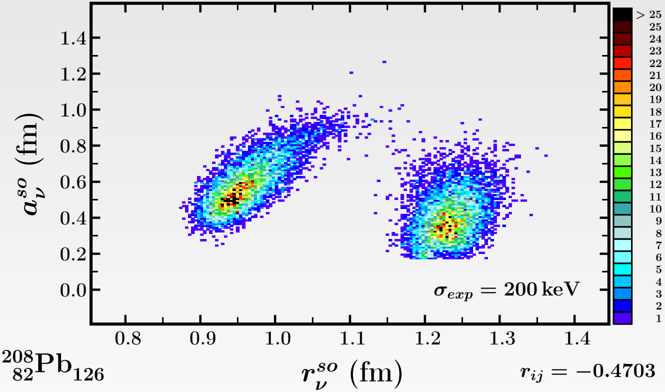
Next:

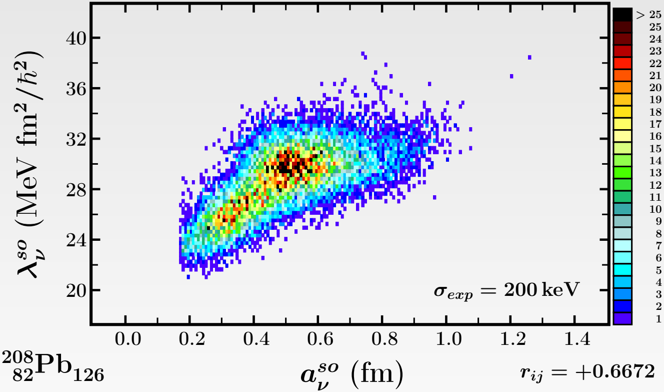
Checking the Spin-Orbit Potential

- **Using Monte Carlo simulations and imposing $\sigma_{exp} = 200$ keV on the experimental neutron single particle energy levels of ^{208}Pb we find two distributions:**



- **These results show that the spin-orbit diffuseness and the spin-orbit radius parameters are correlated: $r_{ij} \approx -0.5$**

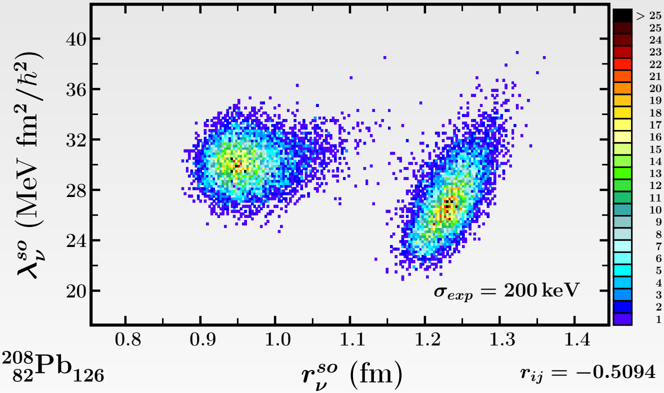
- **Using Monte Carlo simulations and imposing $\sigma_{exp} = 200$ keV to the experimental neutron single particle energy levels of ^{208}Pb we find a linear-like relation**



- **These results show that the spin-orbit diffuseness and the spin-orbit strength parameters are correlated: $r_{ij} \approx +0.7$**

Spin-Orbit Potential: New Forms of Correlations

- **Using Monte Carlo simulations and imposing σ_{exp} = 200 keV to the experimental neutron single particle energy levels of ^{208}Pb we find two distributions:**



- **These results show that the spin-orbit radius and spin-orbit strength parameters are correlated: $r_{ij} \approx -0.5$**

CONCLUSIONS:

The Spin-Orbit potential contains complex correlations:
Double-hump structures

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Double-hump structures

We identify two solutions for the spin-orbit parameters depending on the two 'optimal values' of r_ν^{so}, generating two hump maxima:

- **Compact configuration,** $r_\nu^{so} \sim 0.93$ fm
- **Non-compact configuration,** $r_\nu^{so} \sim 1.22$ fm

CONCLUSIONS:

The Spin-Orbit potential contains complex correlations: Double-hump structures

We identify two solutions for the spin-orbit parameters depending on the two 'optimal values' of r_ν^{so}, generating two hump maxima:

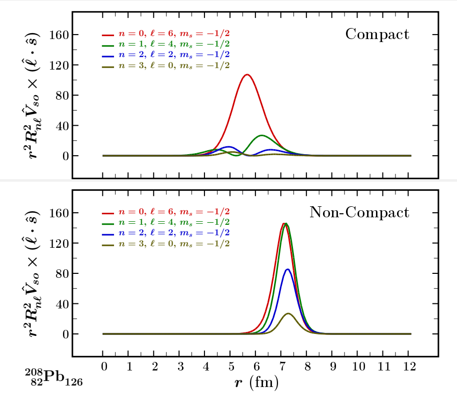
- **Compact configuration,** $r_\nu^{so} \sim 0.93$ fm
- **Non-compact configuration,** $r_\nu^{so} \sim 1.22$ fm

A question arises:
What is a possible physical difference between these solutions?

Comparing $\hat{V}_{so}$ Integrand Profiles

- **The potential 'communicates with the spectrum' via matrix elements**

$$\langle n\ell|\hat{V}_{\rm so}|n'\ell'\rangle \propto \int \underbrace{r^2 R_{n\ell}(r)\hat{V}_{\rm so}(r)R_{n'\ell'}(r)}_{\textbf{Integrand}}\,dr$$



- **Clearly the compact solution manifests some microscopic structure absent in the other**

Comparing $\hat{V}_{so}$ Integrand Profiles

- Compact and Non-Compact solutions produce microscopically different structures

- The compact solution in contrast to the non-compact one manifests microscopic sub-structures and offers better r.m.s. deviations

Type/name	neutron ^{208}Pb-r.m.s. [MeV]
compact	0.18
non-compact	0.29

- This is an interesting observation: The wave-functions in the nuclear interior carry seemingly a very useful structural information

- Moreover, N. Schunck has shown that the compact solutions generate systematically better rotational properties of nuclei!!

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

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

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

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

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

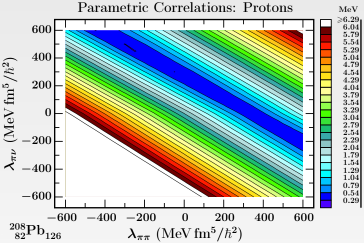
$$\hat{V}_{so}^{\pi} = \lambda_{\pi\pi} \frac{1}{r} \frac{d\rho_\pi}{dr} + \lambda_{\pi\nu} \frac{1}{r} \frac{d\rho_\nu}{dr} \qquad \text{Eq.(A)}$$

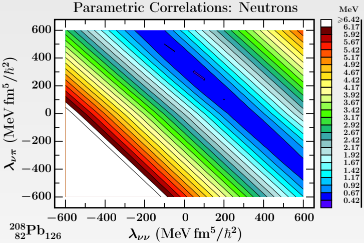
$$\hat{V}_{so}^{\nu} = \lambda_{\nu\pi} \frac{1}{r} \frac{d\rho_\pi}{dr} + \lambda_{\nu\nu} \frac{1}{r} \frac{d\rho_\nu}{dr} \qquad \text{Eq.(B)}$$

Advantages: The new expression includes the iterative self-consistency condition like in the microscopic HF approach rather than pure phenomenology and contains 4 parameters rather than 6. What are their correlations?

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

- **Correlation on the planes $(\lambda_{\pi\pi}, \lambda_{\pi\nu})$ and $(\lambda_{\nu\nu}, \lambda_{\nu\pi})$ for ^{208}Pb**



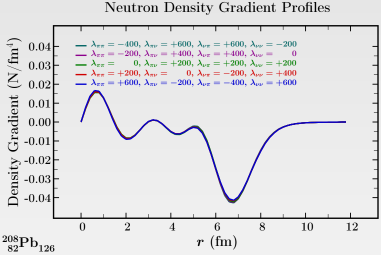


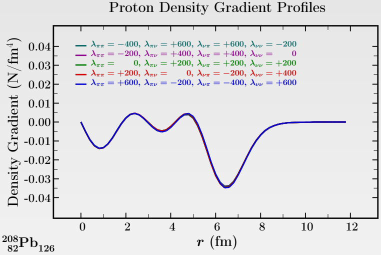
- **Realistic calculations indicate that the density-dependent spin-orbit potential parameters are correlated – but the correlations are perfectly linear**

$$\lambda_{qq'} = \alpha \cdot \lambda_{qq} + \beta$$

Microscopic Justification: Density-Dependent Profiles

• The <u>self-consistent</u> density gradient does not depend much on the choice of the strength-parameters $\{\lambda\}$





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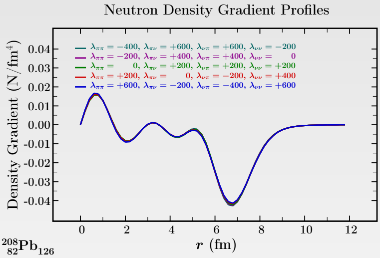

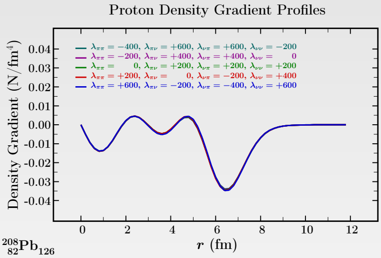

- For big-r values, corresponding to the vicinity of the nuclear surface Σ

$$\nabla\rho_\pi(r) \propto \nabla\rho_\nu(r) \Longrightarrow \nabla\rho_{q'}(r) \approx \mu\nabla\rho_q(r)$$

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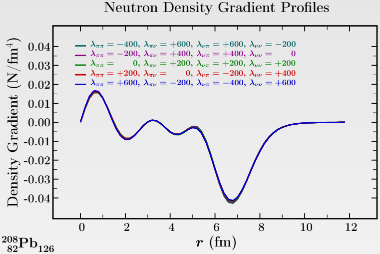

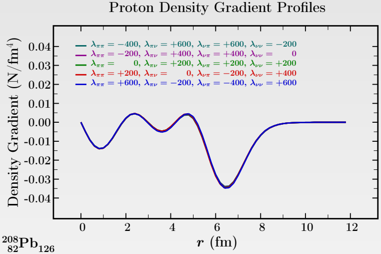

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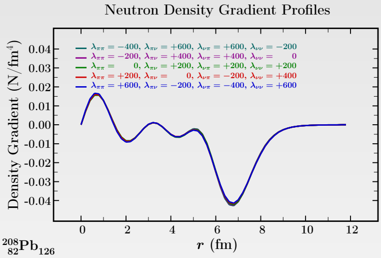

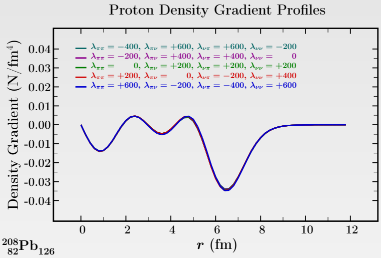

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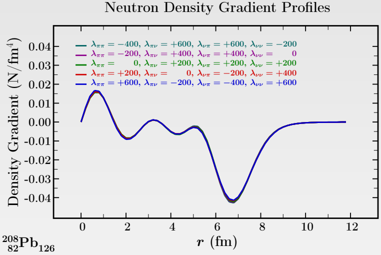

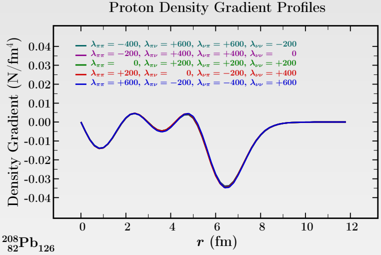

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A Working Conclusion

- A more detailed analysis shows that the valleys on the planes

$$(\lambda_{\pi\pi}, \lambda_{\pi\nu}) \text{ and } (\lambda_{\nu\nu}, \lambda_{\nu\pi})$$

cross at the common point for all the nuclei analysed where:

$$\lambda_{\pi\pi} \approx \lambda_{\pi\nu} \approx \lambda_{\nu\nu} \approx \lambda_{\nu\pi}$$

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We may significantly decrease the number of independent spin-orbit potential parameters thus eliminating correlations

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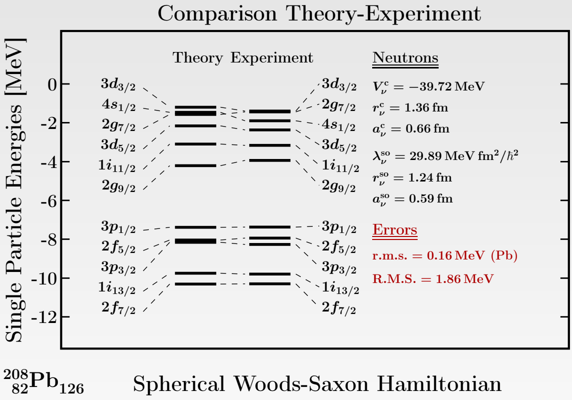
- **Conclusion:**

We may significantly decrease the number of independent spin-orbit potential parameters thus eliminating correlations

$\Longrightarrow$ **But: Do we loose/gain something? What?**

We Fit All the Six Parameters of Traditional $\hat{V}_{so}$

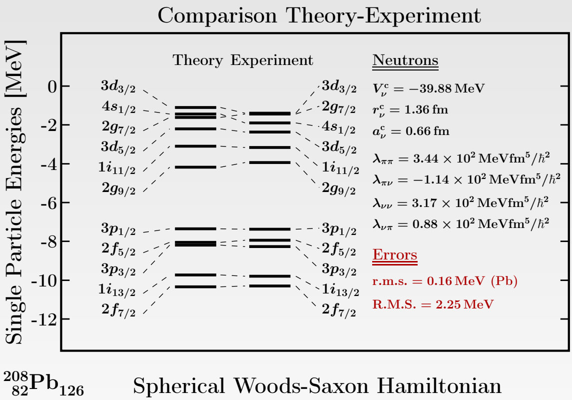
- We fit six parameters - $\{\lambda_\pi^{so}, r_\pi^{so}, a_\pi^{so}\}$ for protons and $\{\lambda_\nu^{so}, r_\nu^{so}, a_\nu^{so}\}$ for neutrons



- Results for ^{208}Pb: Neutrons → **Resulting r.m.s. = 0.16 MeV**
- Results for 8 nuclei, neutrons: ^{16}O, ^{40}Ca, ^{48}Ca, ^{56}Ni, ^{90}Zr, ^{132}Sn, ^{146}Gd, ^{208}Pb
  Parameters fitted to ^{208}Pb only: Neutrons → **Resulting R.M.S. = 1.86 MeV**

We Fit All the Four Parameters of the Density-Dependent $\hat{V}_{so}[\rho(r)]$

- We fit $\lambda_{nn}, \lambda_{np}, \lambda_{pn}, \lambda_{pp}$ of the **density-dependent – WS** to ^{208}Pb levels

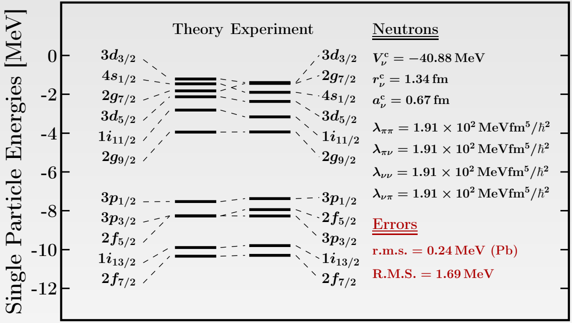


- ^{208}Pb-neutrons → **Results r.m.s. = 0.16 MeV** (unchanged)

- Results for ^{16}O, ^{40}Ca, ^{48}Ca, ^{56}Ni, ^{90}Zr, ^{132}Sn, ^{146}Gd, ^{208}Pb, the same parameters
8 nuclei neutrons → **Results R.M.S. = 2.25 MeV** (huge deterioration!)

- We introduce the constraint $\lambda_{nn} = \lambda_{np} = \lambda_{pn} = \lambda_{pp} \equiv \lambda$, and fit ^{208}Pb levels

Comparison Theory-Experiment



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

- ^{208}Pb-neutrons → **Results r.m.s. = 0.24 MeV** (small deterioration)
- Results for ^{16}O, ^{40}Ca, ^{48}Ca, ^{56}Ni, ^{90}Zr, ^{132}Sn, ^{146}Gd, ^{208}Pb, the same parameters 8 nuclei neutrons → **Solution R.M.S. = 1.69 MeV** (improvement!)
- Conjecture: **Equivalent to 1 parameter - common for protons and for neutrons**

What If We Increase the Sampling?

- We fit the parameters to ^{132}Sn and ^{208}Pb energy levels

- Neutron Results:

	^{208}Pb r.m.s. [MeV]	R.M.S. [MeV]
Density Dependent SO - 4 parameters	0.30	1.58
Density Dependent SO - 1 parameter	0.30	1.20

- Proton Results:

	^{208}Pb r.m.s. [MeV]	R.M.S. [MeV]
Density Dependent SO - 4 parameters	0.20	1.67
Density Dependent SO - 1 parameter	0.35	1.17

- **Conclusion I**: individual ^{208}Pb r.m.s. increased for both protons and neutrons, but still it can be considered a very good description

- **Conclusion II**: global R.M.S. improved for both protons and neutrons

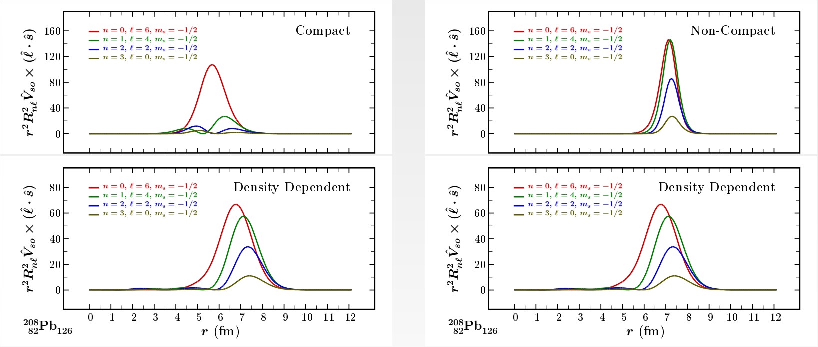
$\Longrightarrow$**Improvement in terms of Predictive Power!**

Back to Physical Significance of the Compact vs. Non-Compact Spin-Orbit Variants

Comparing $\hat{V}_{so}$-Density Dependent Integrand Profiles

- **The potential 'communicates with the spectrum' via matrix elements**

$$\langle n\ell|\hat{V}_{\rm so}|n'\ell'\rangle \propto \int \underbrace{r^2 R_{n\ell}(r)\hat{V}_{\rm so}[\rho(r)]R_{n'\ell'}(r)}_{\textbf{Integrand}}\, dr$$



- **The density dependent spin-orbit manifests similarities with the compact solution!**
- **These structures deserve attention since they improve the r.m.s-deviations!!**
- **In this project they were discovered when of analysing parametric correlations**

FINAL CONCLUSIONS:

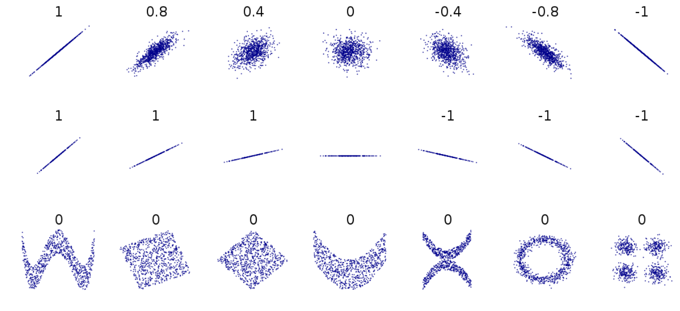
The self-consistent density-dependent,
and thus 'more microscopic' spin-orbit potential,
depends effectively on one parameter rather than six

- **By introducing the density-dependent spin-orbit potential we arrive at the eliminating of all parametric correlations → thus the implied problems**
- **We obtain better or equal quality of comparison with experiment**
- **Parametric correlations in the form of double hump distributions**
- **We show the microscopic background of the compact spin-orbit potential and certain parallels with the density-dependent one**

Thank you!

ANNEXE - Extra slides

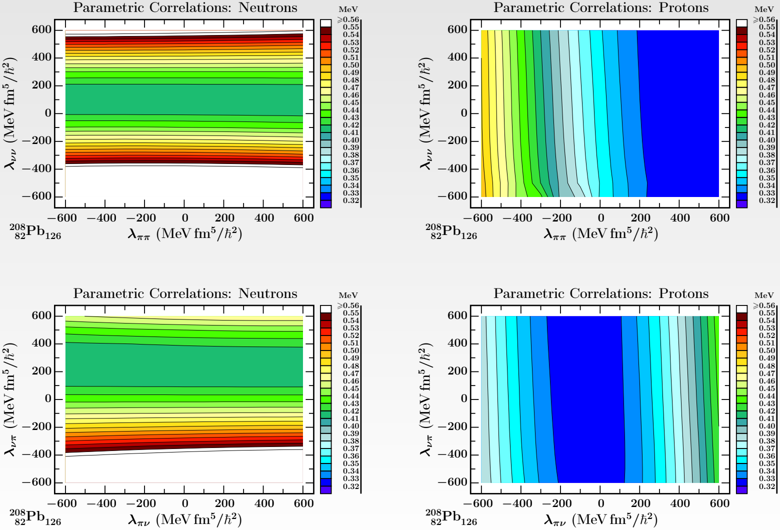
• From *Wikipedia*: two-dimensional (x, y) distributions of data-points with their corresponding values of Pearson Coefficient r_{ij}.



• **Observation**: the bottom row results show **correlated distributions which give $r_{ij} \approx 0$**

No Correlations in the Density-Dependent Spin-Orbit

- χ^2-projection onto the planes $(\lambda_{\pi\pi}, \lambda_{\nu\nu})$ and $(\lambda_{\pi\nu}, \lambda_{\nu\pi})$



Parametric Correlations

[Illustrations for Skyrme Hartree-Fock Hamiltonian]

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

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

Parameter-Correlations in Skyrme-HF

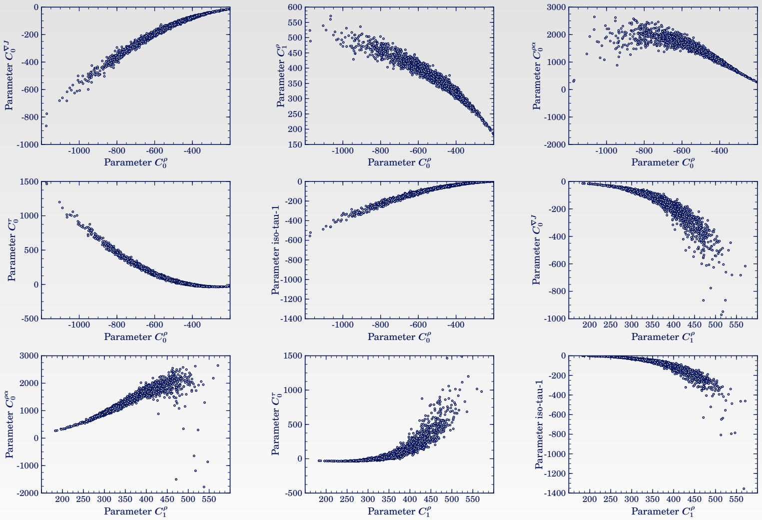


Illustration shows that majority of these parameters are strongly correlated excluding the prediction capacities of the model [B. Szpak, PhD thesis]

Parametric Correlations:

Strongly Present the Skyrme-Hartree-Fock Mean Fields

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The presence of parametric correlations implies that no stable extraneous predictive power can be obtained with this type of the Hamiltonians

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Strongly Present the Skyrme-Hartree-Fock Mean Fields

The presence of parametric correlations implies that no stable extraneous predictive power can be obtained with this type of the Hamiltonians

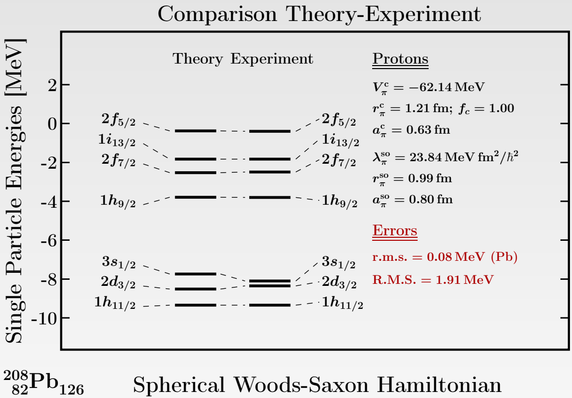
In other words: This type of the Hamiltonian may very well allow to fit the data: Stable extraneous predictions is another issue*)

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

We repeat the test for the protons

How Many Degrees of Freedom Does the V_{so} Have?

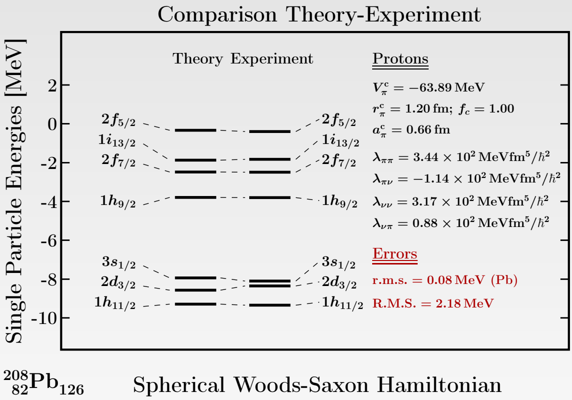
- We fit all the **traditional – WS** potential parameters to ^{208}Pb levels



- Results for ^{208}Pb-neutrons → **Solution r.m.s. = 0.08 MeV**
- Results for 8 nuclei neutrons → **Solution R.M.S. = 1.91 MeV**
- The answer: **6 parameters** - $\{\lambda^{so}, r_0^{so}, a_0^{so}\}$ for protons and $\{\lambda^{so}, r_0^{so}, a_0^{so}\}$ for neutrons

How Many Degrees of Freedom Does the V_{so} Have?

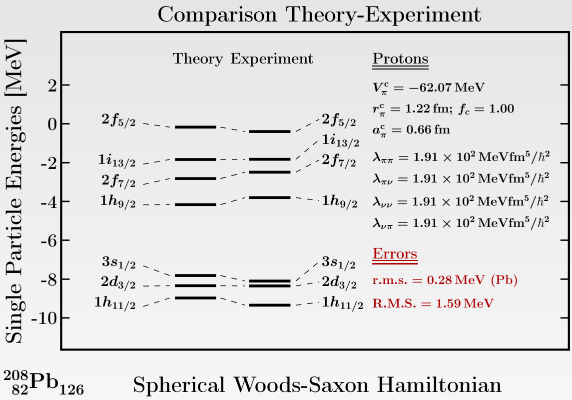
- We fit the **density-dependent – WS**: $\lambda_{nn}, \lambda_{np}, \lambda_{pn}, \lambda_{pp}$, to ^{208}Pb levels



- Results for ^{208}Pb-neutrons → **Solution r.m.s. = 0.08 MeV** (unchanged)
- Results for 8 nuclei neutrons → **Solution R.M.S. = 2.18 MeV** (huge deterioration!)
- The answer: **4 parameters** - for protons and neutrons

How Many Degrees of Freedom Does the V_{so} Have?

- We fit the **density-dependent – WS**: $\lambda_{nn} = \lambda_{np} = \lambda_{pn} = \lambda_{pp} \equiv \lambda$, to ^{208}Pb levels



- Results for ^{208}Pb-neutrons → **Solution r.m.s. = 0.28 MeV** (small deterioration)
- Results for 8 nuclei neutrons → **Solution R.M.S. = 1.59 MeV** (improvement!)
- The answer: **1 parameter** - common for protons and for neutrons