Predictive Power of Theoretical Modelling of the Nuclear Mean Field: Stochastic Approach

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The Fundamental Method:

Inverse Problem Theory of Applied Mathematics

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

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

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

To determine the optimal parameters of the Hamiltonian

Inverse Problem in Quantum Theories

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

$$\hat{\mathbf{H}}(\mathbf{p}) \rightarrow \{\mathbf{E_p}, \psi(\mathbf{p})\} \leftrightarrow \boxed{\hat{\mathcal{O}}_{\mathbf{H}}(\mathbf{p}) = \mathbf{d}^{\mathbf{th}} \leftarrow \textbf{Direct Problem}}$$

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

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

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

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- Usually we iterate this non-linear problem using Taylor linearization

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

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

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

Inverse Problem in Linearised Representation

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

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

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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 $\mathcal{A}$:

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

Stability of Solutions of Nuclear Inverse Problem

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

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

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

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

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... and even less of prediction capacities!

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

Parametric Correlations
within the Inverse Problem:

a. How to determine their presence?

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

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- From m-tuplets of obtained parameters, $\{p_1, p_2, \ldots\ p_m\}$, we construct the tables and projection plots like the ones which follow

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

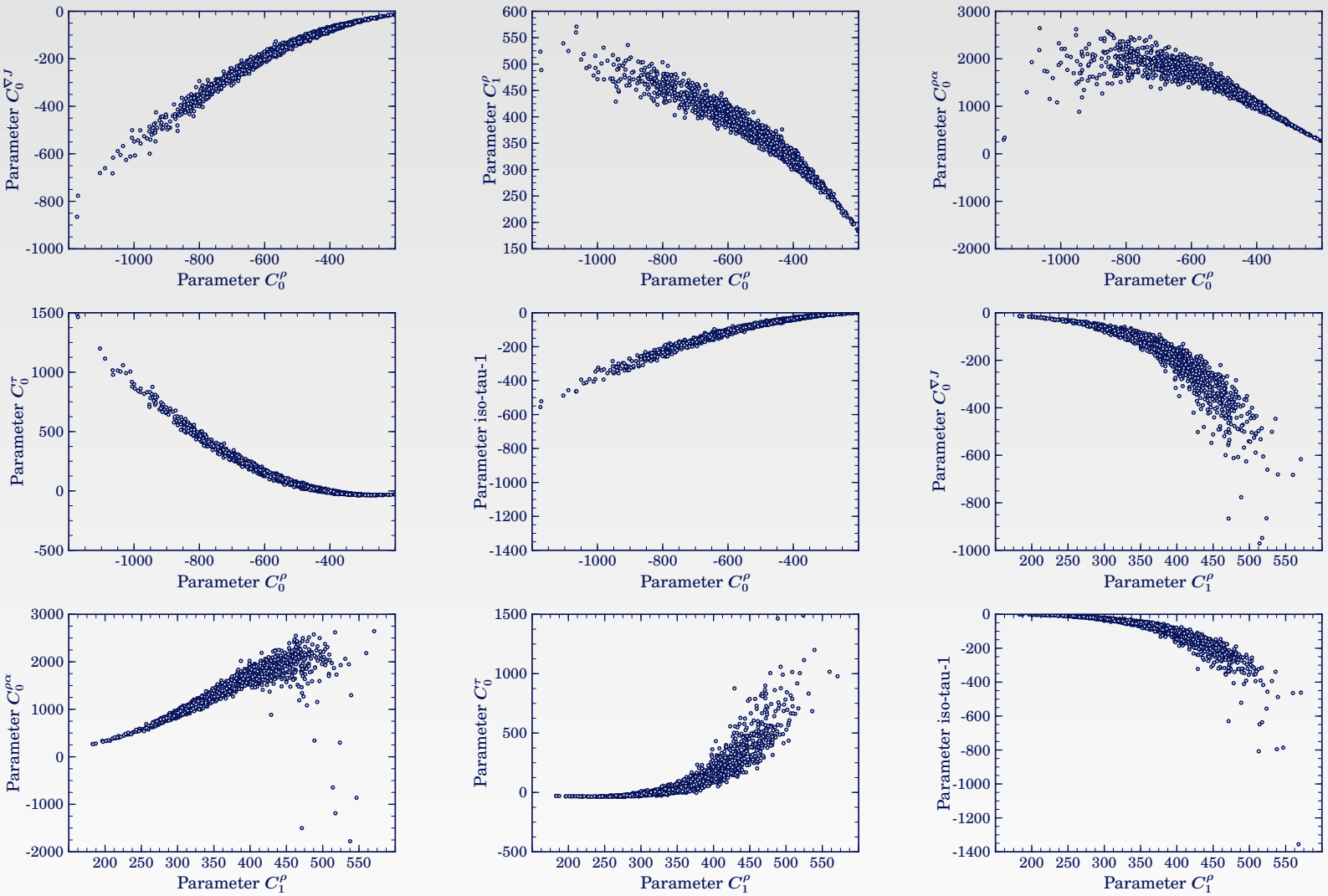

Illustration shows that majority of these parameters are strongly correlated excluding the prediction capacities of the model [B. Szpak, PhD thesis]

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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**

Selection of the Model Mean-Field Hamiltonian for the Project

‘WS Universal’: among Popular Realistic [Toy?] Models

• Here we decided to used the Woods-Saxon Universal Hamiltonian since our preliminary tests have shown much fewer parametric correlations

• This Hamiltonian is among the Popular Realistic Models, and it is used for calculations of deformed nuclei structure

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

• To simplify the task without loosing conceptual generality we limit ourselves to ‘experimentally known’ doubly-magic spherical-nuclei:

$$^{16}_{8}\mathrm{O}_{8},\ ^{40}_{20}\mathrm{Ca}_{20},\ ^{48}_{20}\mathrm{Ca}_{28},\ ^{56}_{28}\mathrm{Ni}_{28},\ ^{90}_{40}\mathrm{Zr}_{50},\ ^{132}_{50}\mathrm{Sn}_{82},\ ^{146}_{64}\mathrm{Gd}_{82},\ ^{208}_{82}\mathrm{Pb}_{126}$$

Woods-Saxon Hamiltonian: Central Potential

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

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

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

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

- In principle each of these parameters can be determined separately thus helping to counteract certain parametric correlations
- The importance – This potential is broadly used for deformed nuclei:

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

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

Woods-Saxon Hamiltonian: Spin-Orbit Potential

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

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

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

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

Back to the Parametric Correlation Problem

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

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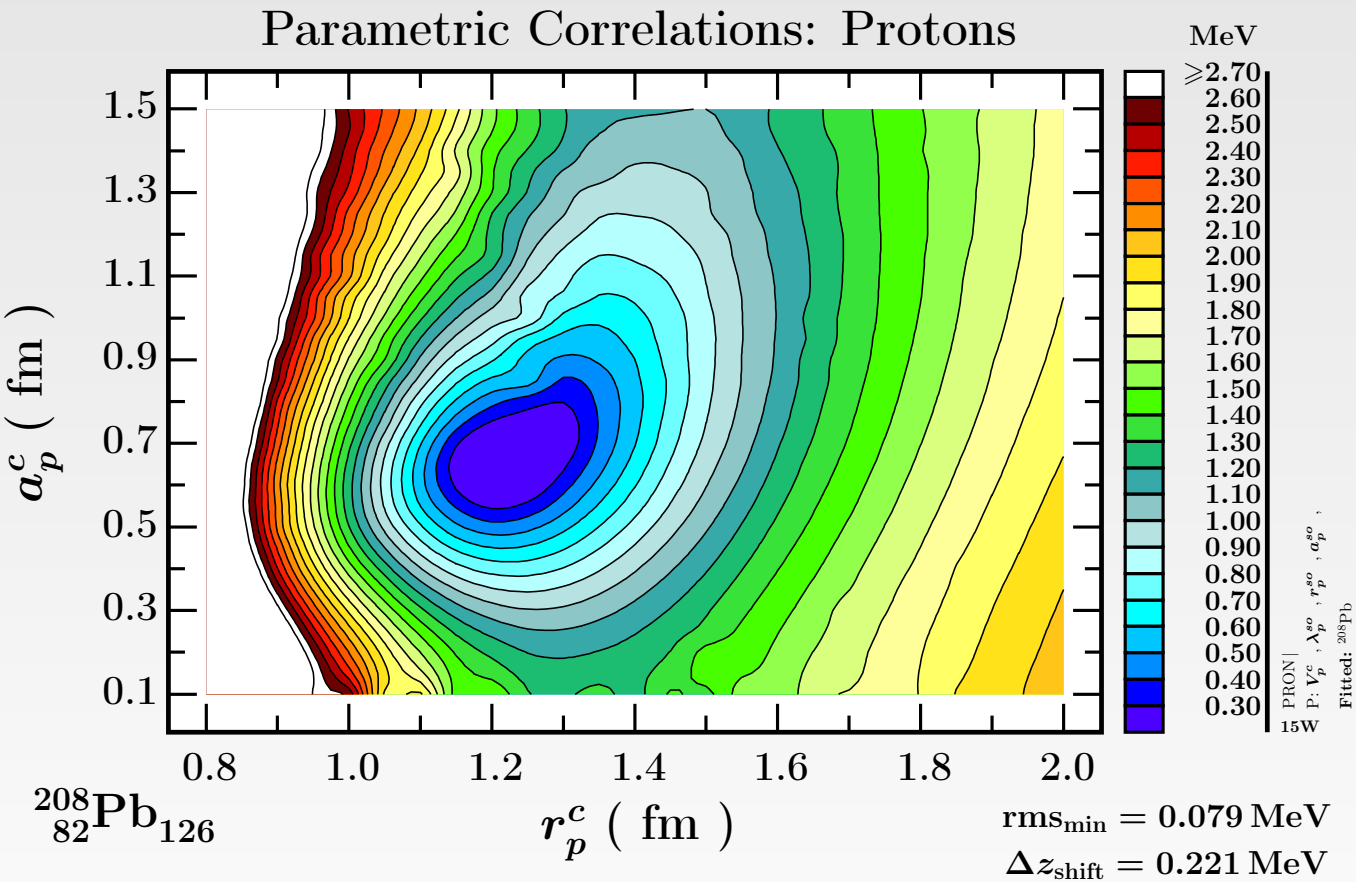

- **As the approximate circular symmetry of this diagram, shows that the central potential radius and central potential diffuseness are not correlated - thus no danger to the predictive power**

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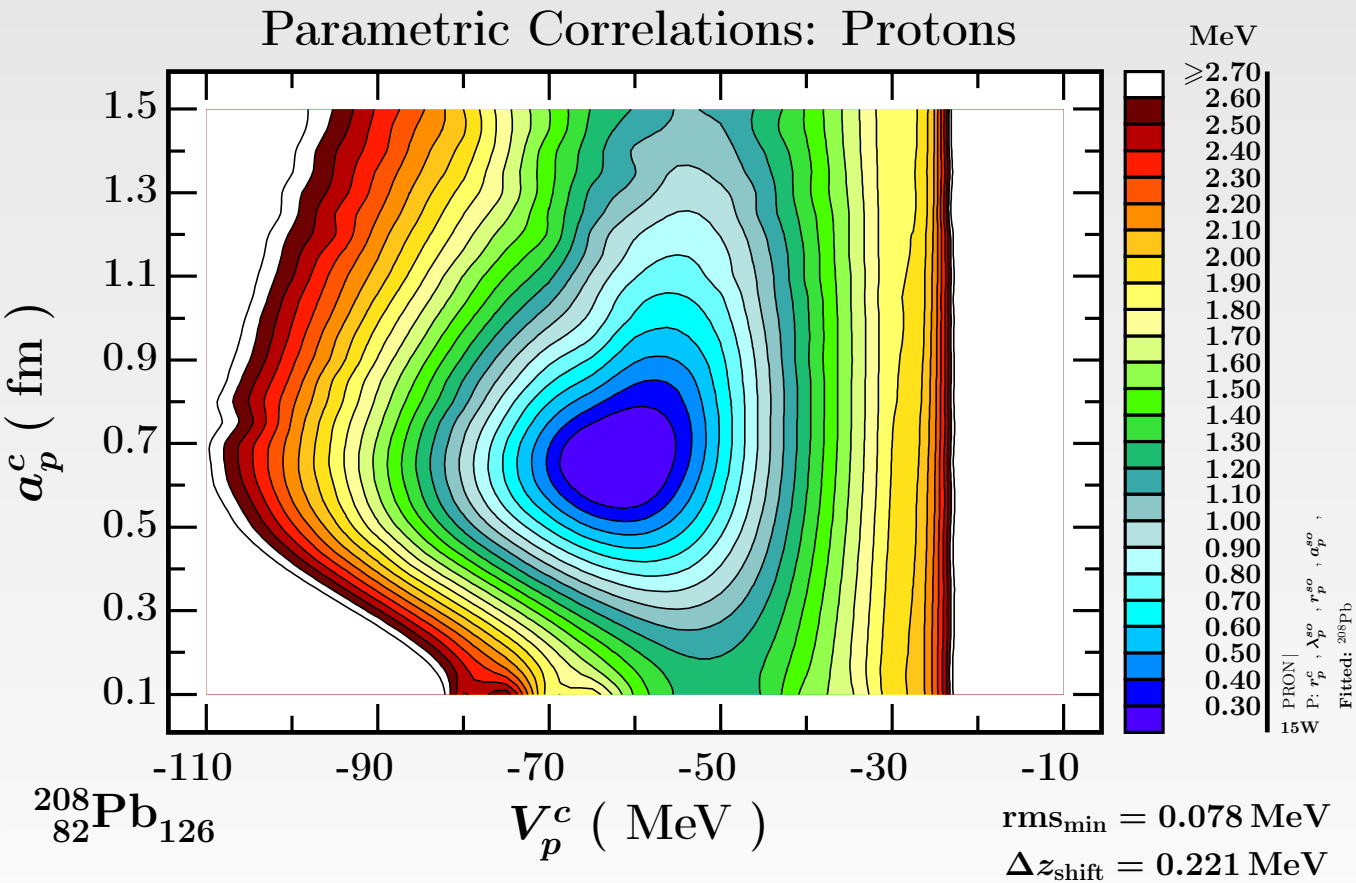

- These results show that the central potential **depth** and central potential **diffuseness** are not correlated - therefore no danger to the predictive power!

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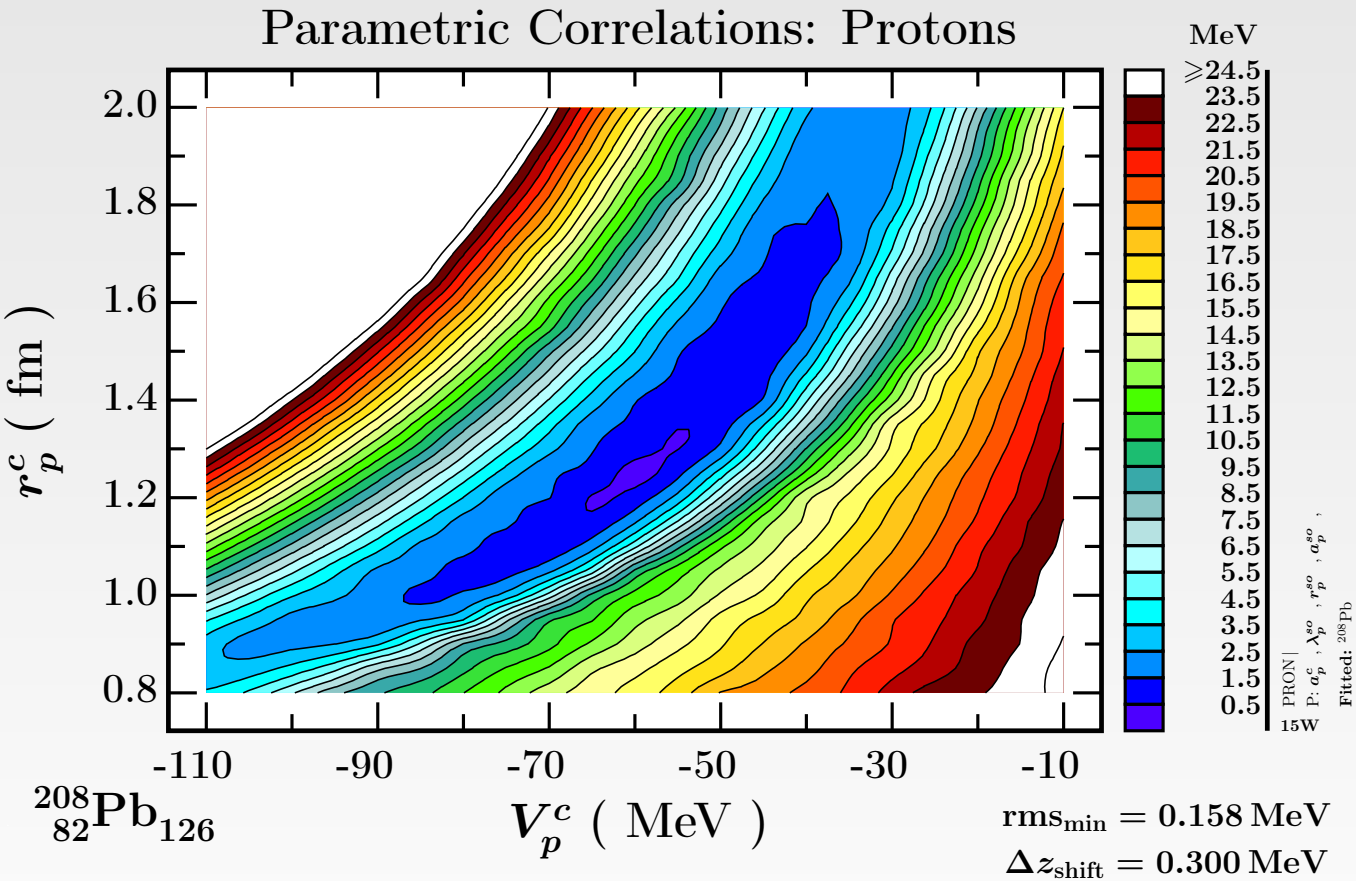

- These results show that the central potential depth and central potential radius are correlated: $V_c \times r_c^2 \approx \mathrm{const.}$ An ad hoc choice: $r_c \rightarrow r_c^{\mathrm{exp.}}$

Conclusion:

The Central Potential is virtually free from correlations

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Next:

Checking the Spin-Orbit Potential

The Spin-Orbit Situation is More Complex

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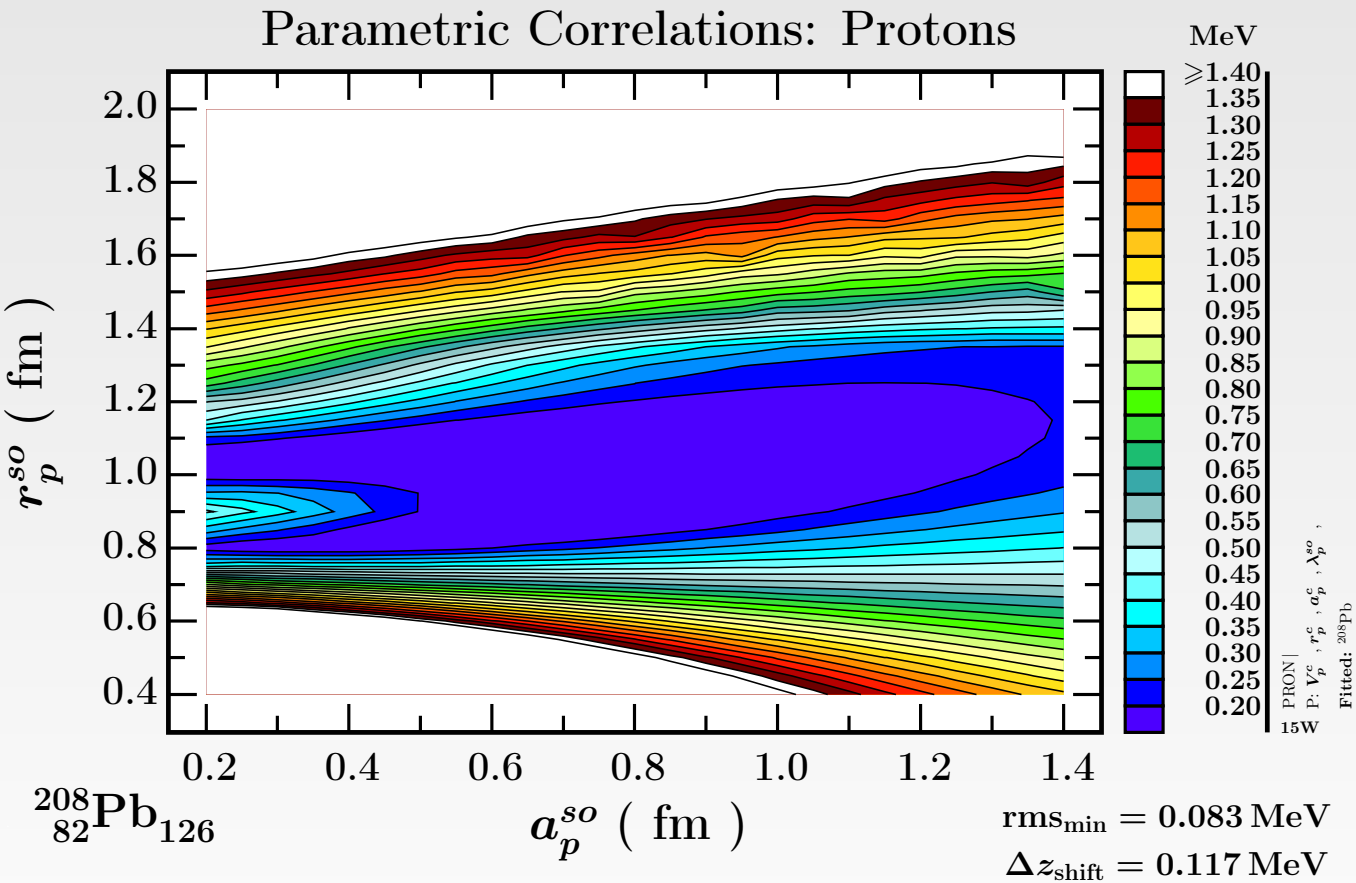

- These results show that the spin-orbit **diffuseness** and spin-orbit **radius** are weakly correlated

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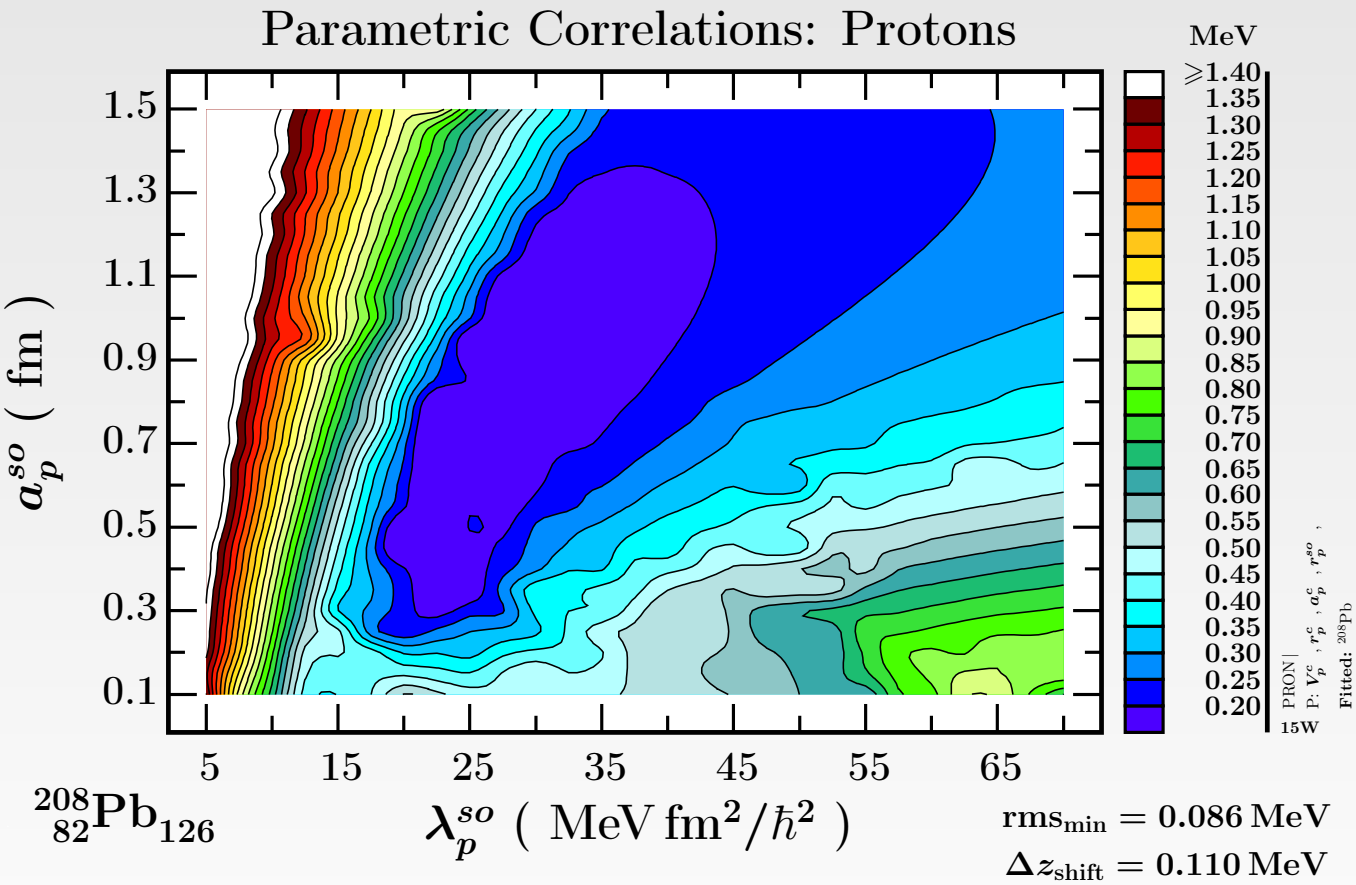

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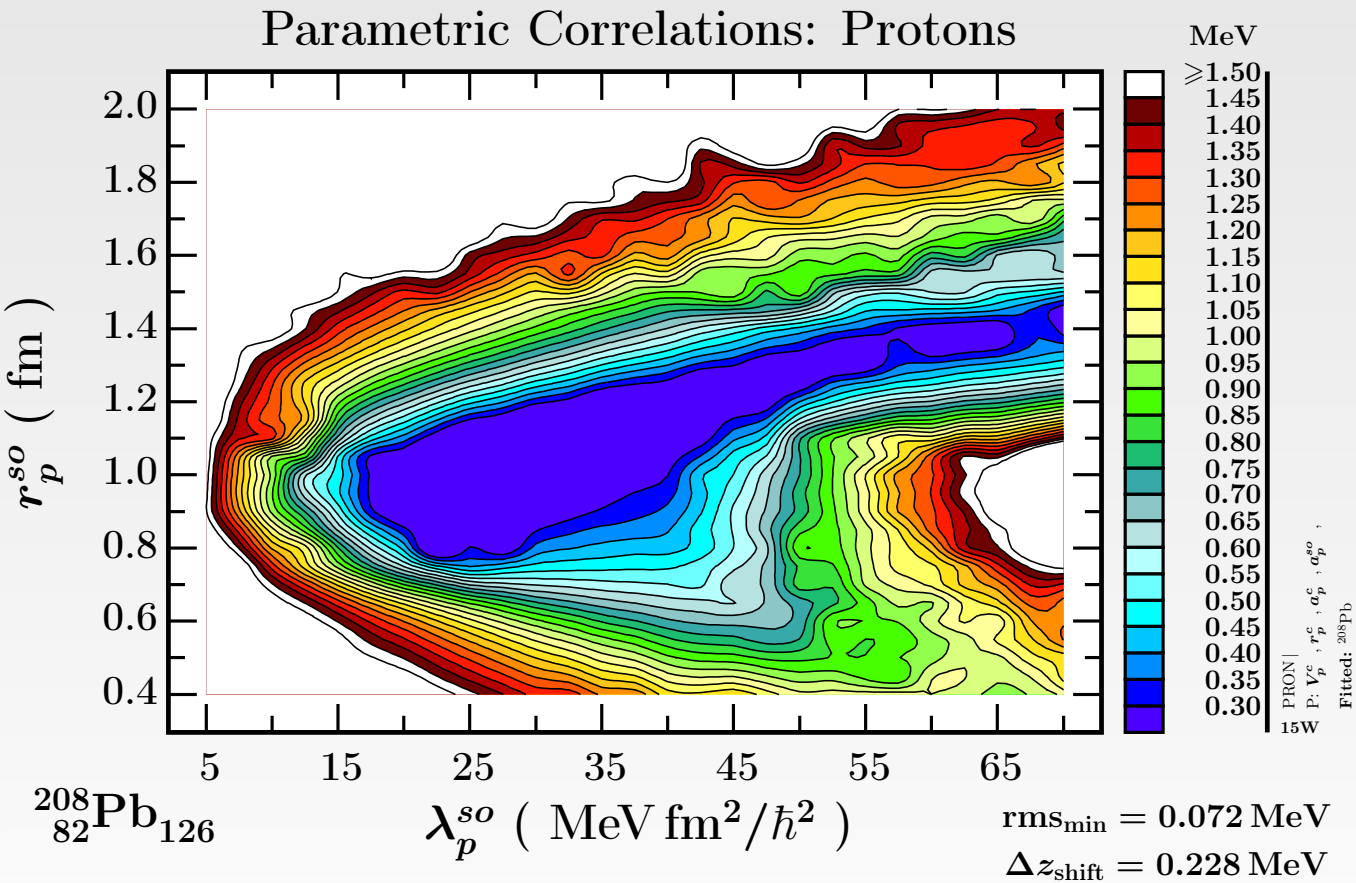

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Our solution:

Seek physics arguments eliminating correlations

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The Spin-Orbit Potential contains weak but complex correlations

Our solution:

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A possible alternative:

Using Applied–Mathematics regularisation–methods, e.g.: 'Truncated Singular Value Decomposition Theorem'

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However, here we follow the first approach $\rightarrow\rightarrow\rightarrow$

Physics-Guided Improvements of the WS Universal

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

$$\hat{\mathbf{v}}_2 \leftrightarrow \hat{\mathbf{v}}_{\mathbf{two-body}}(\vec{\mathbf{r}}_\mathbf{i} - \vec{\mathbf{r}}_\mathbf{j}) \rightarrow \mathbf{V}_{\mathbf{mean-field}}(\vec{\mathbf{r}}_\mathbf{i}) \leftrightarrow \hat{\mathbf{V}}_{\mathbf{mf}}(\vec{\mathbf{r}}_\mathbf{i})$$

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

- Here we follow the 'microscopic generalisaton 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* $\Rightarrow$

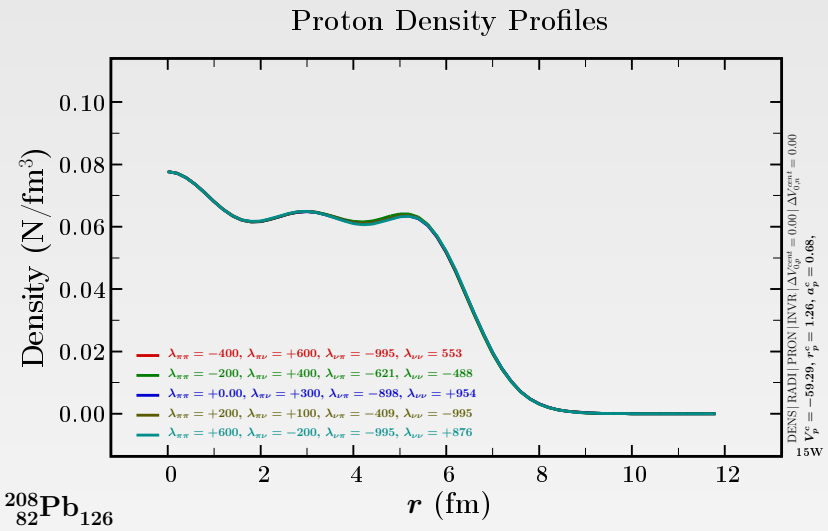
$$\hat{\mathbf{V}}^{\pi}_{\mathbf{so}} = \lambda_{\pi\pi} \frac{\mathbf{1}}{\mathbf{r}} \frac{\mathbf{d}\rho_\pi}{\mathbf{dr}} + \lambda_{\pi\nu} \frac{\mathbf{1}}{\mathbf{r}} \frac{\mathbf{d}\rho_\nu}{\mathbf{dr}} \qquad \textbf{Eq.(A)}$$

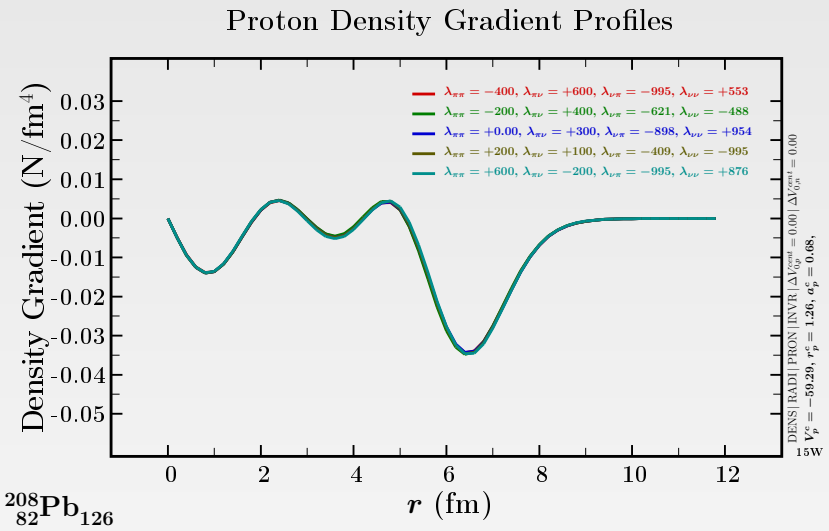
$$\hat{\mathbf{V}}^{\nu}_{\mathbf{so}} = \lambda_{\nu\pi} \frac{\mathbf{1}}{\mathbf{r}} \frac{\mathbf{d}\rho_\pi}{\mathbf{dr}} + \lambda_{\nu\nu} \frac{\mathbf{1}}{\mathbf{r}} \frac{\mathbf{d}\rho_\nu}{\mathbf{dr}} \qquad \textbf{Eq.(B)}$$

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?

Density-Dependent Profiles

- **The first preliminary tests show that the selfconsistent density and the density gradient do not depend much on the choice of the λ parameters**



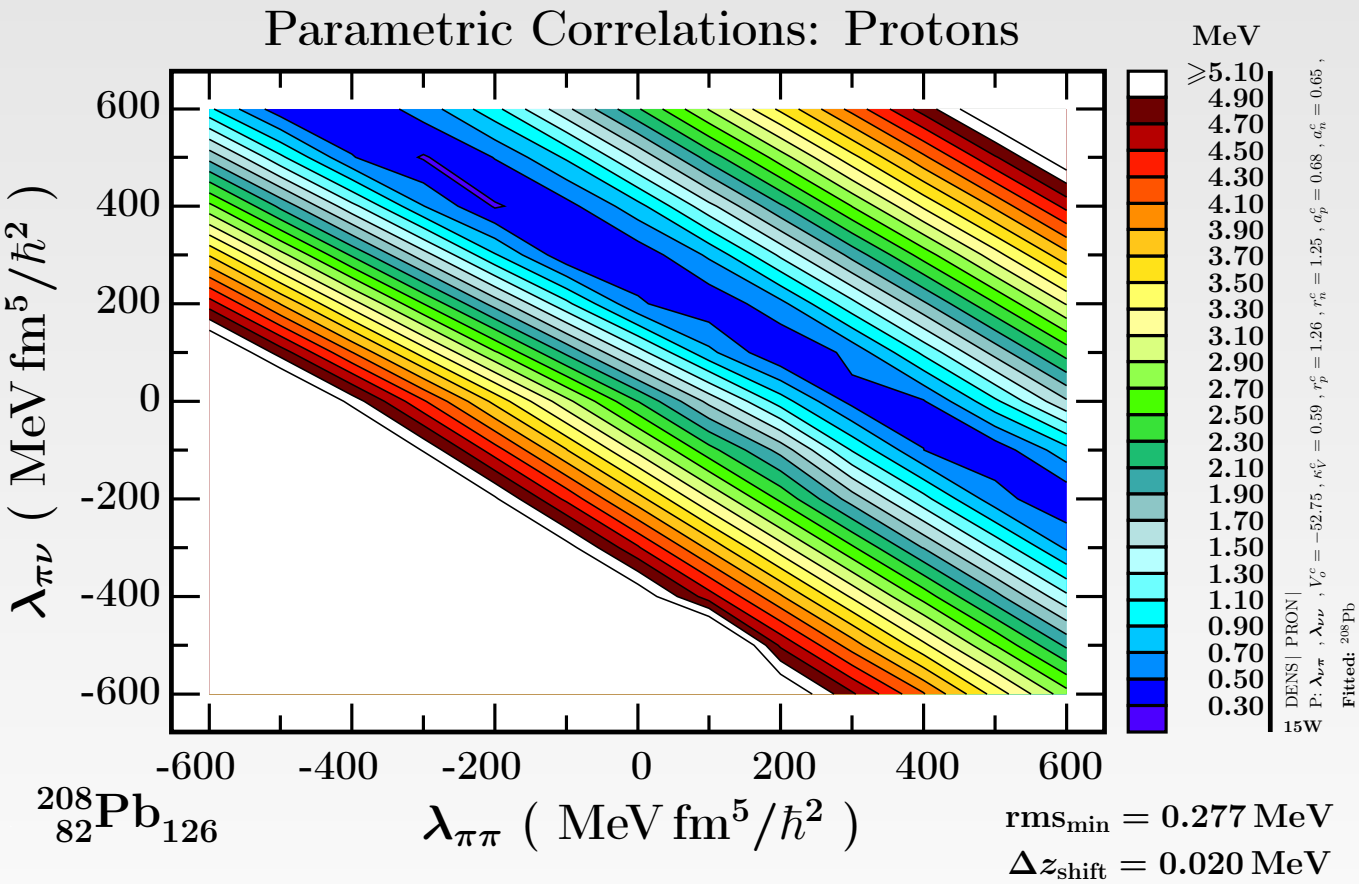


- **This means that after the minimisation, parameters compensate mutually their impact... But this must imply the linear parametric $\lambda - \lambda$ correlations!**

$$\hat{V}_{so}^{\pi} = \lambda_{\pi\pi} \frac{1}{r} \frac{d\rho_{\pi}}{dr} + \lambda_{\pi\nu} \frac{1}{r} \frac{d\rho_{\nu}}{dr}$$

Density-Dependent Spin-Orbit: Linear Correlations

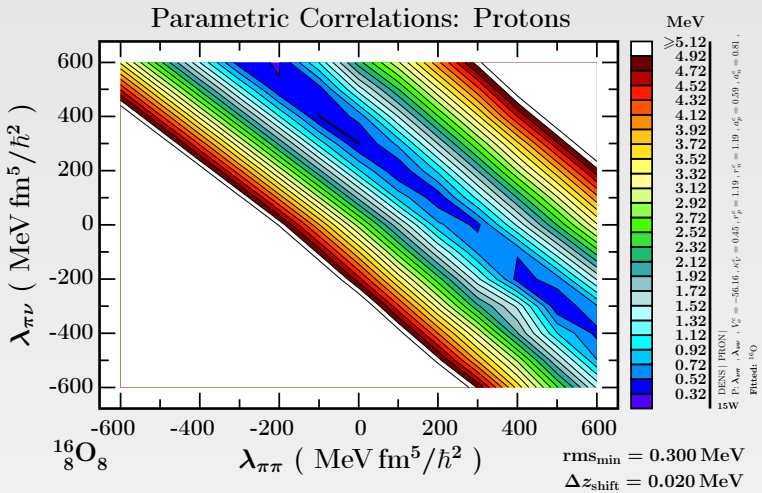
- **Correlation between $\lambda_{\pi\pi}$ and $\lambda_{\pi\nu}$ for ^{208}Pb**

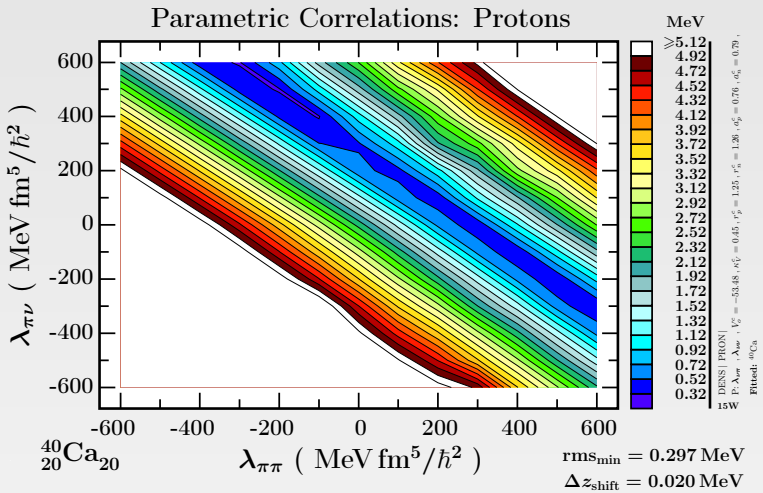


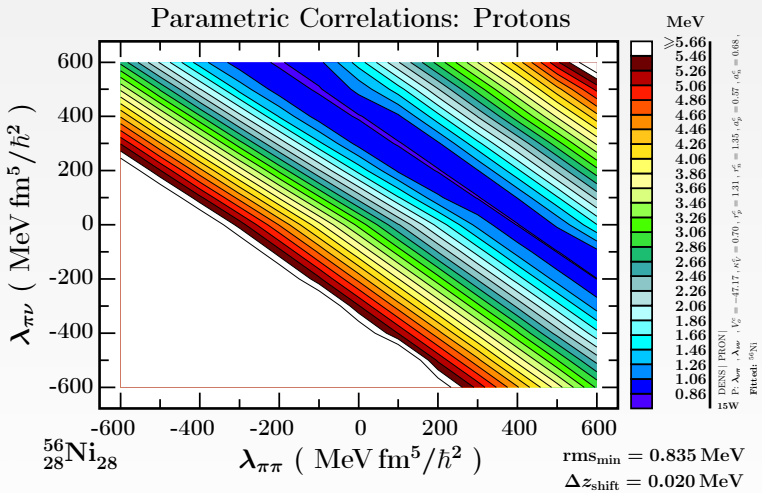
- **Realistic calculations indicate that the density-dependent spin-orbit potential parameters are correlated – but the correlations are perfectly linear**

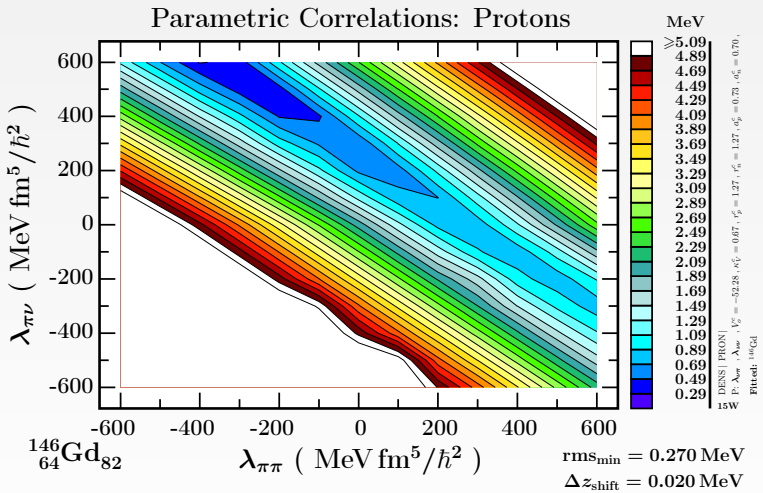
Linear-Correlations in Density-Dependent Spin-Orbit

- **The same as before but for ^{16}O, ^{40}Ca, ^{56}Ni and ^{146}Gd**



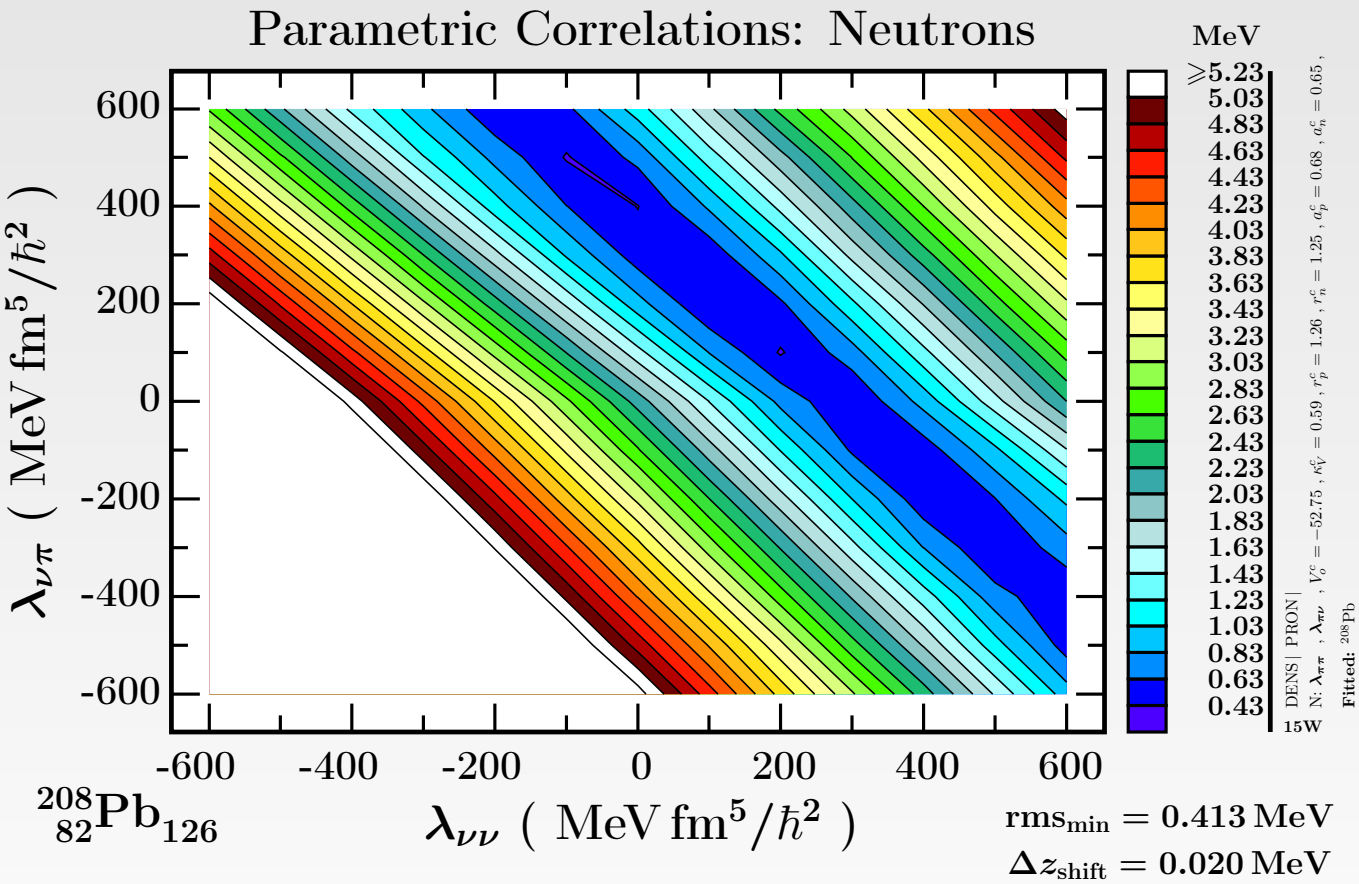






Density-Dependent Spin-Orbit: Linear Correlations

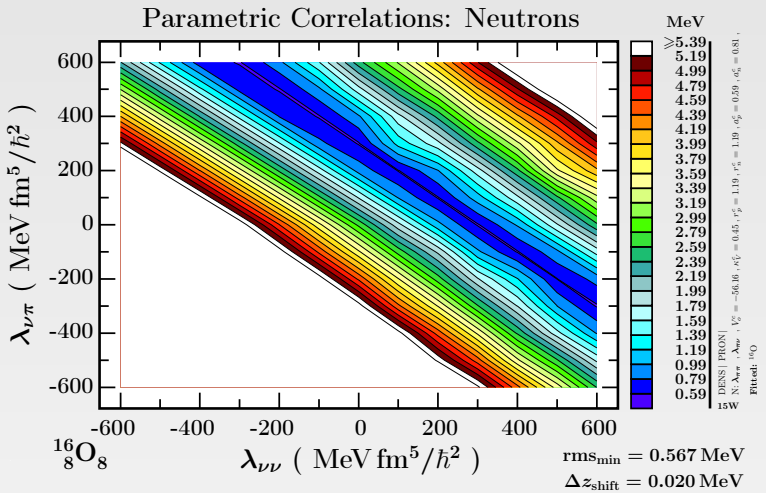
- **Correlation between $\lambda_{\nu\nu}$ and $\lambda_{\nu\pi}$ for ^{208}Pb**

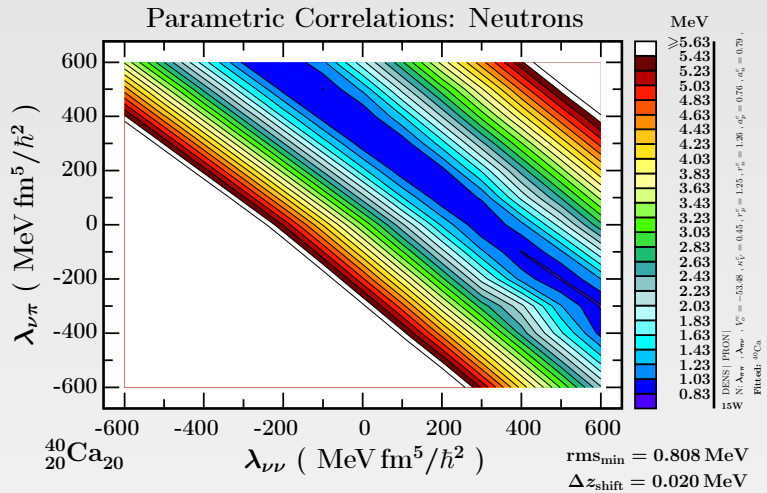


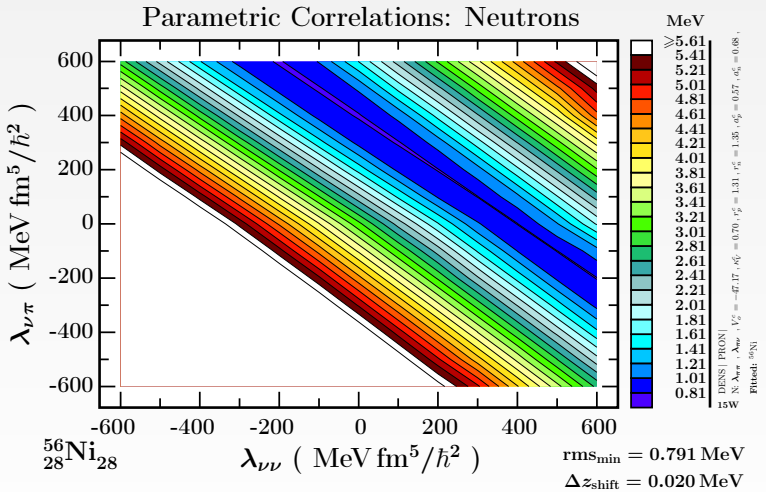
- **Calculations show that the density-dependent spin-orbit potential parameters are correlated – but the $\lambda_{\nu\nu} - \lambda_{\nu\pi}$ correlations are perfectly linear**

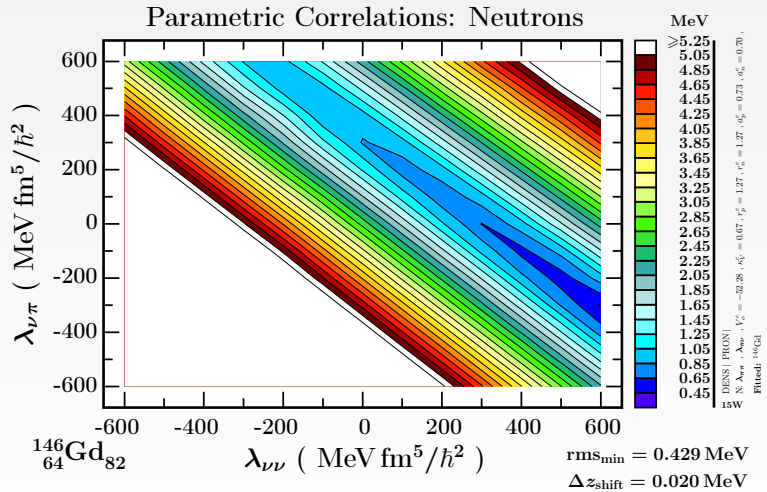
Linear-Correlations in Density-Dependent Spin-Orbit

- **The same as before but for ^{16}O, ^{40}Ca, ^{56}Ni and ^{146}Gd**









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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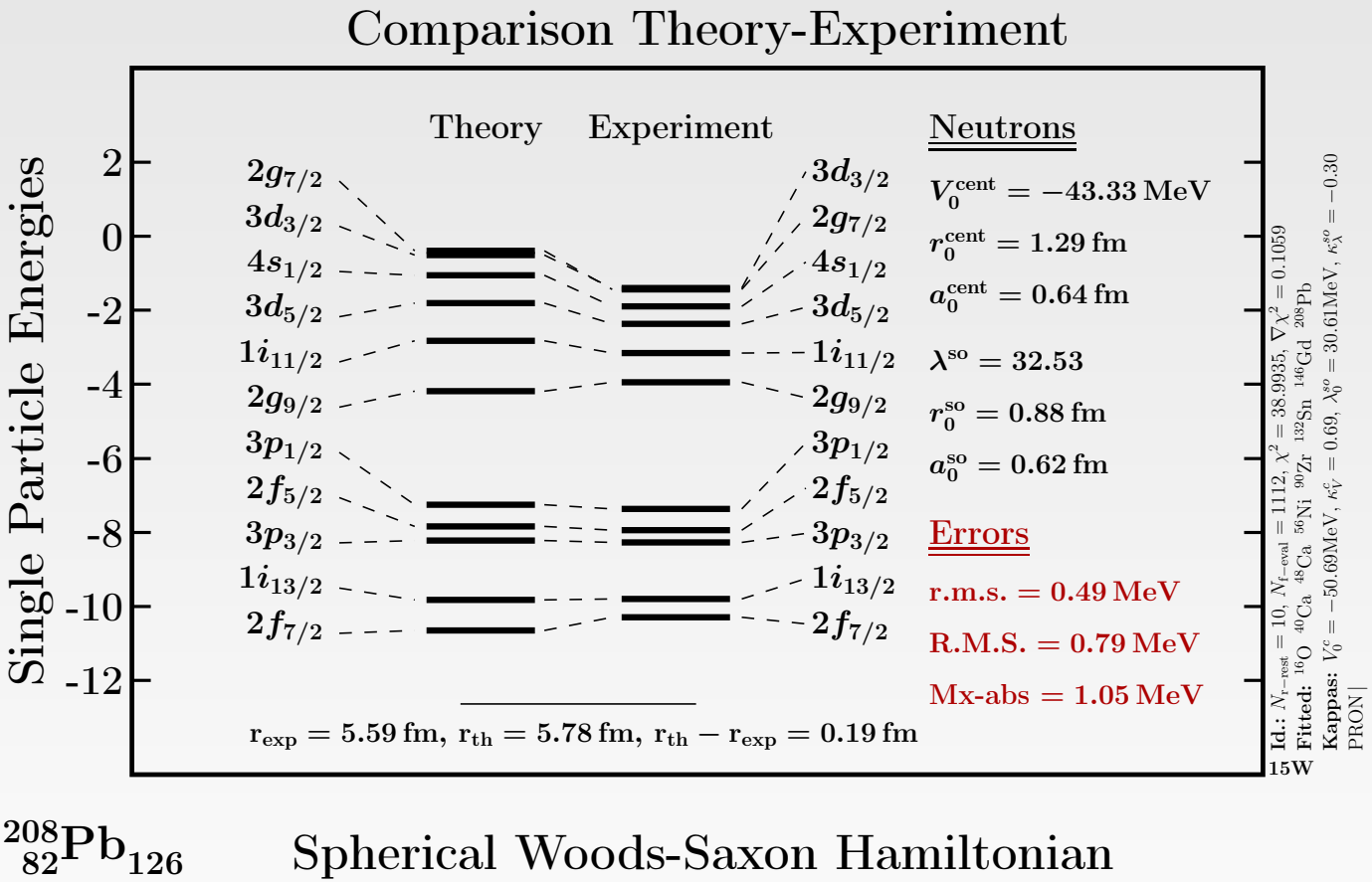
- **Conclusion: We may significantly decrease the number of spin-orbit potential parameters thus eliminating correlations. But: Do we loose something? What?**

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

- **We fit all the traditional WS potential parameters to eight nuclei (60 neutron levels plus 45 proton levels)**

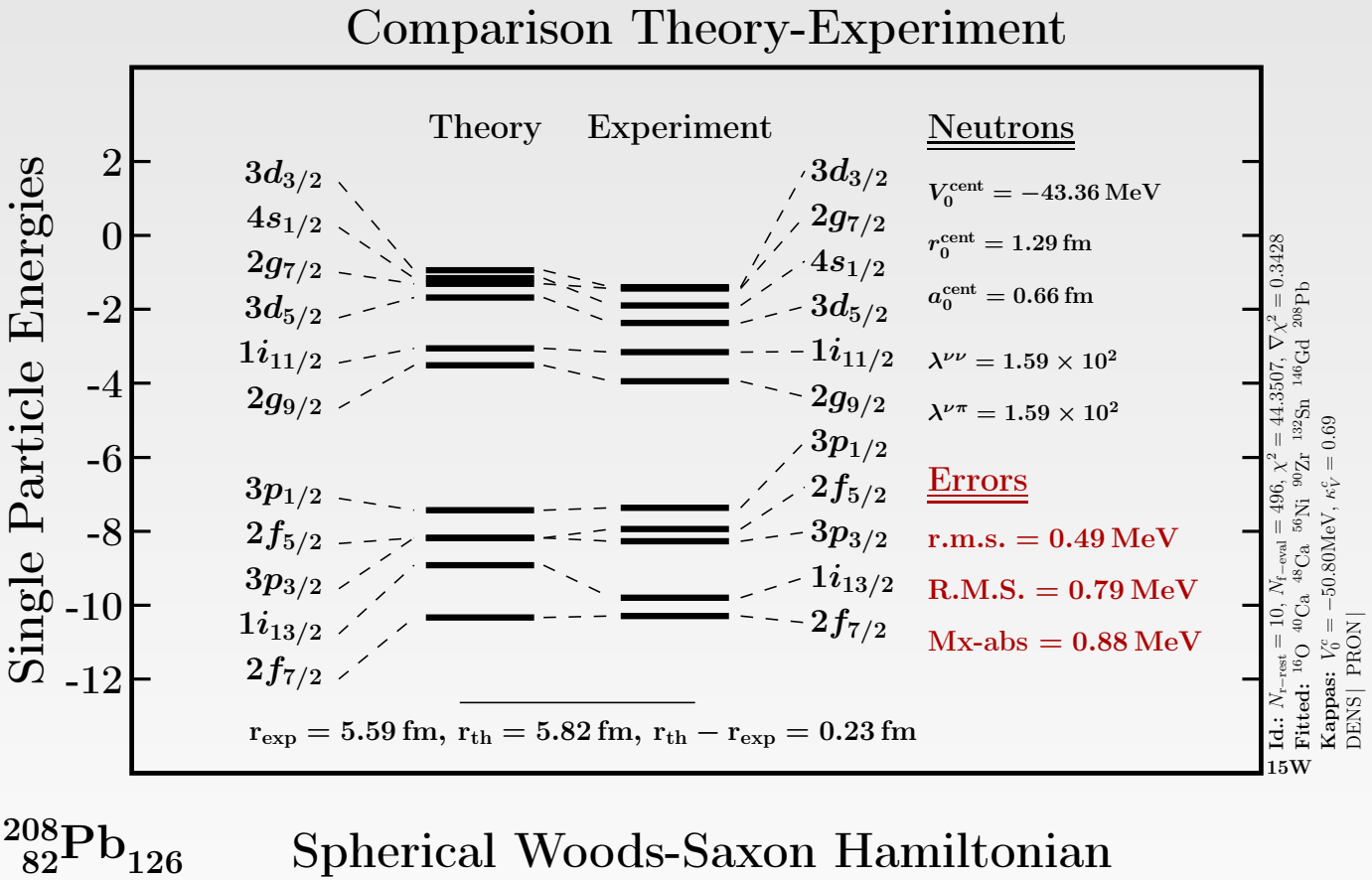


$^{208}_{82}Pb_{126}$ Spherical Woods-Saxon Hamiltonian

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

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

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



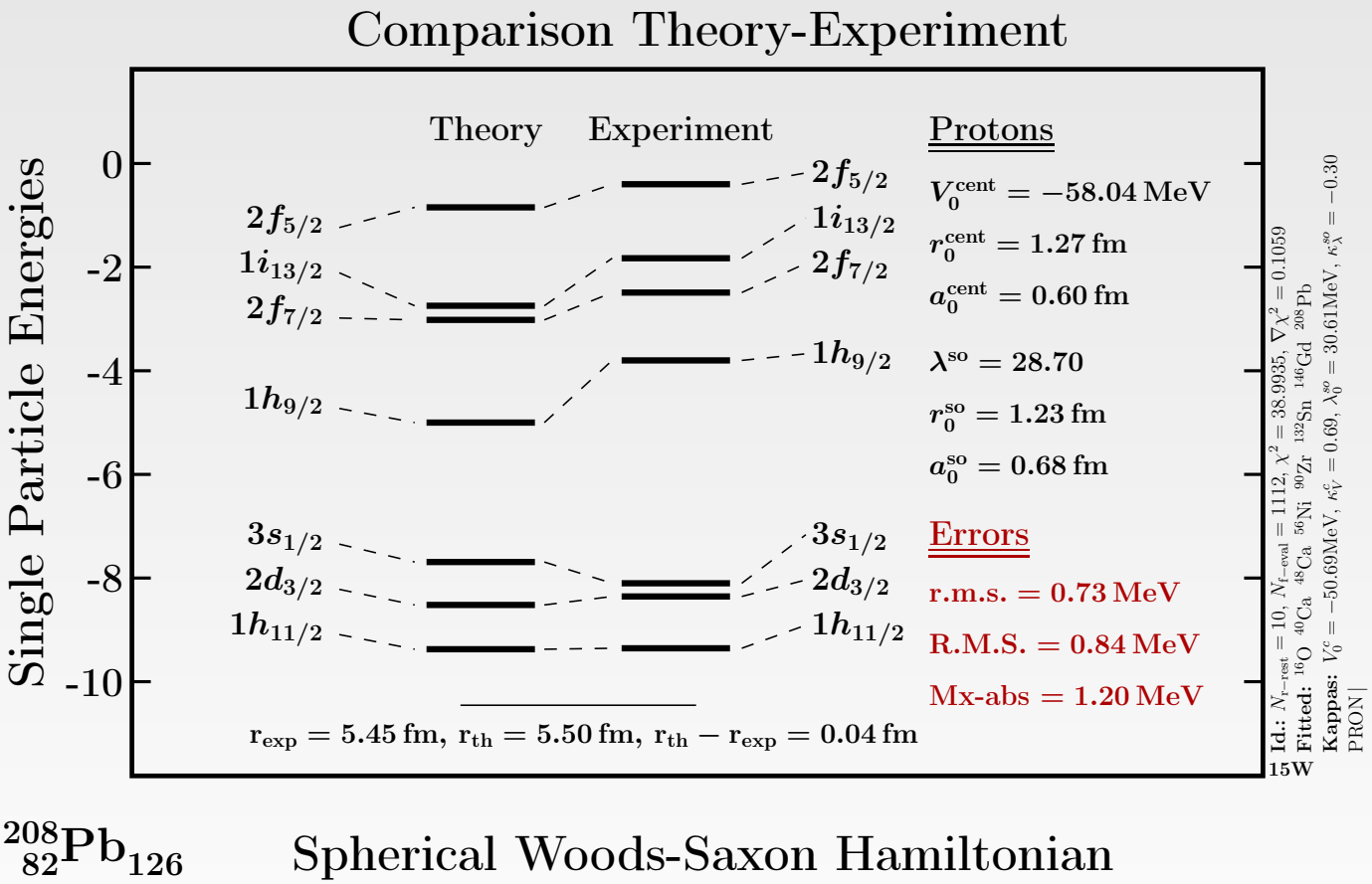
$^{208}_{82}\mathrm{Pb}_{126}$ Spherical Woods-Saxon Hamiltonian

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

We repeat the test for the protons

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

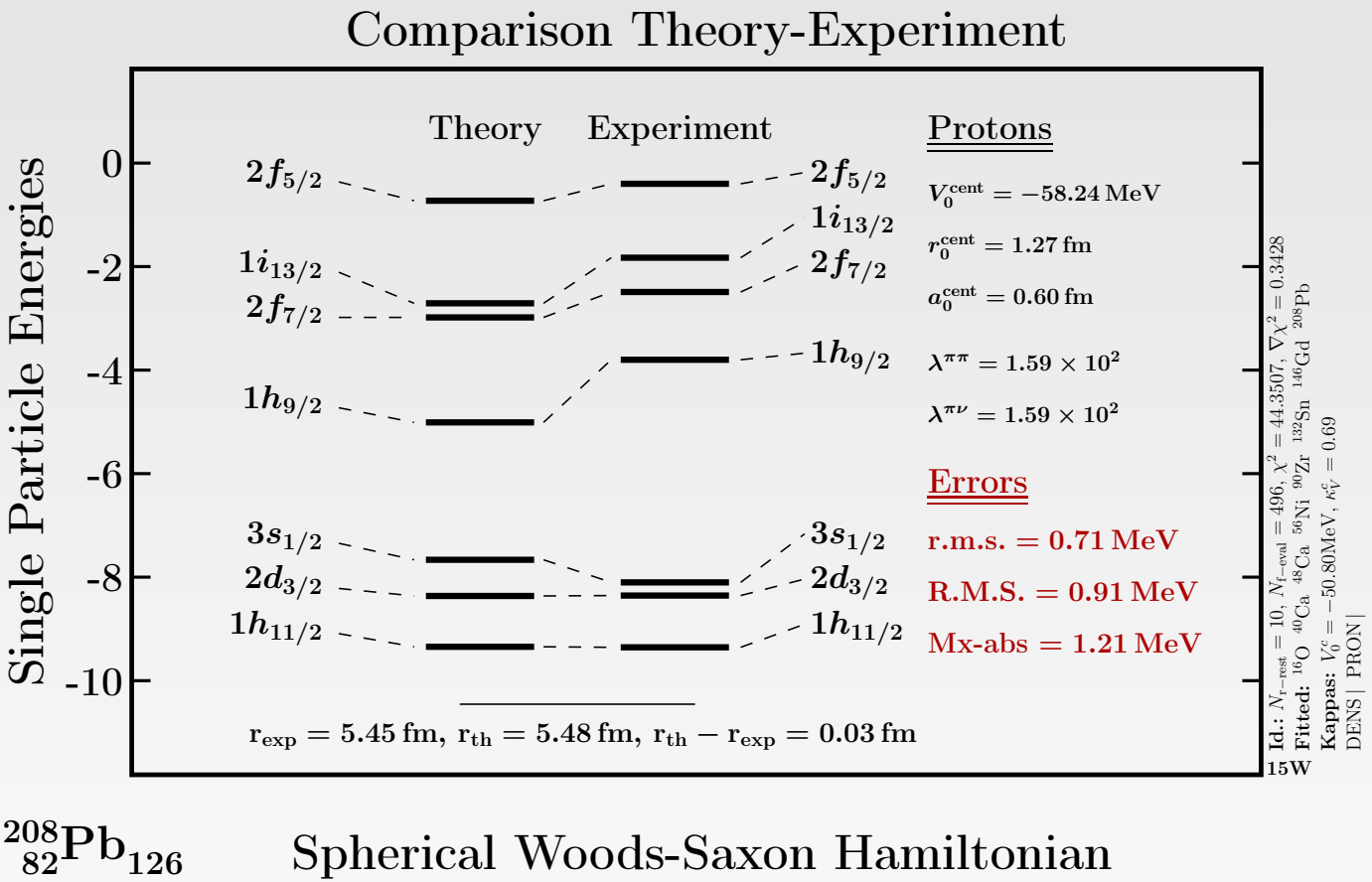
- **We fit all the traditional WS potential parameters to eight nuclei (60 neutron levels plus 45 proton levels)**



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

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

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



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

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

Conclusions & Summary

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Conclusions & Summary

- We need to take into account both the theory uncertainties and the experimental errors in order to determine the uncertainties of the model predictions
- The model needs to be verified for the presence/absence of parametric correlations
- The model predictions need to be verified for their stability
- In the case of presence of parametric correlations, we need to eliminate them.
- We have shown that eliminating the spin-orbit parametric correlations, we obtained better or equal quality result.

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

Conclusions:

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

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

With this strategy in mind:

What are the actualised research directions for the project?

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

• Determine quantitative limitations from the today's constraints such as experimental and theory errors which we cannot bypass today

In other words:

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

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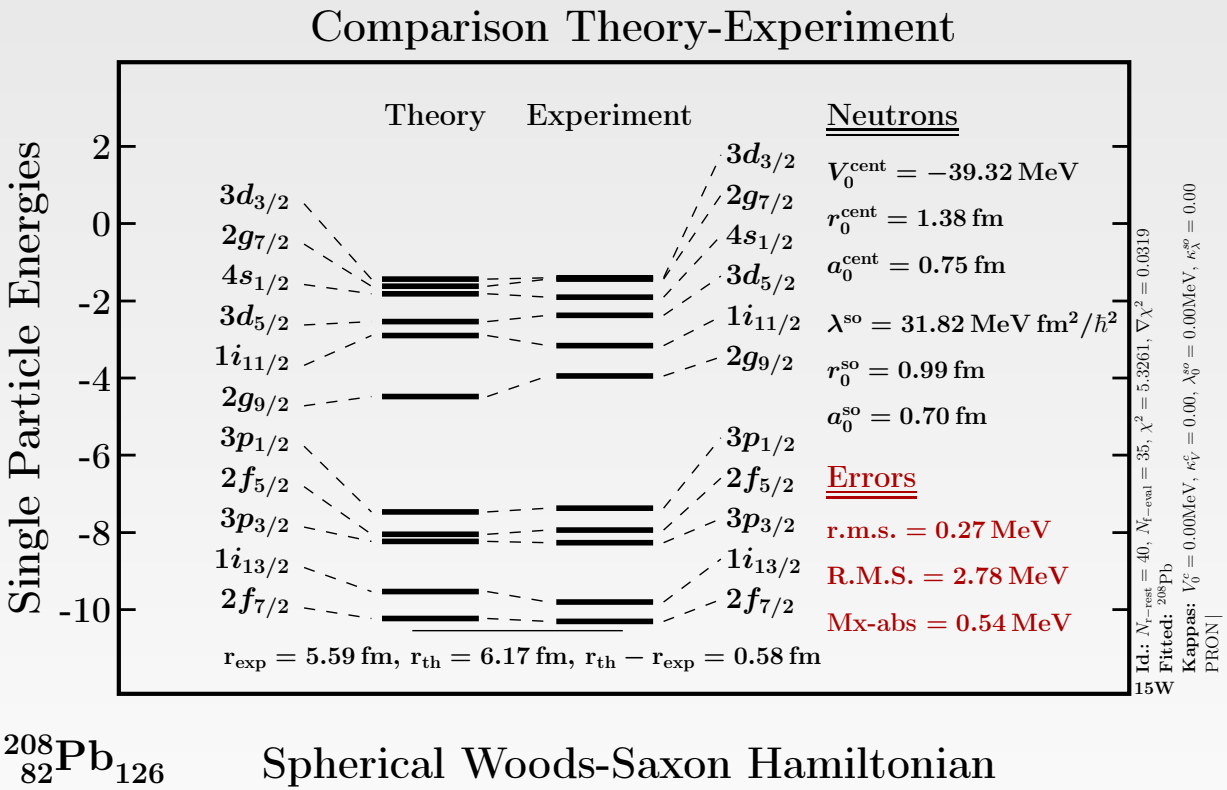
Under these objective constraints we wish to know how (un)certain is what we calculate with our rather complex computer programs?

Uncertainties of Calculated Nucleon Energies

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

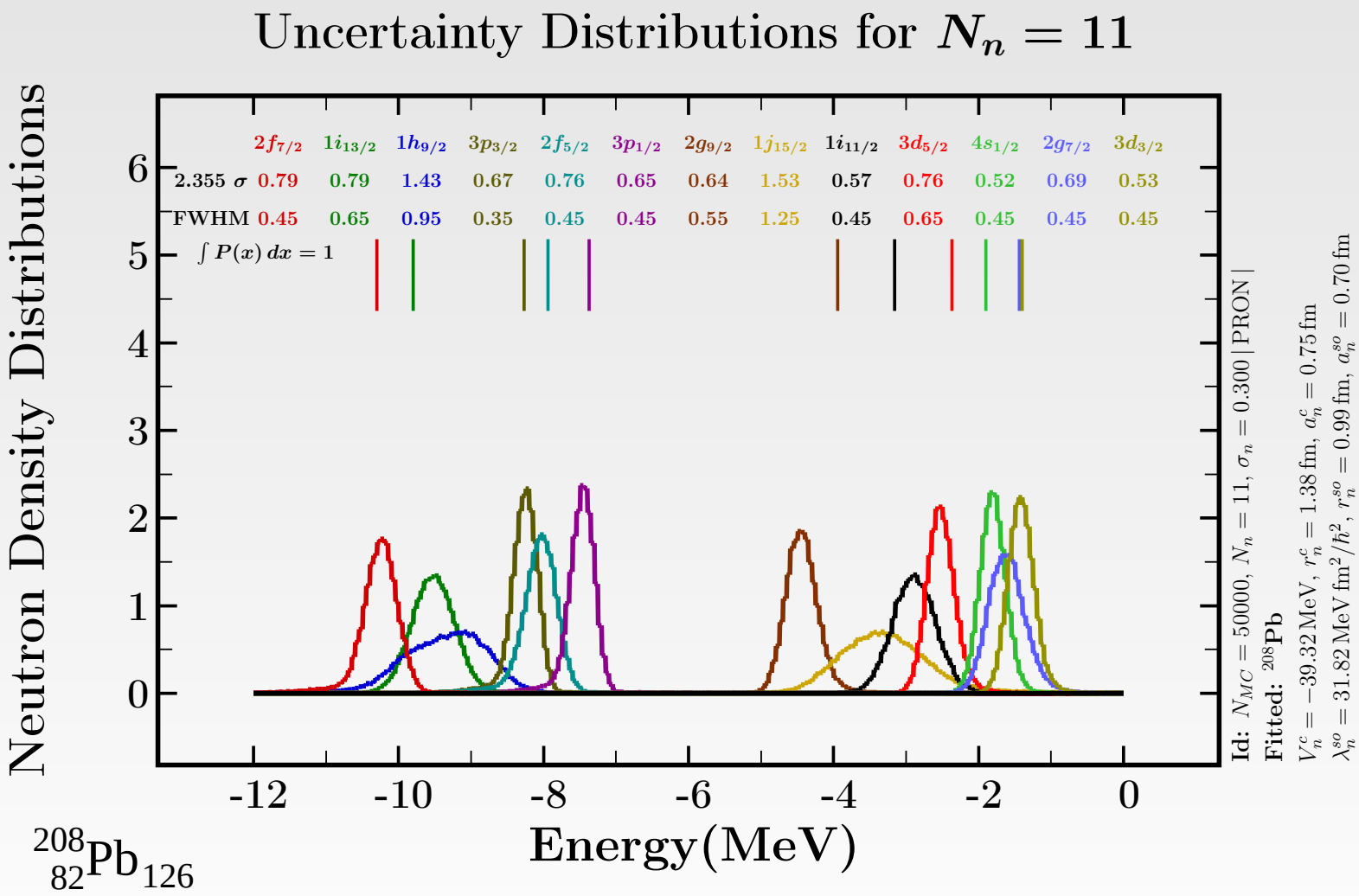


$^{208}_{82}\mathrm{Pb}_{126}$ Spherical Woods-Saxon Hamiltonian

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

Uncertainties of Calculated Nucleon Energies

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



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

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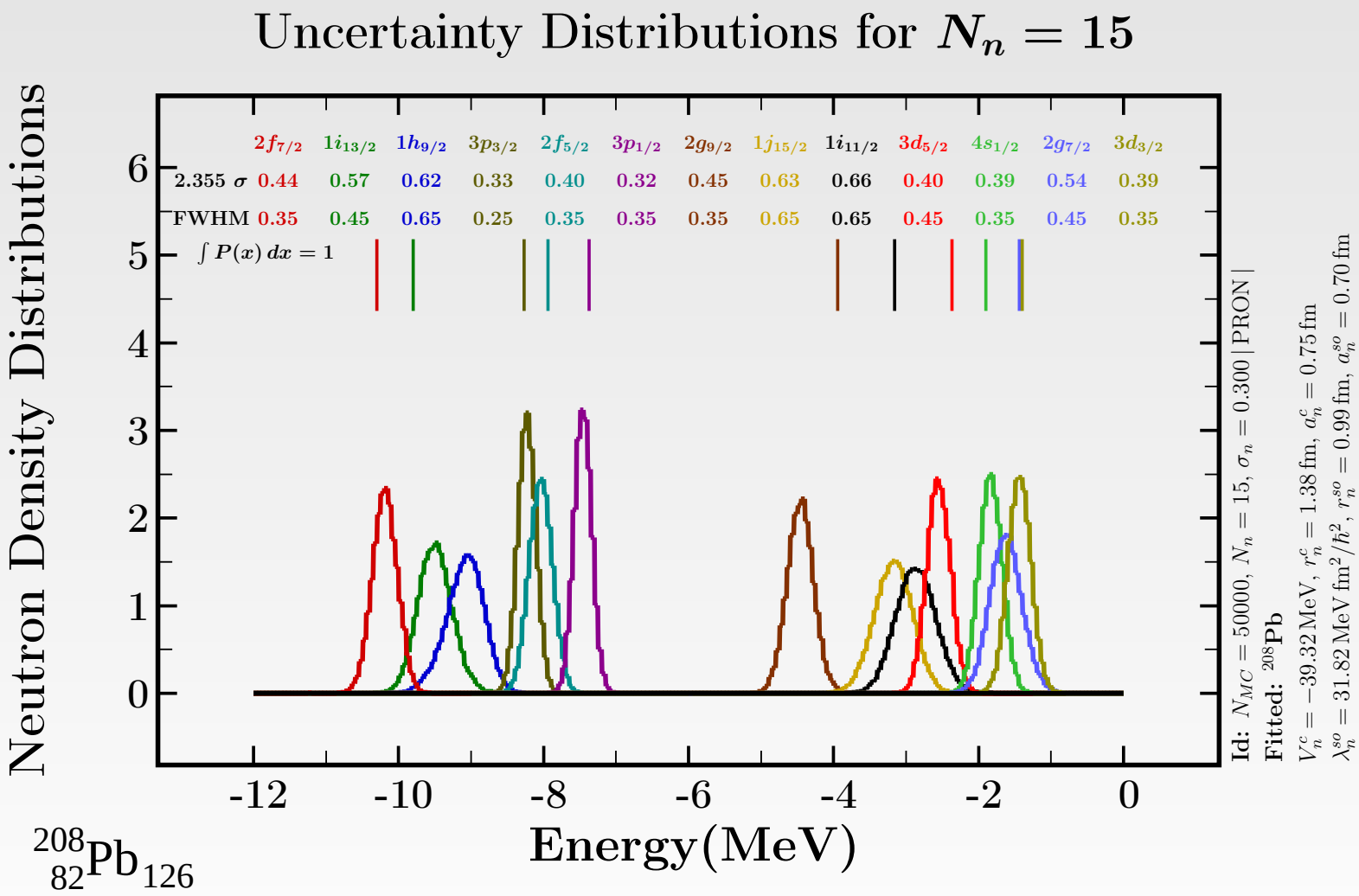

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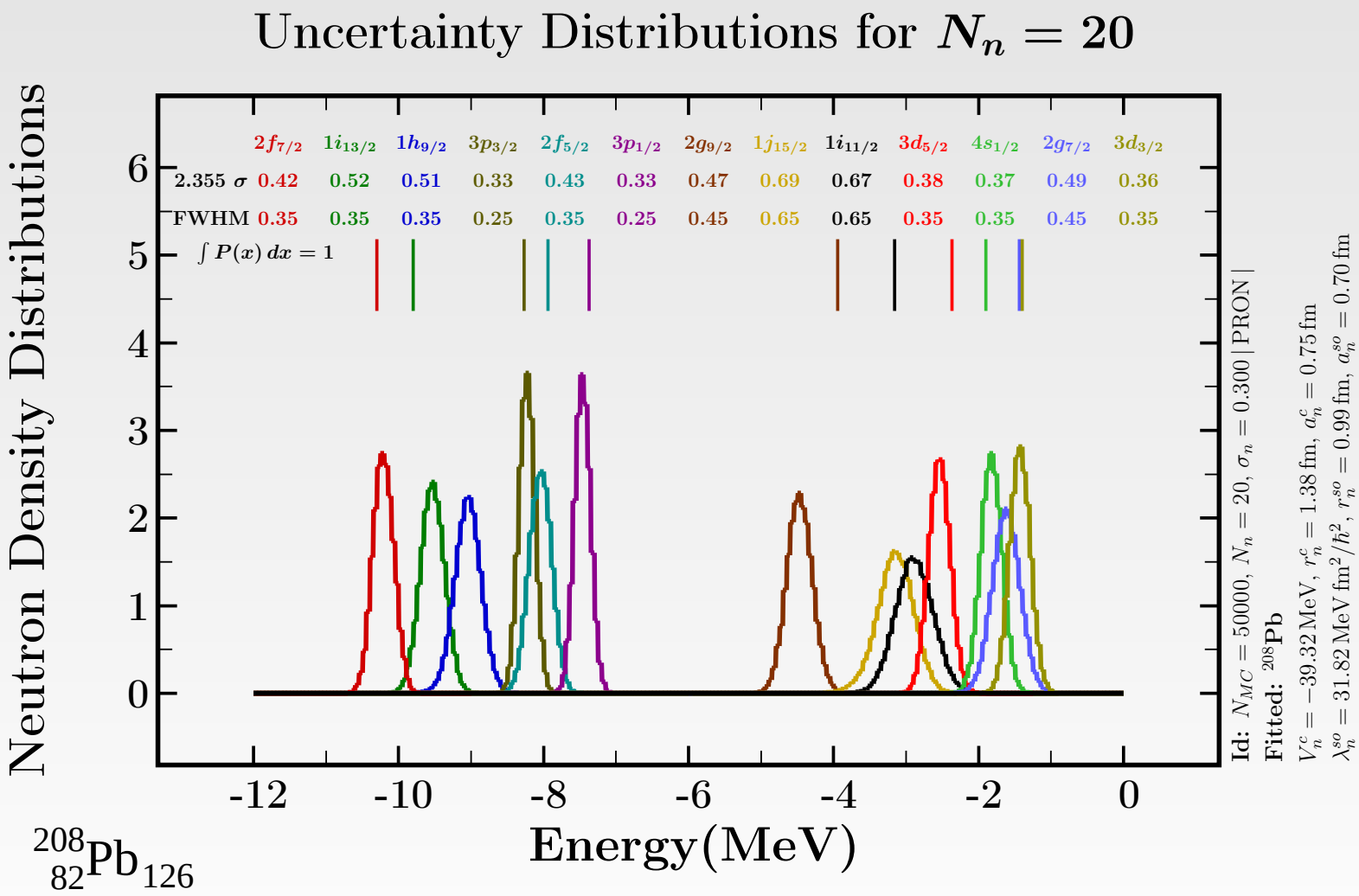

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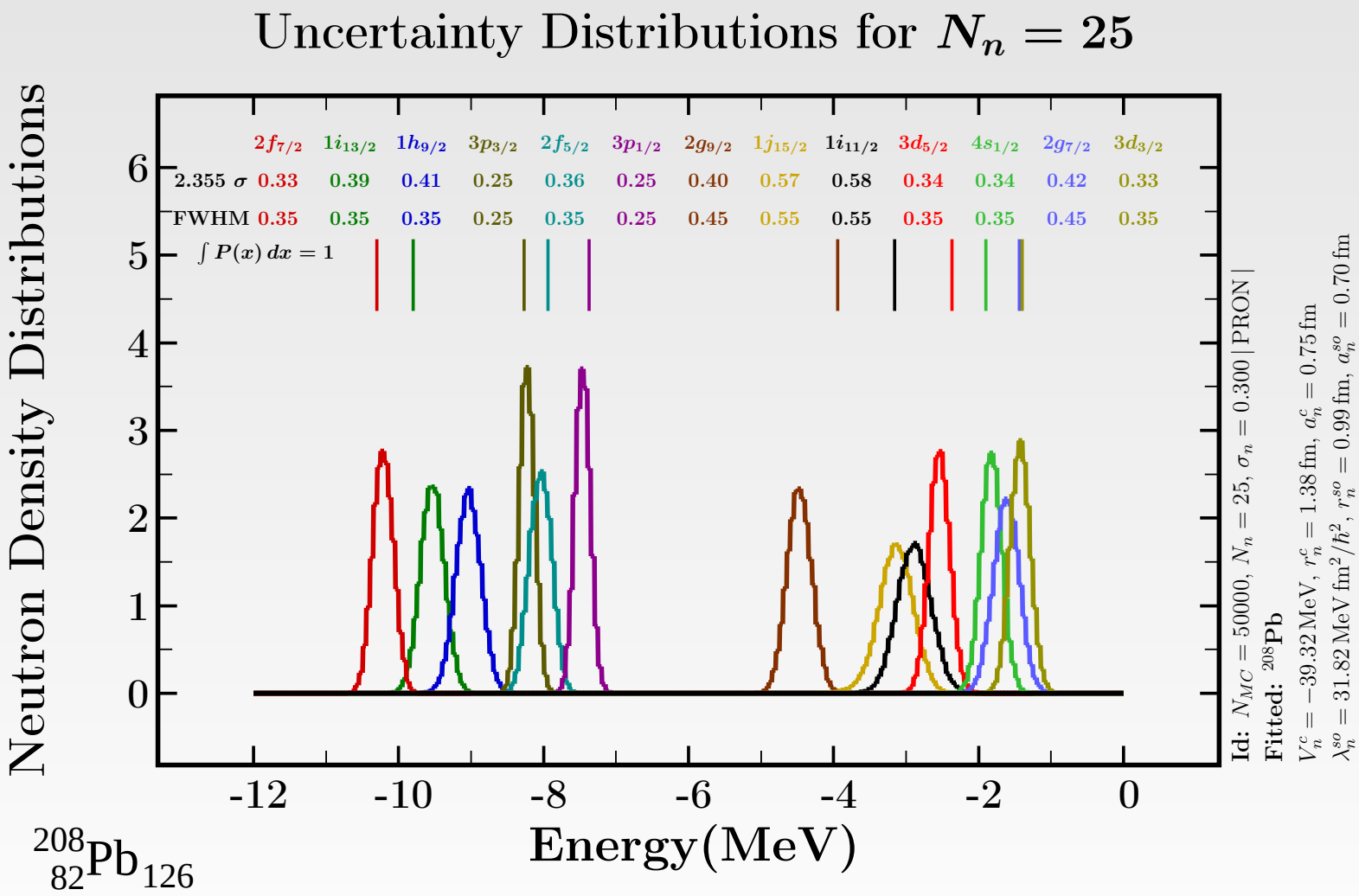

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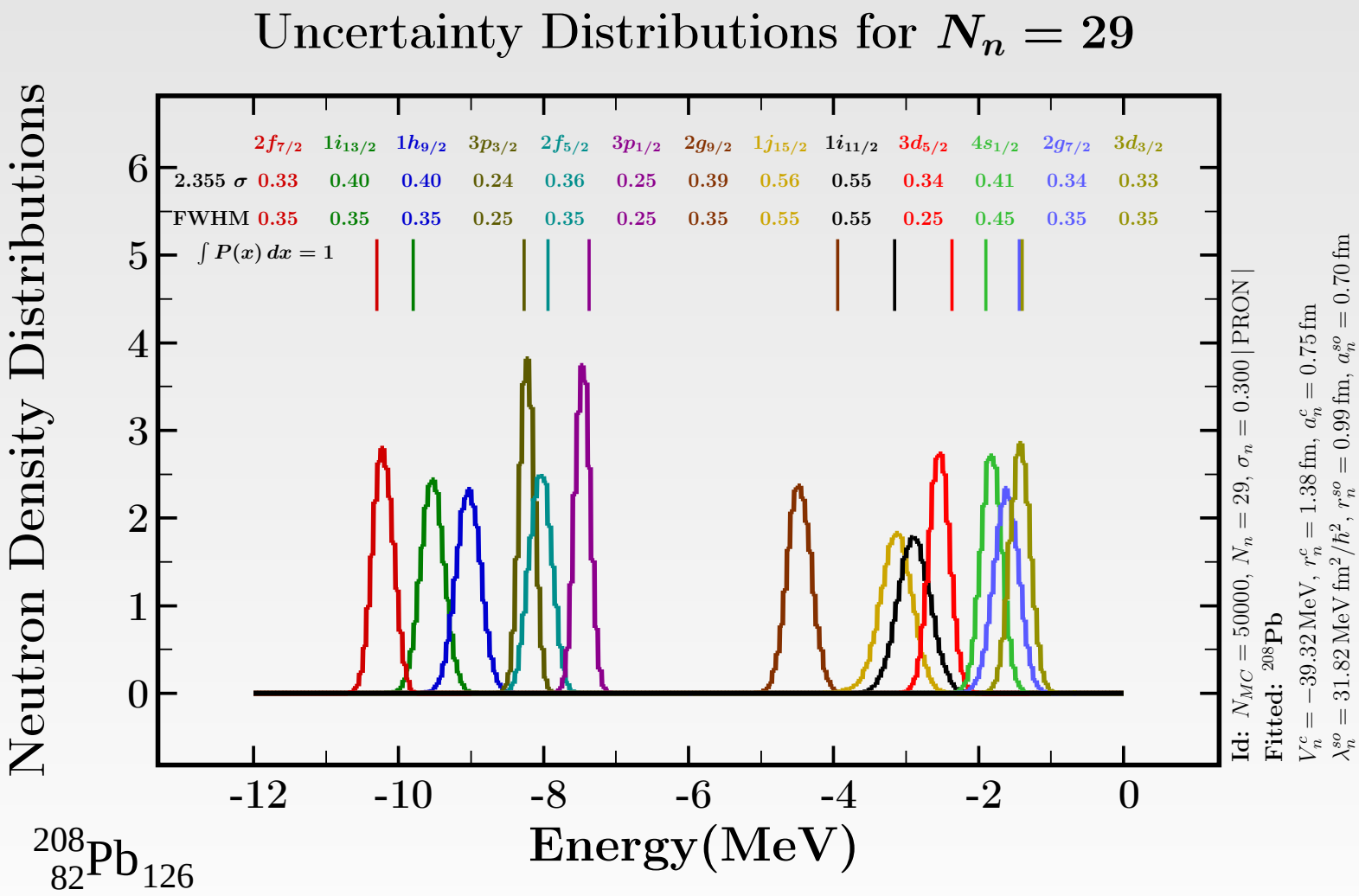

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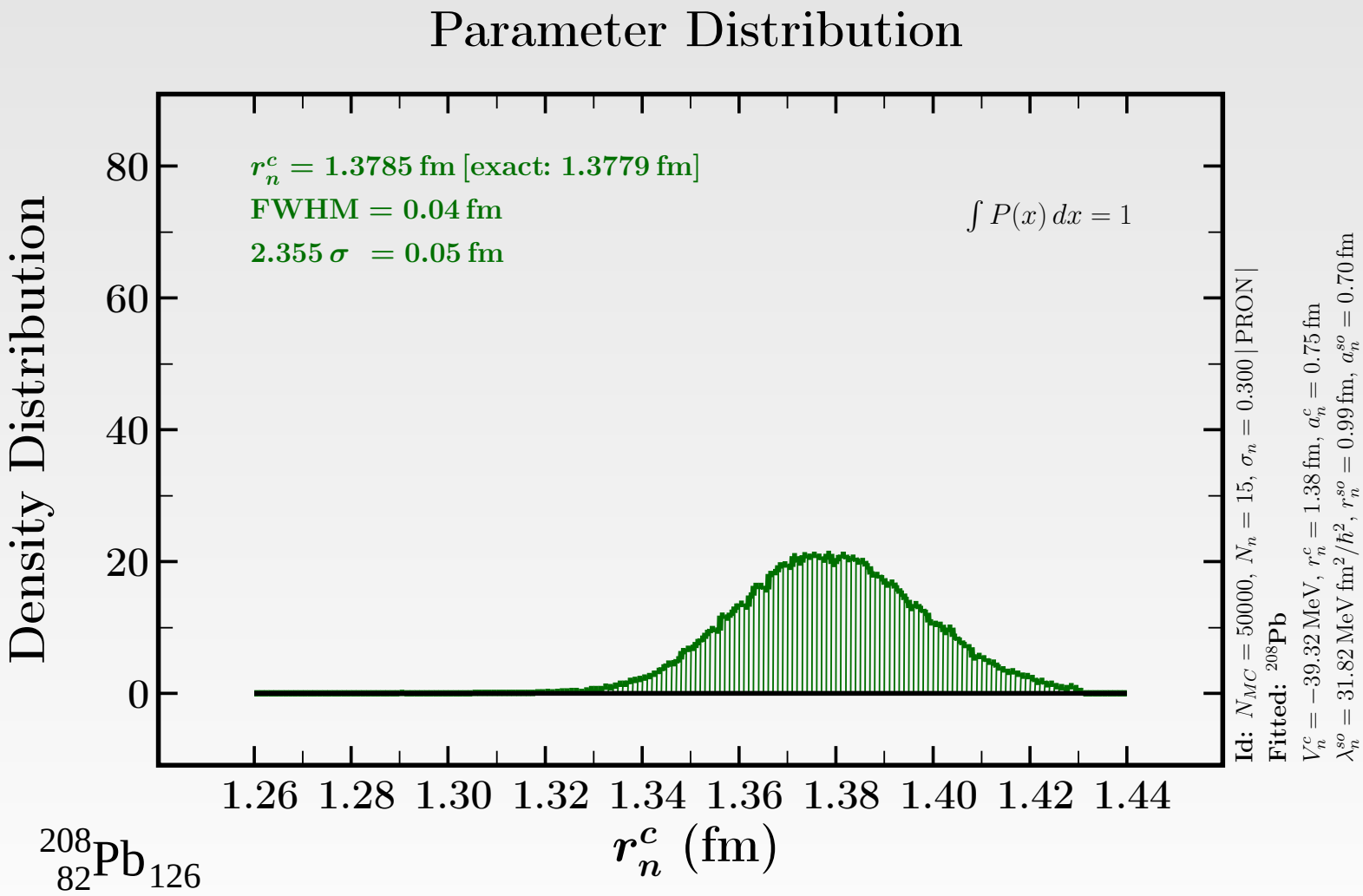
Thank you!

Central Radius Uncertainties

Uncertainties of the Optimal Parameters: $\mathbf{r_n^c}$

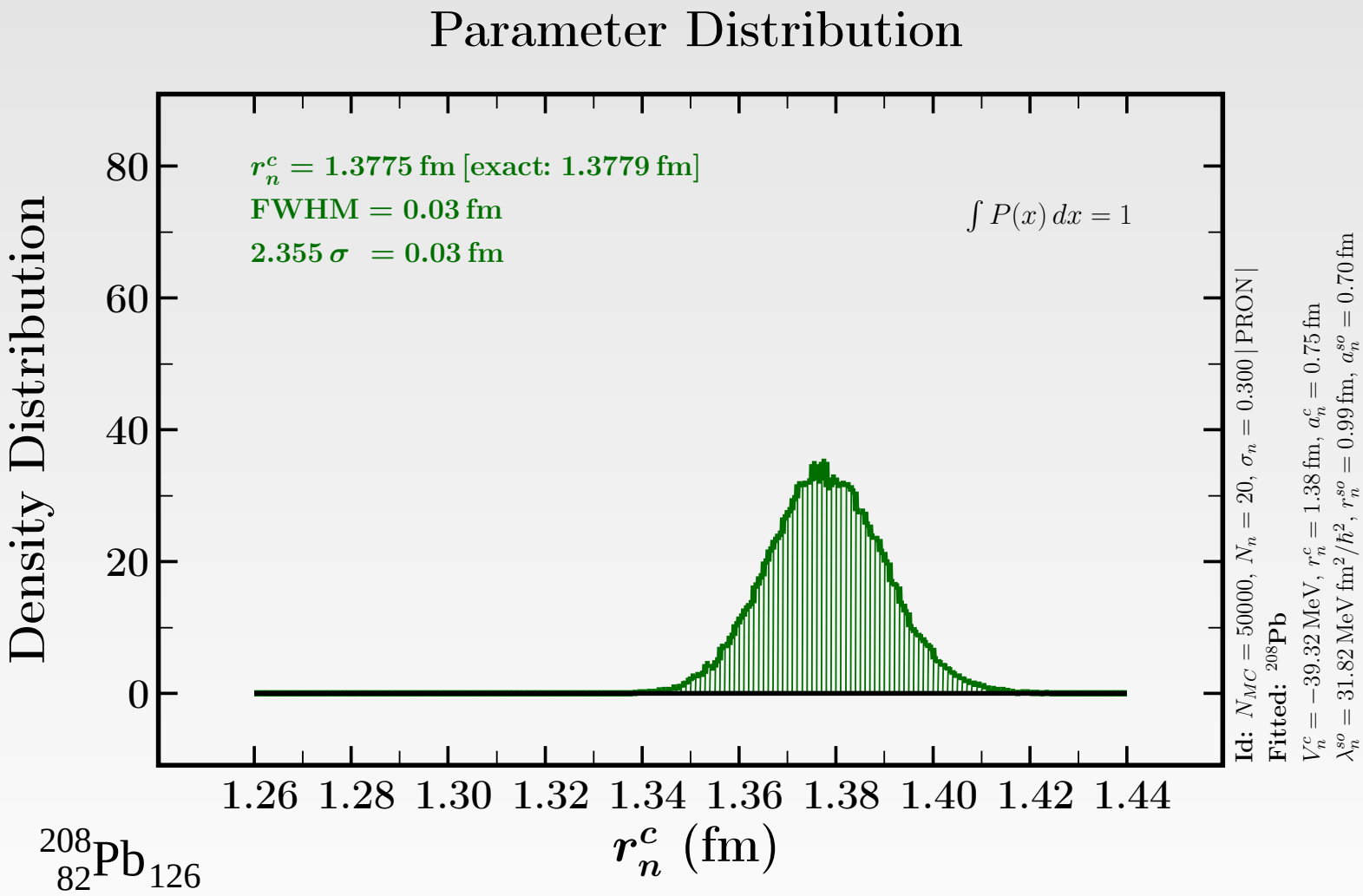
- Pseudo-experimental levels: Parameter uncertainties ← increasing 'sampling'



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

Uncertainties of the Optimal Parameters: $\mathbf{r_n^c}$

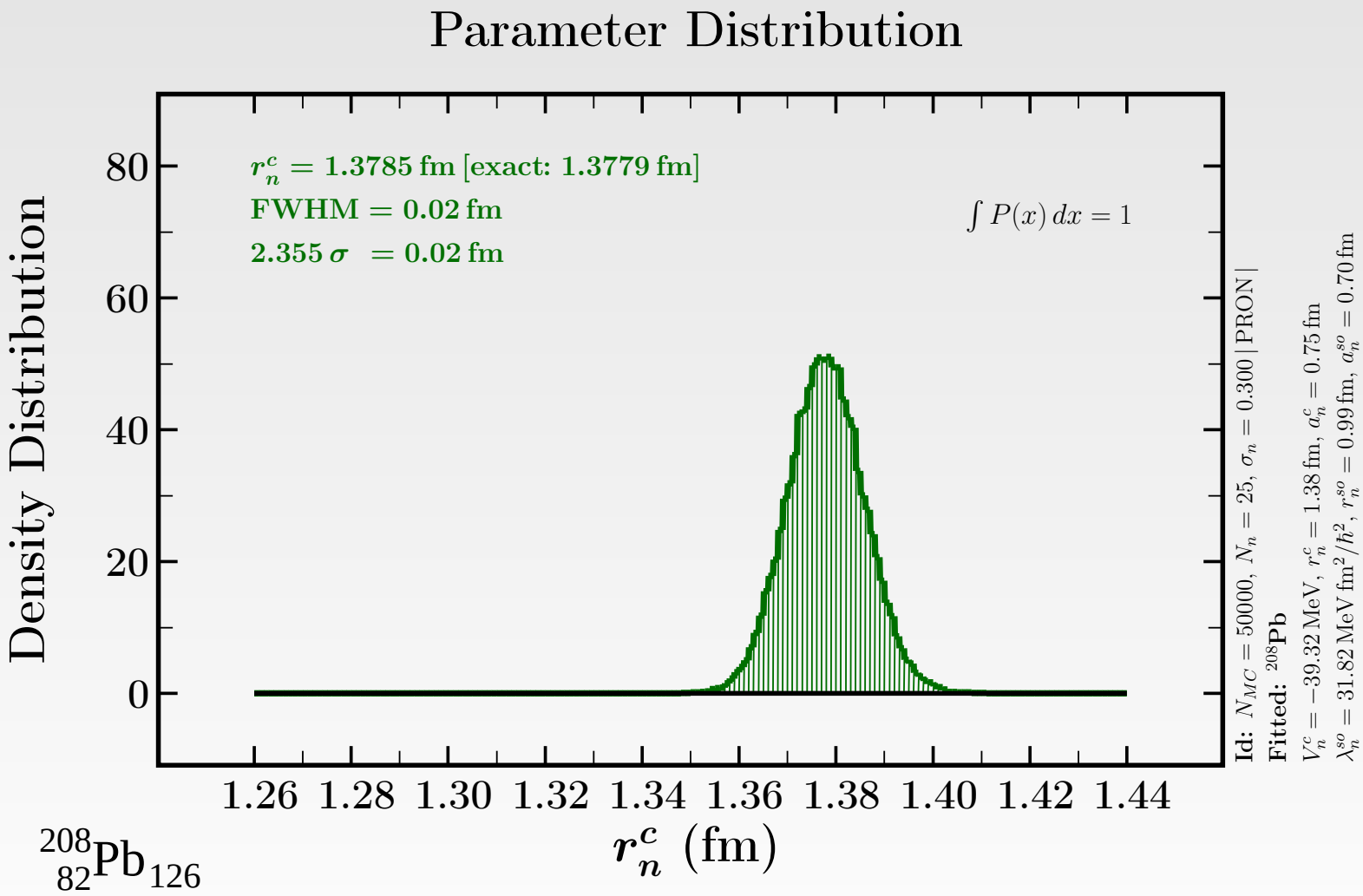
- Pseudo-experimental levels: Parameter uncertainties ← increasing 'sampling'



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

Uncertainties of the Optimal Parameters: $\mathbf{r_n^c}$

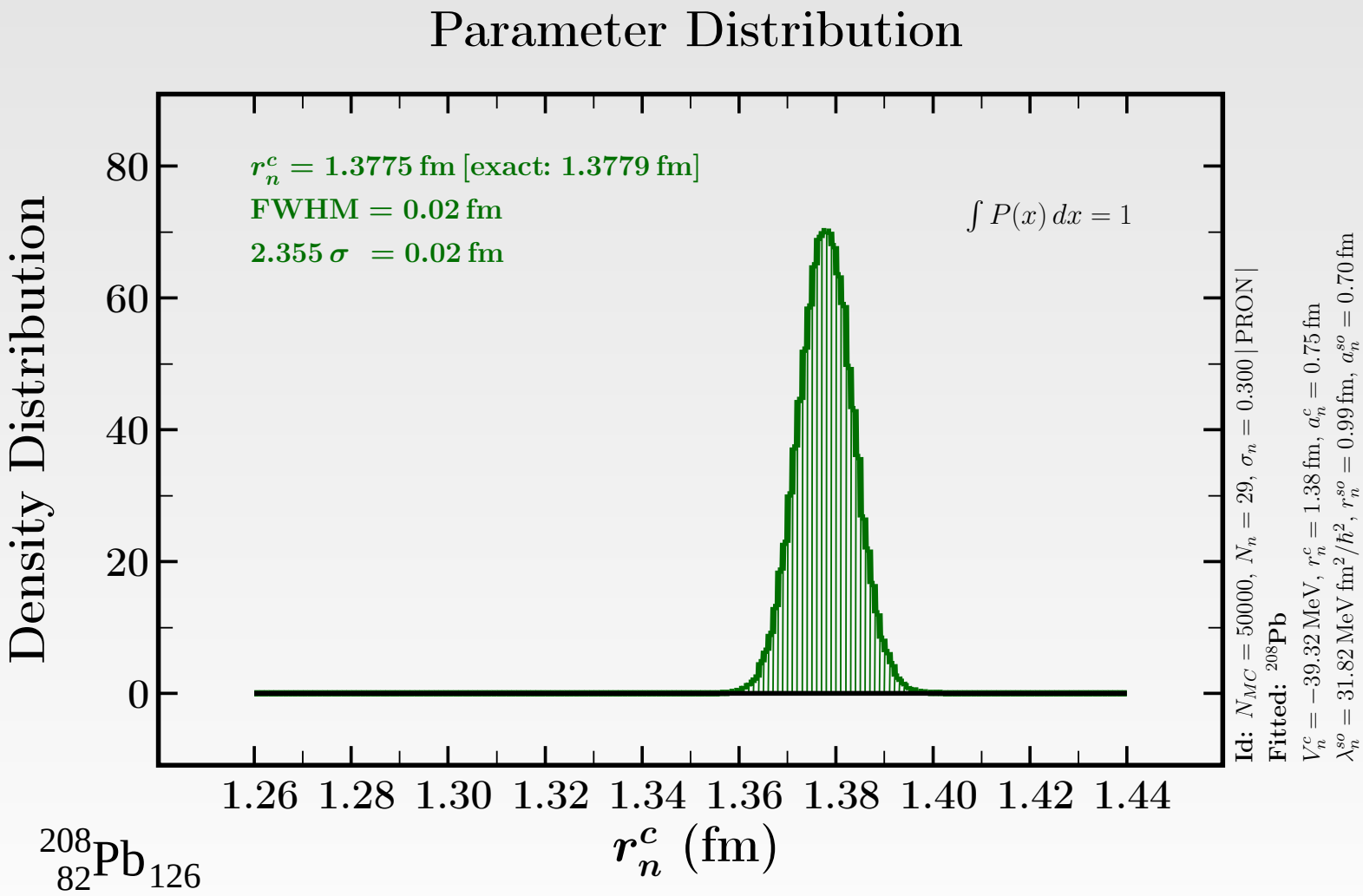
- Pseudo-experimental levels: Parameter uncertainties ← increasing 'sampling'



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

Uncertainties of the Optimal Parameters: $\mathbf{r_n^c}$

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

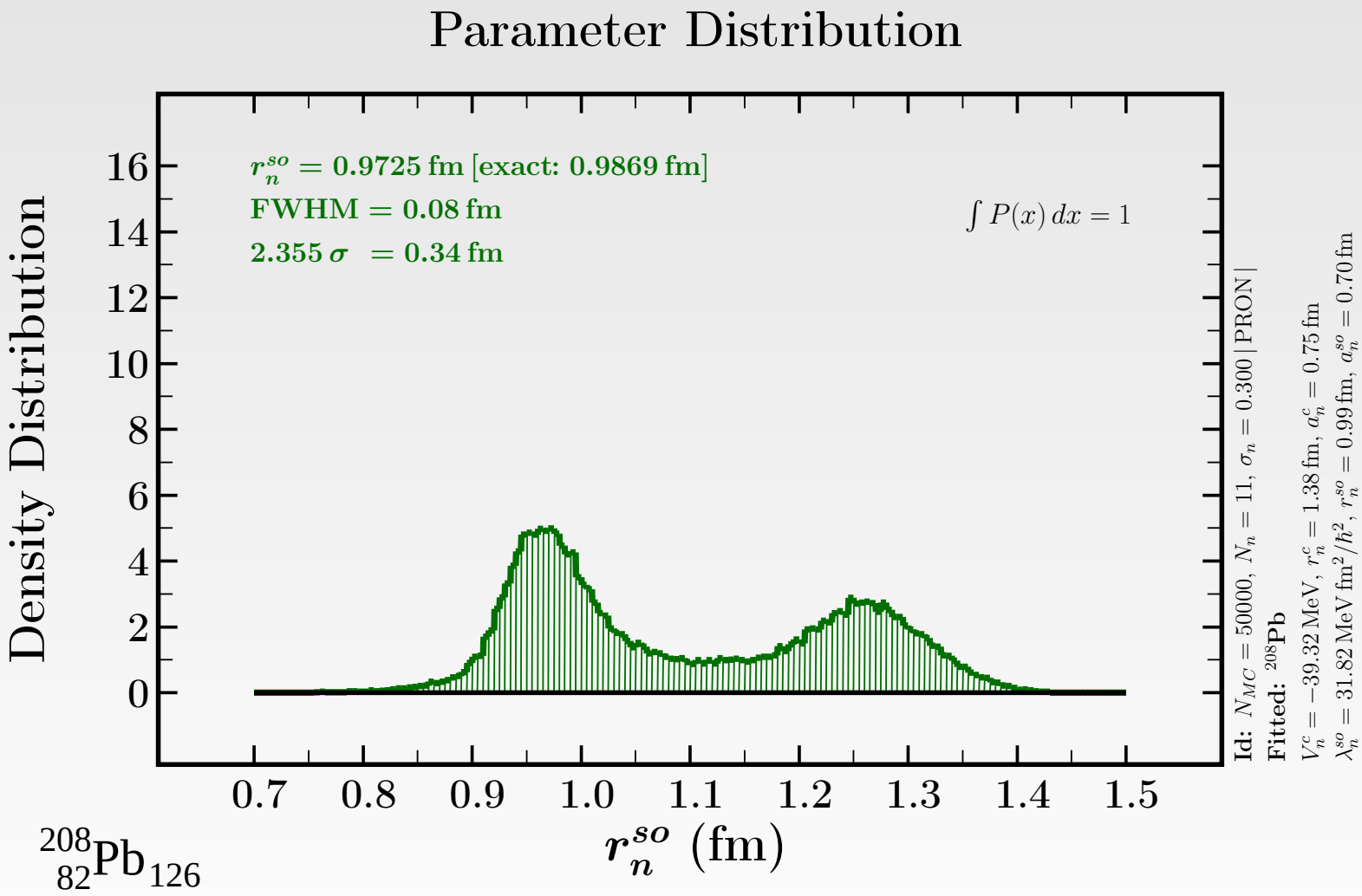


- Here: Sampling composed of 29 levels around the Fermi level

Spin-Orbit Radius Uncertainties

Uncertainties of the Optimal Parameters: r_n^{so}

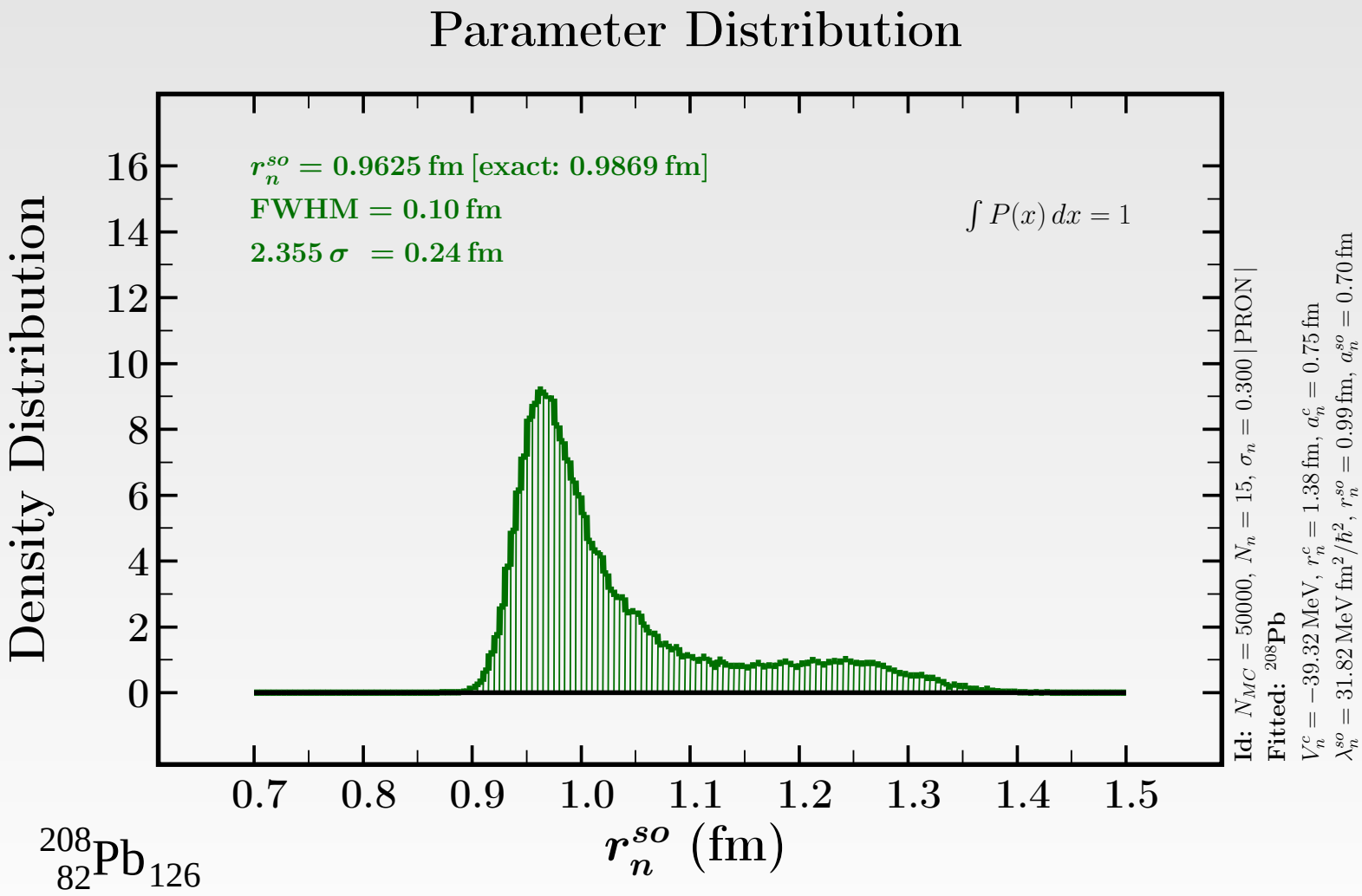
- Pseudo-experimental levels: Parameter uncertainties ← increasing 'sampling'



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

Uncertainties of the Optimal Parameters: r_n^{so}

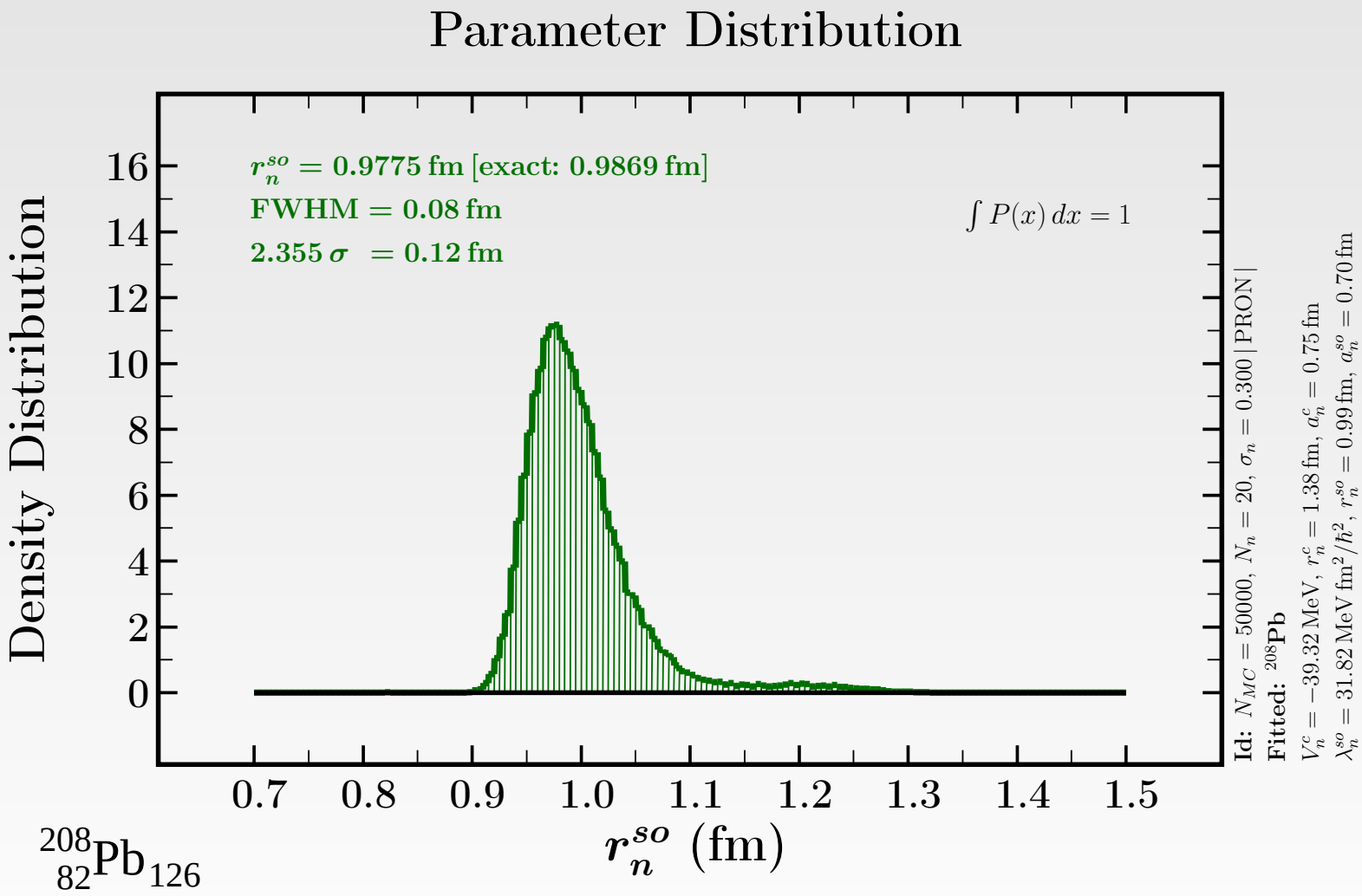
- Pseudo-experimental levels: Parameter uncertainties ← increasing 'sampling'



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

Uncertainties of the Optimal Parameters: r_n^{so}

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



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

Uncertainties of the Optimal Parameters: r_n^{so}

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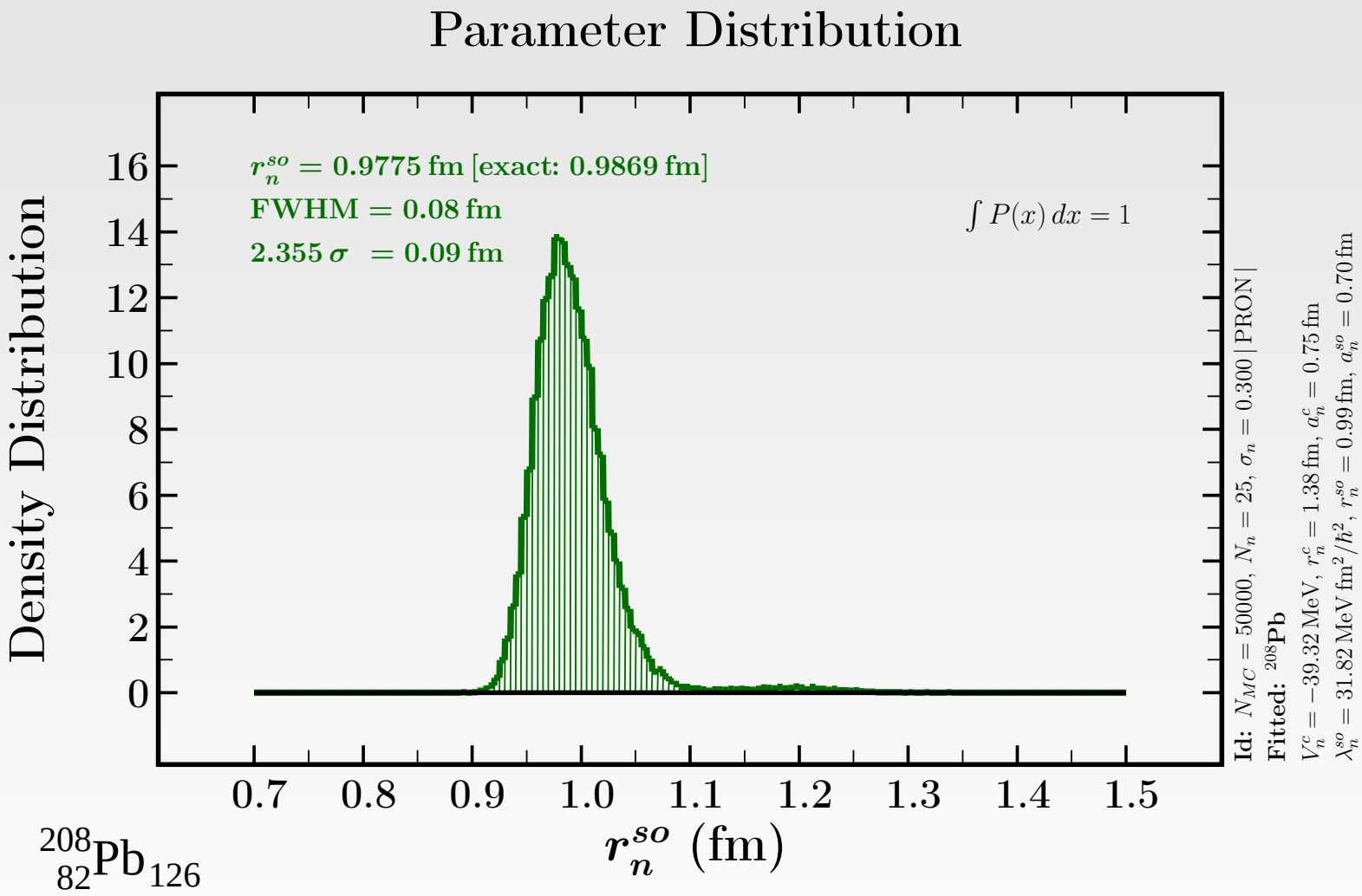
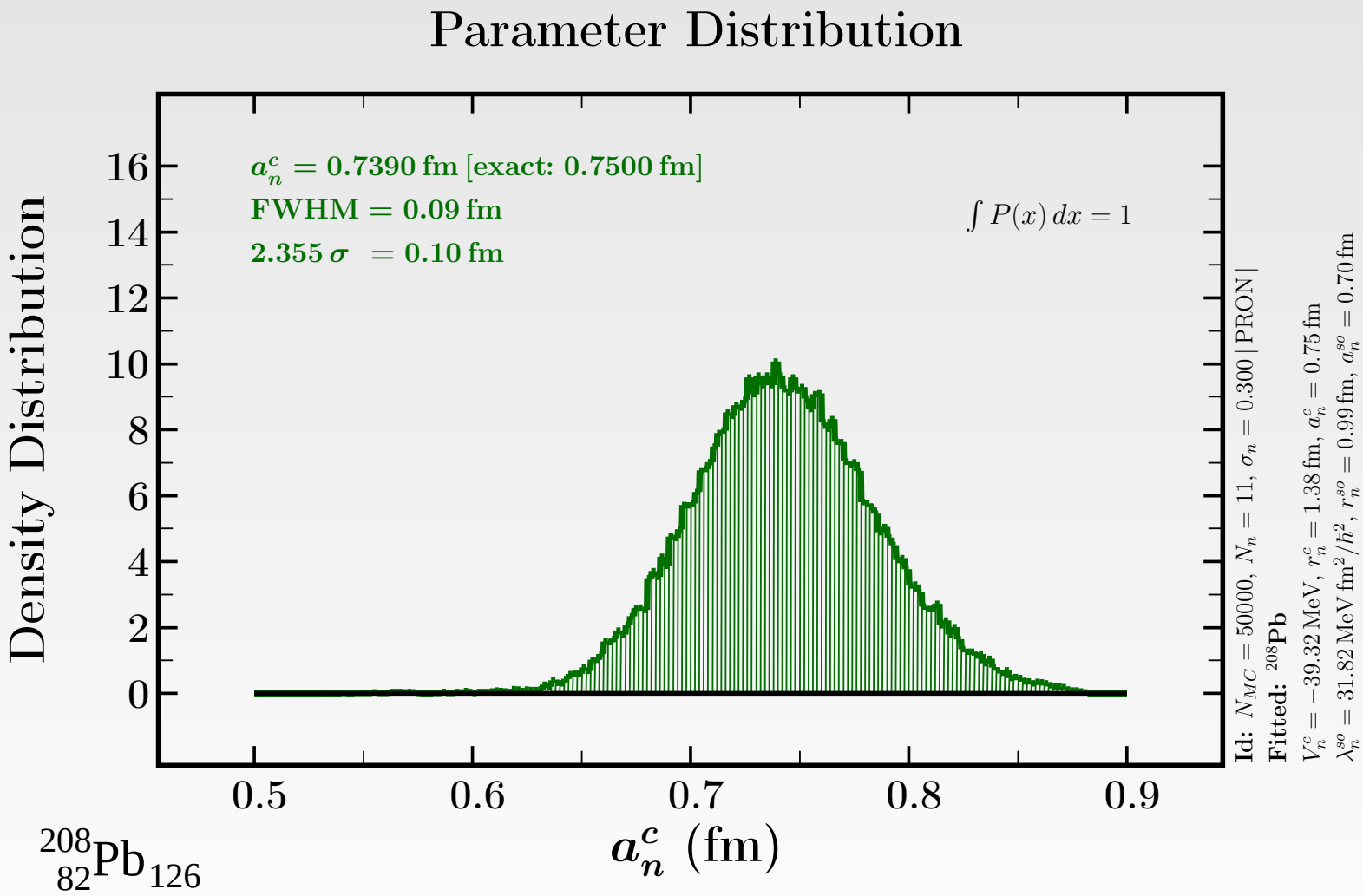


- Here: Sampling composed of 25 levels around the Fermi level

Diffusivity Parameter Uncertainties

Uncertainties of the Optimal Parameters: $\mathbf{a_n^c}$

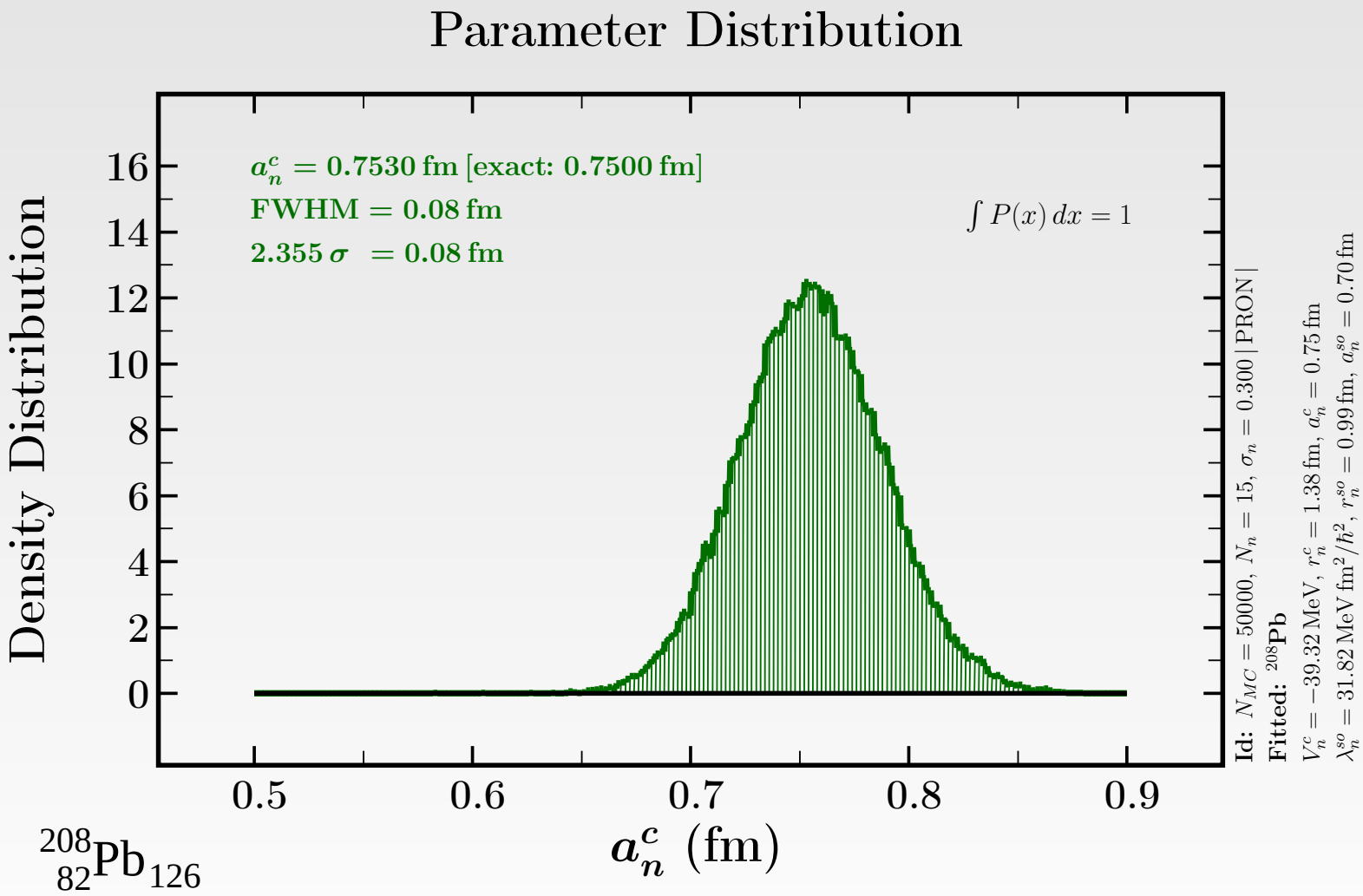
- Pseudo-experimental levels: Parameter uncertainties ← increasing 'sampling'



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

Uncertainties of the Optimal Parameters: a_n^c

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



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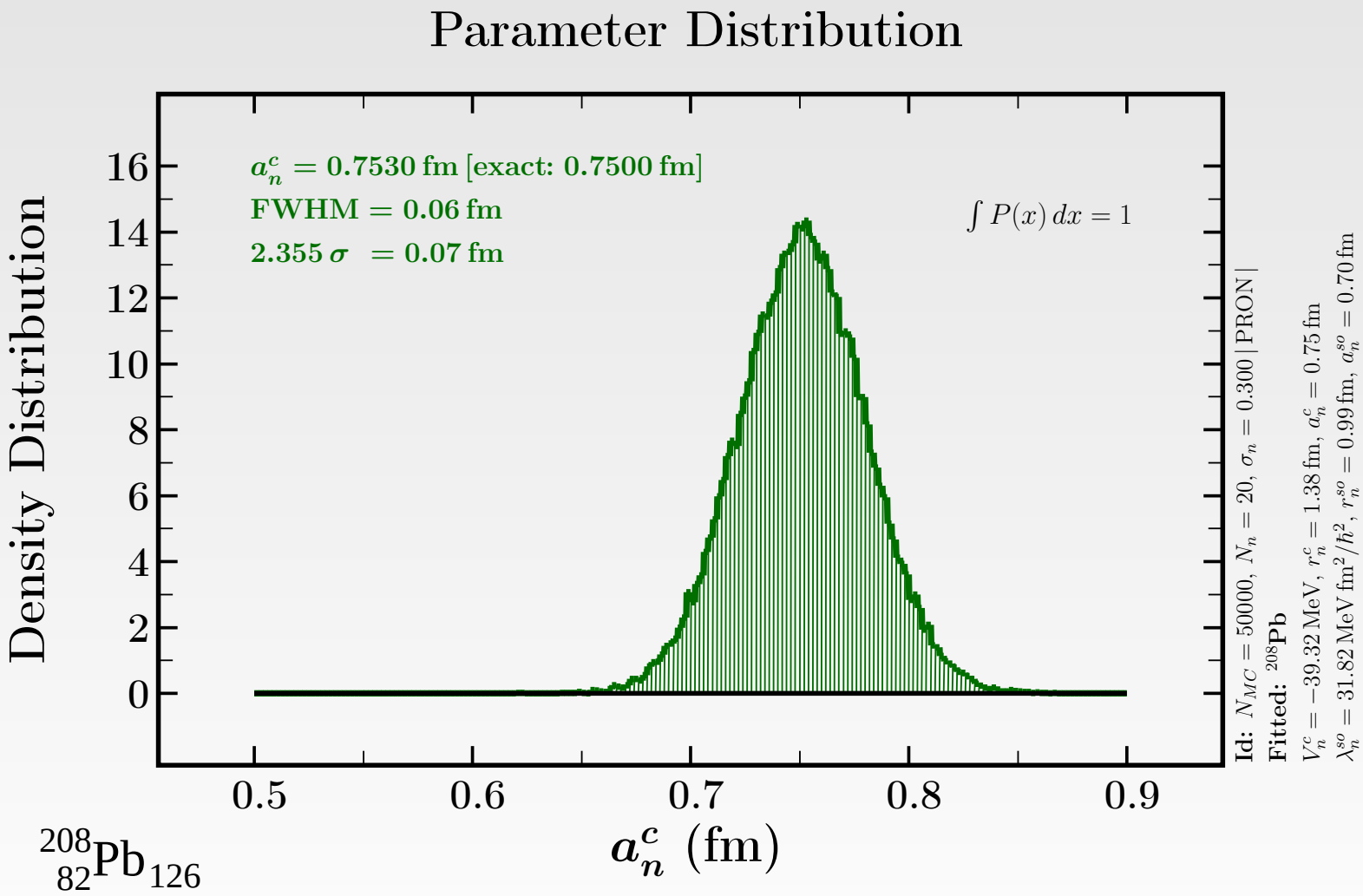
Uncertainties of the Optimal Parameters: a_n^c

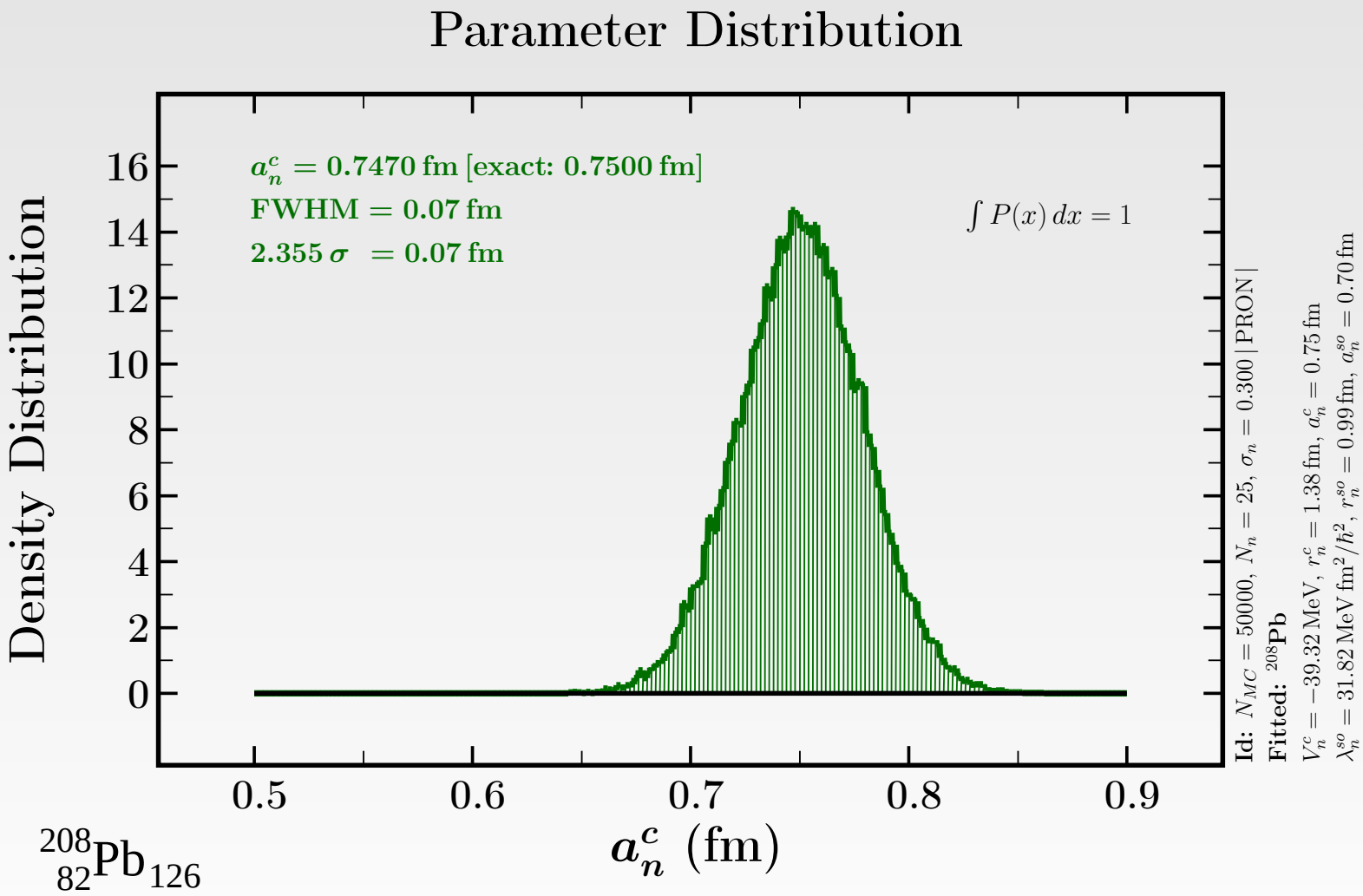
- Pseudo-experimental levels: Parameter uncertainties ← increasing 'sampling'



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

Uncertainties of the Optimal Parameters: a_n^c

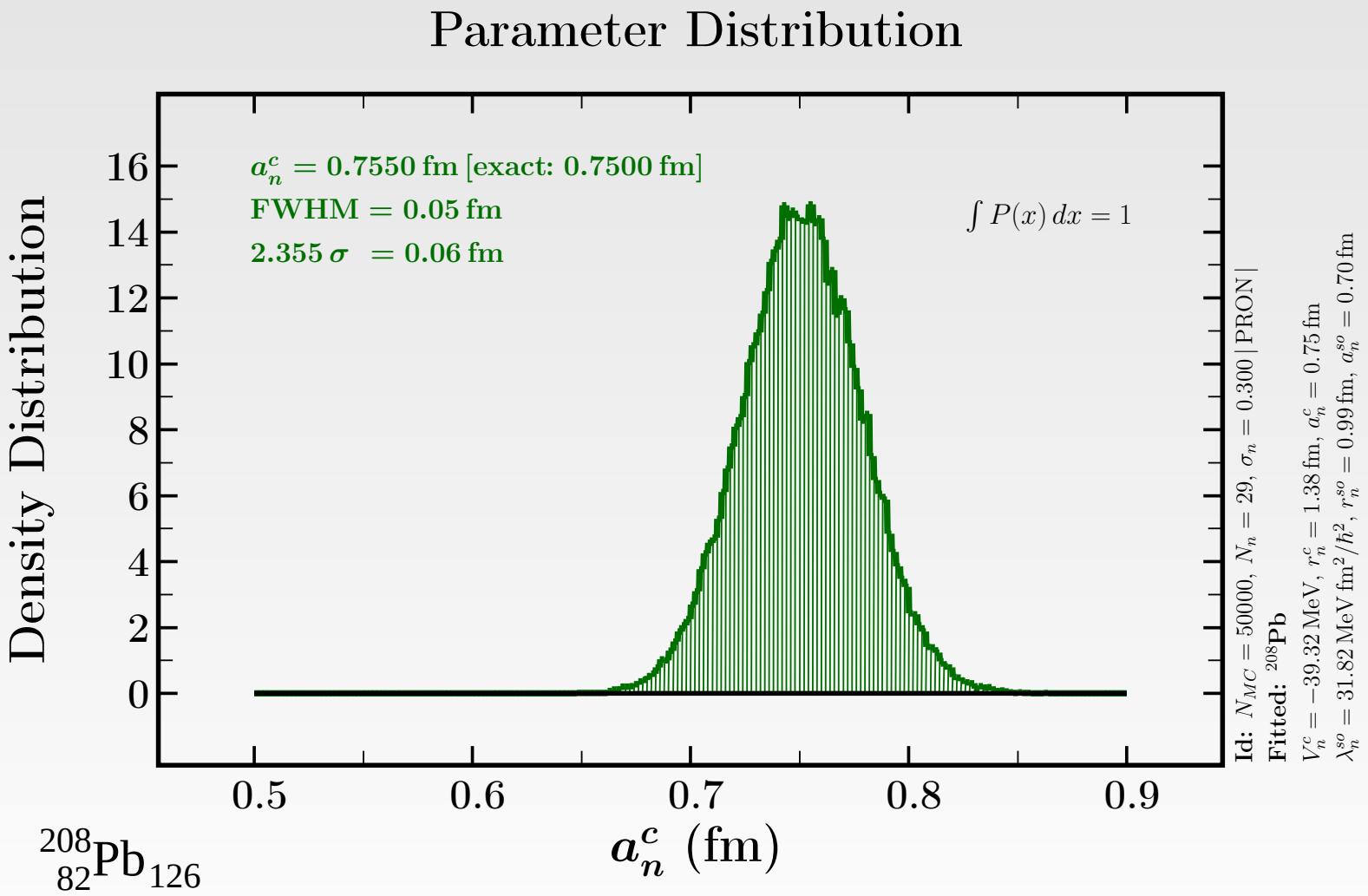
- Pseudo-experimental levels: Parameter uncertainties ← increasing 'sampling'



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

Uncertainties of the Optimal Parameters: a_n^c

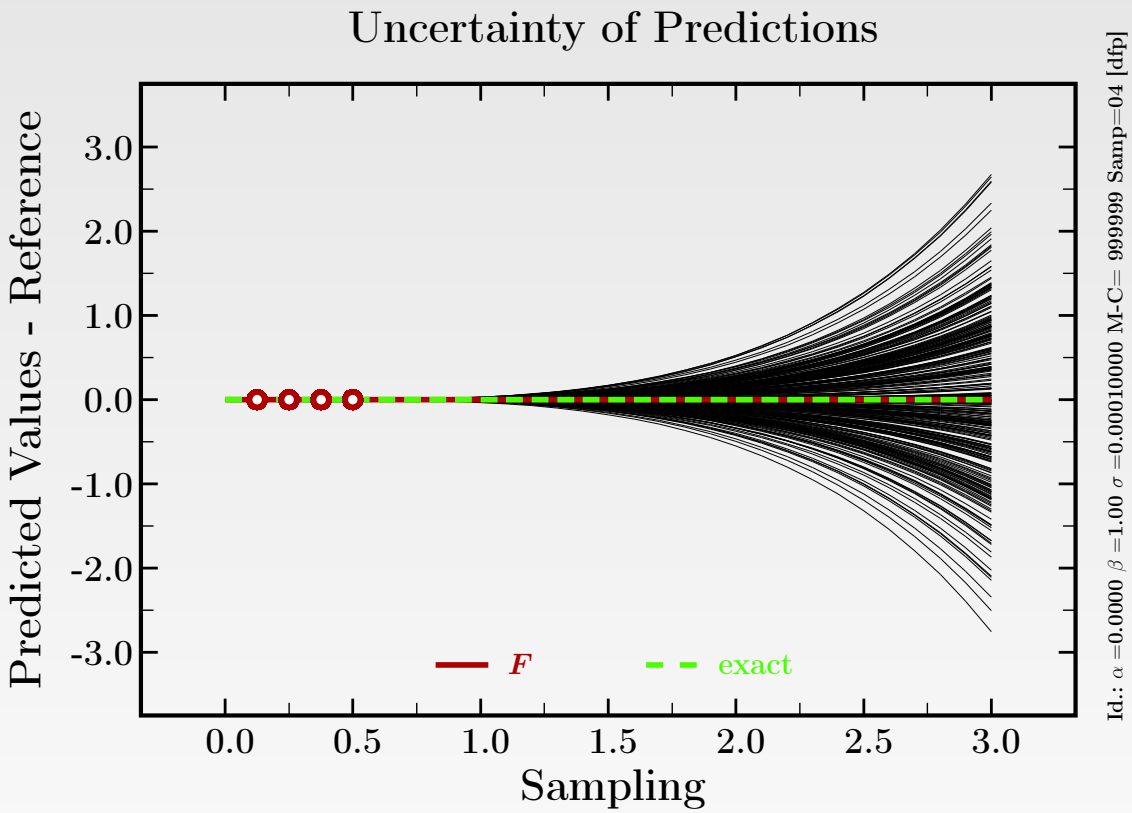
- Pseudo-experimental levels: Parameter uncertainties ← increasing 'sampling'



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

Monte Carlo: Propagation of Uncertainties

• Monte-Carlo Simulation prediction curves, fitting the parameters to 4 sampling points. The exact solution curve has been subtracted for easy reading.



• Observe that the uncertainties near the sampling points are usually minute. Suppose that at 'sampling=2' – for the successful description we need the precision of 0.1. The simulation assures us that we MUST NOT use this exact theory at this required precision level.