Empir – MetroBeta : WP1

Theoretical Calculations of Beta Spectra

In partnership: CEA (X. Mougeot) and UMCS (J. Dudek)

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Part II

Microscopic Input for Theoretical Calculations of Beta Spectra

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Microscopic Input for Theoretical Calculations of Beta Spectra

Jerzy DUDEK

University of Marie Curie-Skłodowska, Poland

In partnership: CEA (X. Mougeot) and UMCS (J. Dudek)

This presentation contains the result obtained in collaboration
with
Irene DEDES
University of Marie Curie-Skłodowska, Poland

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- To summarise: Our starting point is a well tested so-called

Phenomenological Universal Woods-Saxon Hamiltonian

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• They all use WS-Universal Hamiltonian for the nuclear structure calculations

• There are hundreds of nuclear structure articles using this particular nuclear mean-field Hamiltonian published every year because of its Predictive Power!

The Purpose:

Optimise and stabilise the parametrisation of the Hamiltonian – thus the spectra

The Method Employed:

Inverse Problem Theory
[A Branch of Applied Mathematics]

Inverse Problem in Quantum Theories

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

$$\hat{H}(p) \rightarrow \{E_p, \psi(p)\} \leftrightarrow \boxed{\hat{O}_H(p) = d^{th} \leftarrow \textit{Direct Problem}}$$

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$$\boxed{p^{opt} = \hat{O}_H^{-1}(d^{exp}) \leftarrow \textit{Inverse Problem}}$$

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

Inverse Problem in Algebraic [Matrix] Representation

- One may show introducing an equivalent algebraic representation →

$$\frac{\partial \chi^2}{\partial p_i} = 0 \;\rightarrow\; (J^T J) \cdot p = J^T\, b(d^{\text{exper}}) \;\leftrightarrow\; J^T J \overset{df}{=} \mathcal{A}$$

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

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

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

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

Possibly Loosing the Correlation Data $\leftrightarrow$ Parameters

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

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

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

Ill-Posed $\rightarrow$ Correlation between parameters and the data is lost!

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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?

Woods-Saxon Hamiltonian: Central Potential

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

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

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:

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

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

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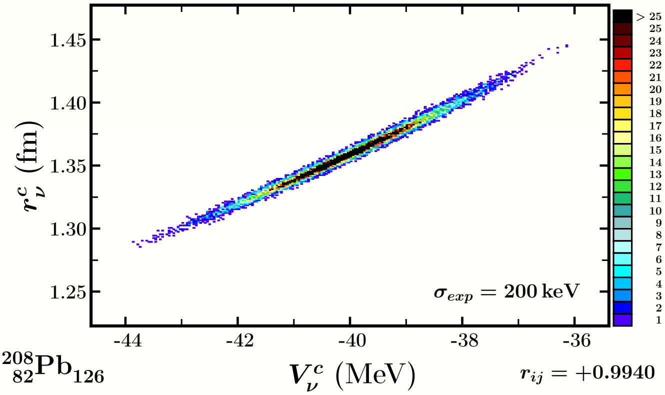

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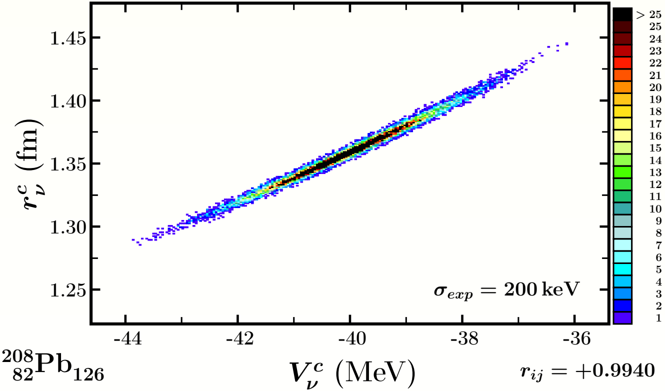

• **These results show that the central potential depth and central potential radius are correlated: $V_c \times r_c^2 \approx$ const.** **A possible ad hoc choice: $r_c \rightarrow r_c^{exp}$**

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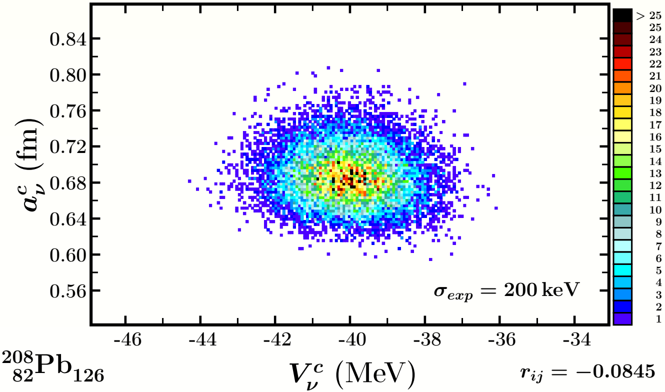

• **An approximate circular symmetry of this diagram shows ($r_{ij} \approx 0$) that the central potential depth and the central potential diffuseness are not correlated - therefore no danger to the predictive power!**

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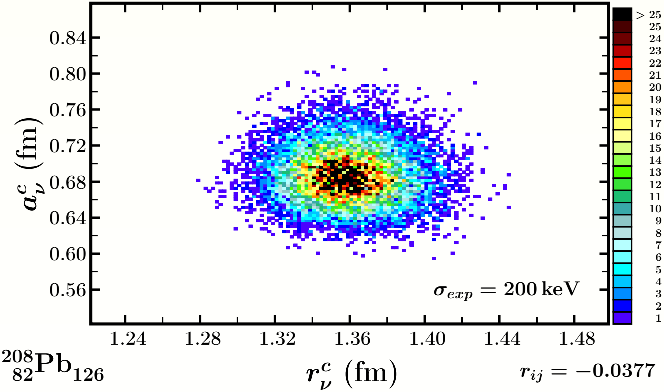

• **Once again, the circular symmetry of this diagram shows ($r_{ij} \approx 0$) that the central potential radius and central potential diffuseness are not correlated - therefore no danger to the predictive power either → Just one parametric correlation!**

Conclusion:

The central potential has only one correlation among 3 parameters

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

easy to remove

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Next:

Checking the Spin-Orbit Potential

Similar tests show that the Spin-Orbit potential contains complex parametric correlations

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- **We decided to resign from the simple phenomenology of the spin-orbit potential in favour of the more microscopic, Hartree-Fock type structure**

- **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***

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

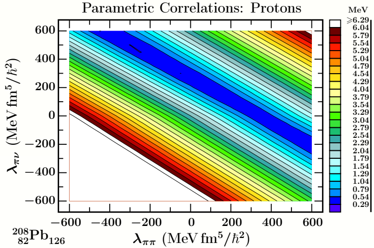
$$\hat{V}_{so}^{\nu} = \lambda_{\nu\pi}\frac{1}{r}\frac{d\rho_\pi}{dr} + \lambda_{\nu\nu}\frac{1}{r}\frac{d\rho_\nu}{dr} \qquad \textbf{Eq.(B)}$$

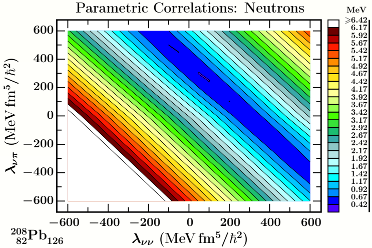
Advantages: The new expression includes the iterative self-consistency condition like in the microscopic HF approach rather than pure phenomenology and contains 4 parameters rather than 6. What are their correlations?

Density-Dependent Spin-Orbit: Linear 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:** $\quad \min_{i \neq j,k} \chi^2(p_1, p_2, \ldots p_m)$

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



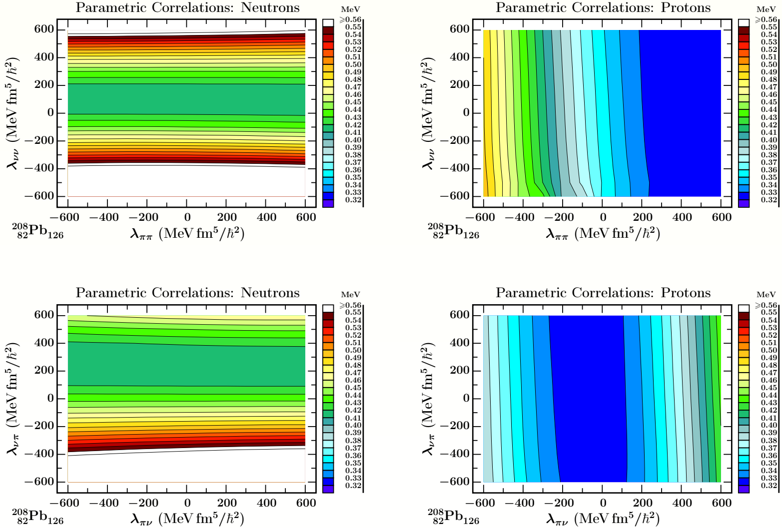


- **Realistic calculations indicate that the density-dependent spin-orbit potential parameters are correlated – but the correlations are perfectly linear**

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

No Correlations in Other S-O Parameter Combinations

- **Horizontal/vertical valleys: χ^2-projection onto $(\lambda_{\pi\pi}, \lambda_{\nu\nu})$ and $(\lambda_{\pi\nu}, \lambda_{\nu\pi})$**



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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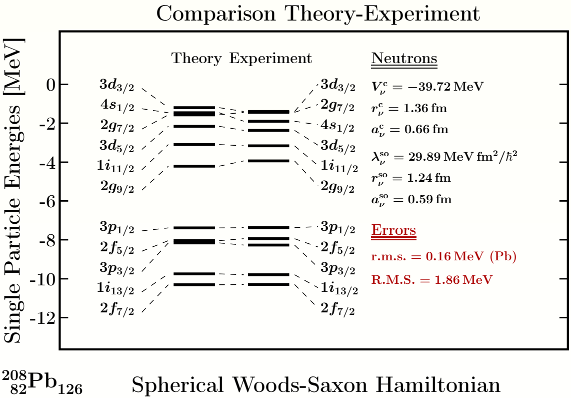
→ Original potential 6 parameters
→ Density dependent 4 parameters
→ Correlation removal → 1 free spin-orbit parameter left !!!

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

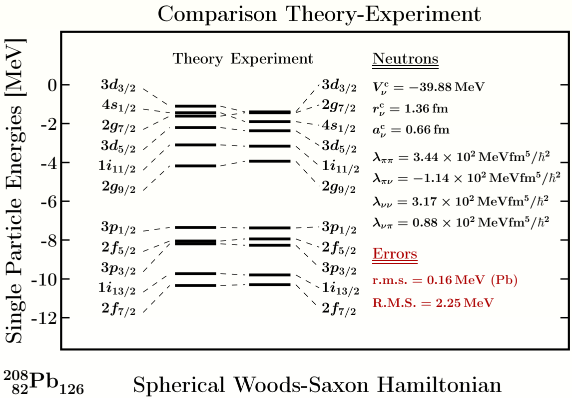
- We fit six parameters - $\{\lambda_\pi^{so}, r_\pi^{so}, a_\pi^{so}\}$ for protons and $\{\lambda_\nu^{so}, r_\nu^{so}, a_\nu^{so}\}$ for neutrons



- Results for ^{208}Pb: Neutrons, traditional $\hat{V}_{so}$ → **Resulting r.m.s. = 0.16 MeV**

Fit All Four Parameters of the Density-Dependent SO

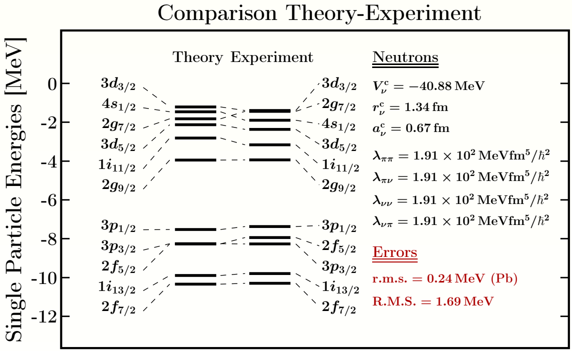
- **We fit { λ_{nn}, λ_{np}, λ_{pn}, λ_{pp} } of the density-dependent – SO to ^{208}Pb levels**



- ^{208}Pb: Density-dependent $\hat{V}_{so}$ → **Resulting r.m.s. = 0.16 MeV (unchanged)**

Fitting Just 1 Parameter in the Density-Dependent SO

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

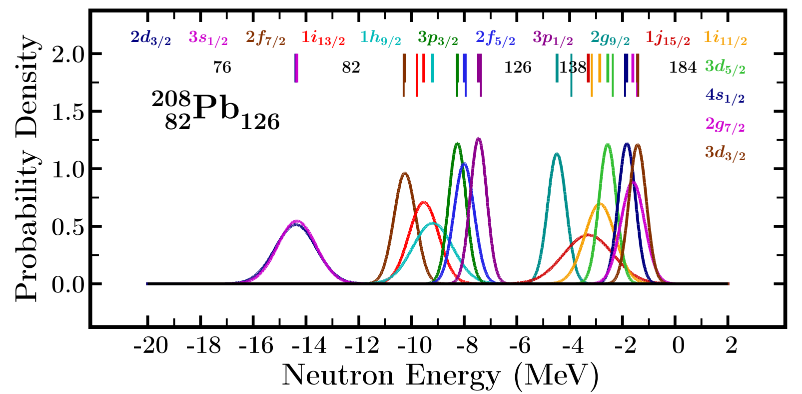


$^{208}_{82}$Pb$_{126}$ Spherical Woods-Saxon Hamiltonian

- ^{208}Pb: Just 1 free parameter → **Results r.m.s. = 0.24 MeV (small deterioration)**
- Conjecture: **Equivalent to 1 parameter - common for protons and for neutrons**

Monte-Carlo Simulations of Uncertainty Distributions

- **Prediction-uncertainty distributions and $\{e_\nu\}$-comparison with experiment**



- Example of realistic simulations corresponding to actual experimental errors
- Notice a strong state-dependence of the resulting uncertainty-distribution width

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- **Global simultaneous fits to these nuclei confirm above conclusions**

Amazing but True: 40 Years Old Parameterisation !!

- Our starting point Hamiltonian has been tested in thousands of published articles (preceding page) and is being used continually

- The *Universal Woods-Saxon Hamiltonian* and associated, so-called 'universal parametrisation' has been developed in a series of articles:

- J. Dudek and T. Werner, J. Phys. G: Nucl. Phys. **4**, 1543 (1978),

- J. Dudek, A. Majhofer, J. Skalski, T. Werner, S. Cwiok, and W. Nazarewicz, J. Phys. G: Nucl. Phys. **5**, 1359 (1979),

- J. Dudek, W. Nazarewicz, and T. Werner, Nucl. Phys. A **341** 253, (1980)

- J. Dudek, Z. Szymański, and T. Werner, Phys. Rev. C **23**, 920 (1981) and has been summarised in

- S. Ćwiok, J. Dudek, W. Nazarewicz, J. Skalski, and T. Werner, Comp. Phys. Comm. **46**, 379 (1987).

This approach is being used without modifications by many authors also today.