A global data-driven dispersive optical model

Uncertainty-quantified non-local nucleon-nucleus scattering and structure description across the chart

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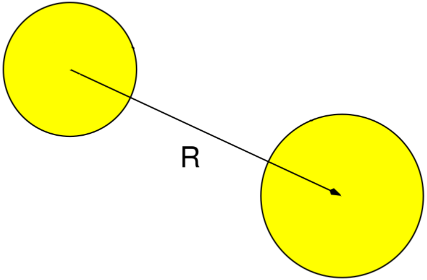
Towards a consistent approach for nuclear structure and reactions:
microscopic optical potentials
ECT*, June 2024

Degrees of freedom: nuclei.
Projection of the Hamiltonian on the elastic channel (Feshbach formalism, e.g. A. Moro, 2019, doi.org/10.3254/978-1-61499-957-7-129)



The projected interaction, U, is the optical-model potential:

$$U = PVP + PVQ \frac{1}{E - QHQ + i\epsilon} QVP \quad P, Q \text{ projections}$$

- A completely consistent U will be complex, non-local, and energy-dependent.
- Imaginary part: flux leaving the elastic channel.
- U cannot be actually computed as above

This work

Goal

Design and train a phenomenological optical model that

- Has all features required for a fully consistent microscopic potential: fully non-local and dispersive.
- Has sound uncertainty quantification, also accounting for model defects. Desirable in more ab-initio models too.
- Provides a good description on a wide area of the chart (global) and can be reliable in extrapolation.

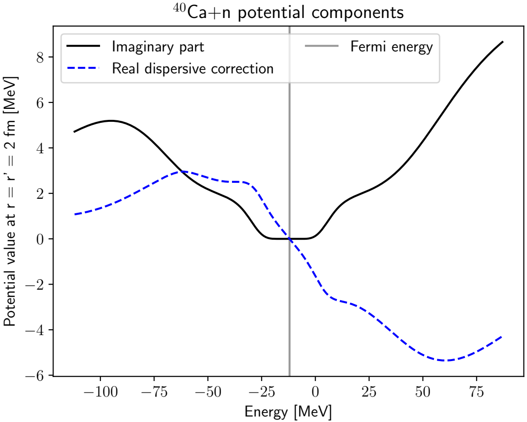
Contents

The dispersive optical model

Causality principle requires (J. S. Toll. *Phys. Rev.* 104.6 (1956))
OMP, U, to follow a dispersion (Kramers-Kronig) relation in energy:

$$U(\alpha, \beta, E) = U_{\mathrm{HF}}(\alpha, \beta) + U_D(\alpha, \beta, E), \quad \mathrm{Re}\, U_D(\alpha, \beta, E) = \frac{1}{\pi}\mathrm{PV}\int_{\mathbb{R}} \frac{\mathrm{Im}\, U_D(\alpha, \beta, \mathcal{E})}{E - \mathcal{E}}\, \mathrm{d}\mathcal{E}$$

Example of
$^{40}\mathrm{Ca+n}$ imaginary potential, and corresponding dispersive correction



Computing the dispersive correction

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In practice, the "usual" (Woods-Saxon, ...) forms are used for

- Energy-independent real part (less parameters)
- Energy-dependent imaginary part, with analytic forms whose integral is known (?).

The energy-dependent real part is then computed as above.

The potential (Hamiltonian) must be defined for all energies, positive and negative, to apply dispersivity.

$\mathrm{Re}\,U(E)$ is connected to $\mathrm{Im}\,U$ at all energies (and vice versa).

Consistent H for negative energies $\rightarrow$ structure information

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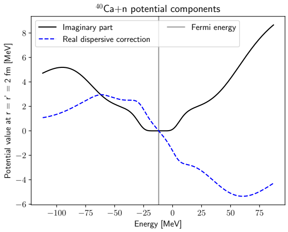
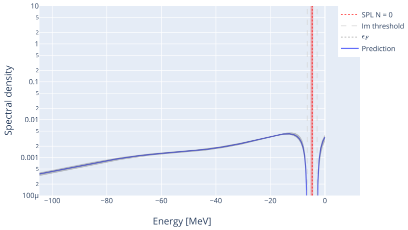
Features of a dispersive optical model

Dispersive optical models:

- Are computationally more expensive (manageable with appropriate analytic forms)
- Are more accurate (a physical condition is being enforced)
- Have less free parameters (the energy dependence of the real part is fixed)
- Describe consistently scattering and bound-state properties





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How to compute spectral functions

1. Define the potential in a basis for the nucleus-nucleon motion $\{\alpha\}$, $V_{\alpha\beta}(E)$.
   E nucleon-nucleus rel. energy
2. Compute the Hamiltonian, $H_{\alpha\beta}(E)$.
3. Compute the propagator, (requires inverting H, i.e. solving the scattering problem)

$$G_{\alpha\beta}(E) = \lim_{\eta \to 0} \frac{1}{E - H_{\alpha\beta}(E) + i\eta}$$

4. The hole spectral functions are

$$S^h_\alpha(E) = \frac{1}{\pi} \operatorname{Im} G_{\alpha\alpha}(E)$$

(analogous for particle spectral functions).

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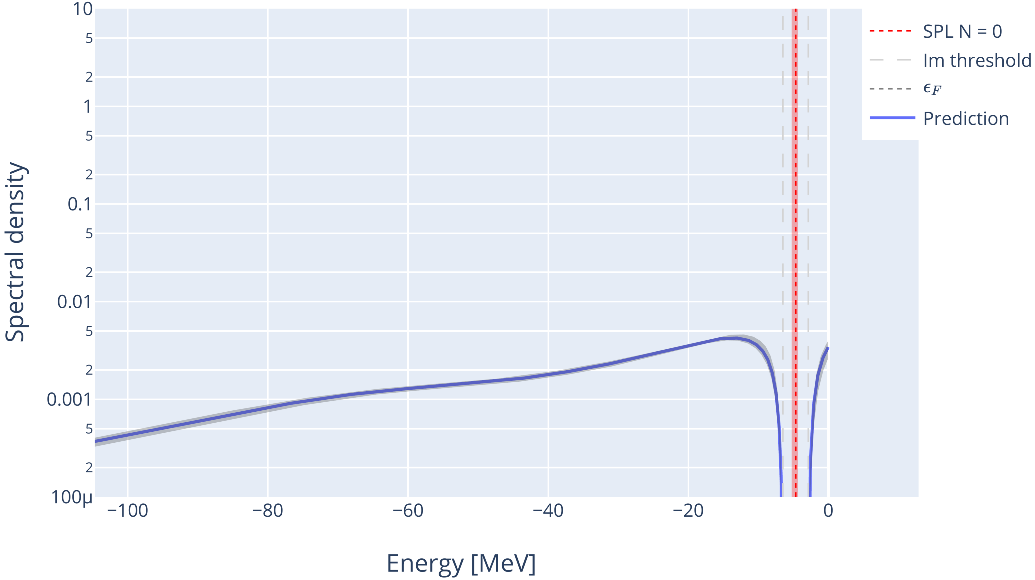
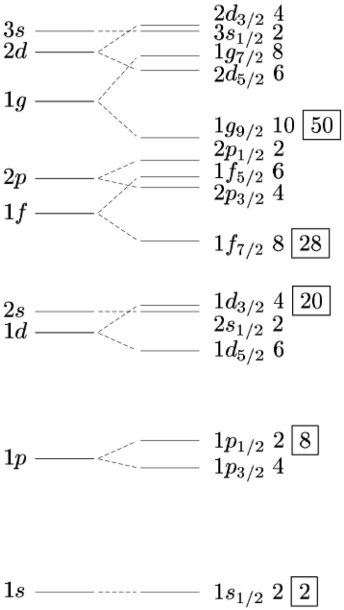
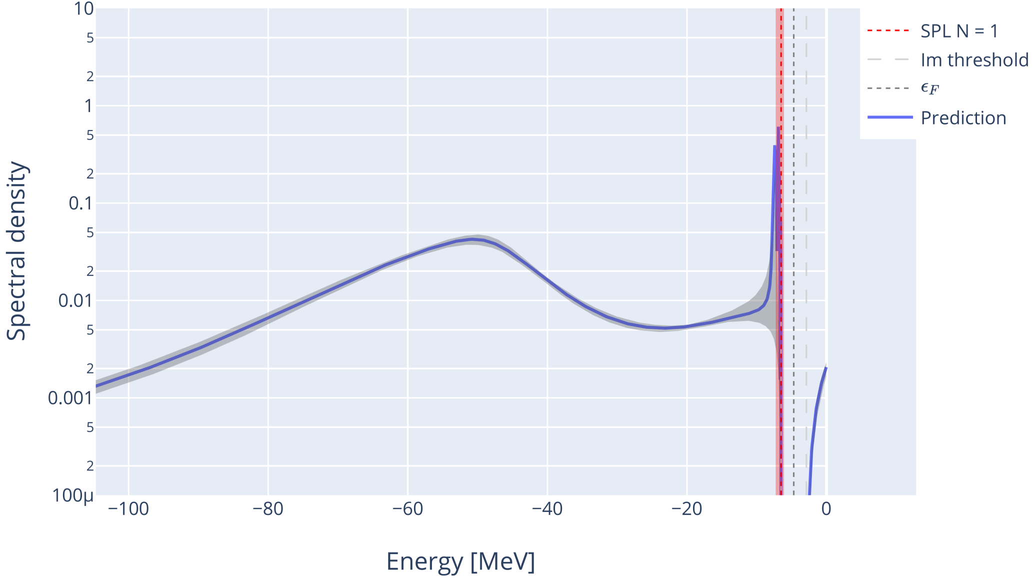


https://en.wikipedia.org/wiki/File:Shells.png



^{40}Ca − p $L = 0$, $J = 1/2$ spectral function (fit on ^{90}Zr, ^{112,124}Sn, ^{208}Pb)



Link to bound-state properties

Given the spectral function $S_\alpha(E)$,

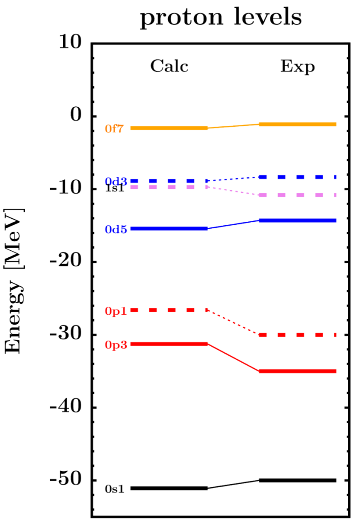
$$\text{one-body density } n_\alpha = \int_{-\infty}^{\mathcal{E}_F} S_\alpha(E)\,\mathrm{d}E \quad , \quad \text{number of particles } n = \sum_\alpha n_\alpha$$

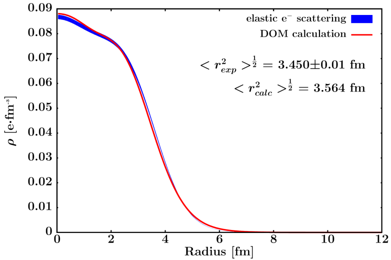
If $\alpha = (\vec{r}, a)$, $\quad n_\alpha =$ density $\rho_a(\vec{r}) \longrightarrow$ charge radius, electromagnetic moments

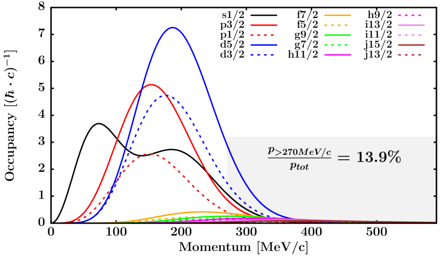
If $\alpha = (r, a)$, $\quad$ "Spectroscopic factors" $S_a(E) = \int S_{a,r}(E)\,\mathrm{d}r$

s.p. energies $E_a = \int_{-\infty}^{\mathcal{E}_F} S_a(E) E\,\mathrm{d}E \longrightarrow$ binding energy

Examples of ^{40}Ca bound-state observable predictions



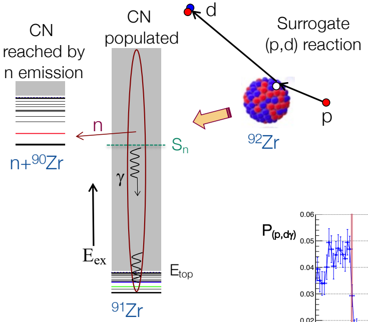


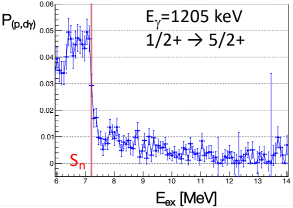


(C. Pruitt, 2019, PhD thesis, 10.7936/hyxx-6e81)

Surrogate reactions method for neutron capture

Escher et al, PRL 121, 052501 (2018)





From theory

To be determined

A Surrogate experiment gives

$$P_{(p,d\gamma)}(E) = \sum_{J,\pi} F_{(p,d)}{}^{CN}(E,J,\pi) \cdot G^{CN}{}_{\gamma}(E,J,\pi)$$

^{90}Zr(n,γ) cross section:

$$\sigma_{(n,\gamma)} = \sum_{J,\pi} \sigma_{n+target}{}^{CN}(E,J,\pi) \cdot G^{CN}{}_{\gamma}(E,J,\pi)$$

From experiment

The new cross section we want

Predicted from optical potential

*Width fluctuation corrections are omitted here, but accounted for in applications.

Contents

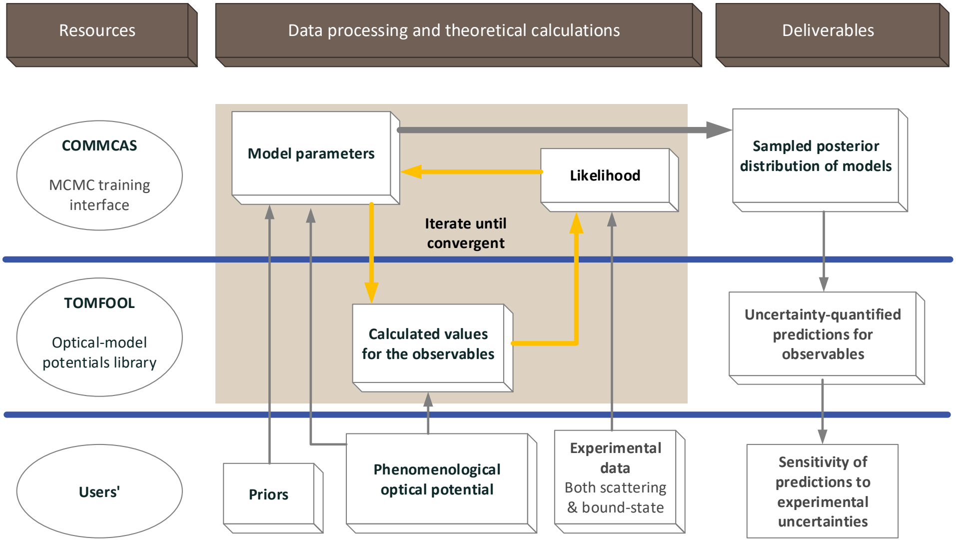
Markov-chain Monte Carlo training

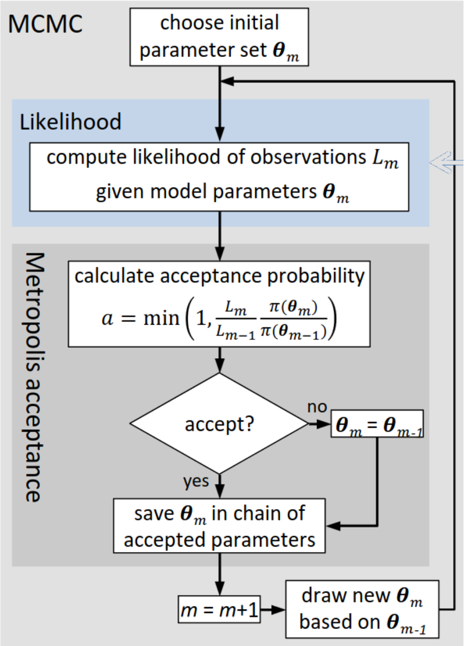
- Highly non-linear model.
- High-dimensional parameter space (e.g. Koning-Delaroche has 46 parameters).
- Need good uncertainty quantification.

→ Fit performed through Markov-chain Monte Carlo (Bayesian):

- Computationally demanding.
- Statistical assumptions more explicit (priors).
- Straightforward and reliable error estimation
  ("fit" yields a sample of posterior distribution of potentials):
  - No truncation to 2^{nd} moments.
  - No Gaussian distribution assumption.

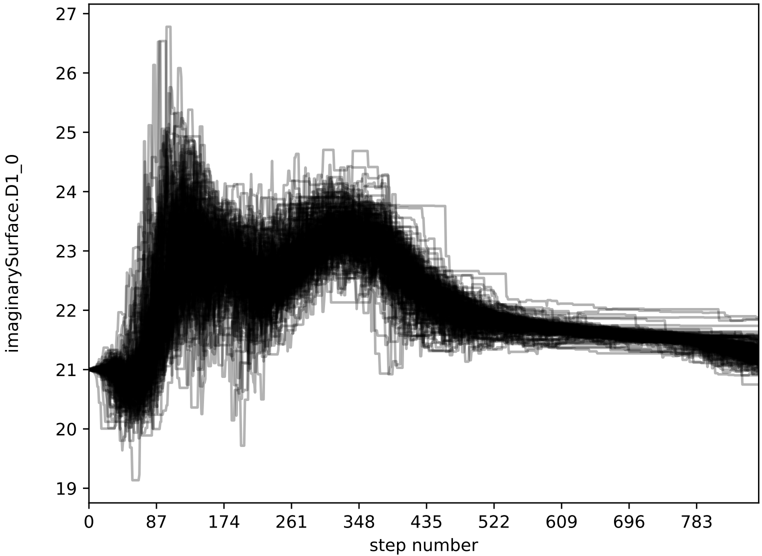
MCMC training of data-driven optical models





ebooks.iospress.nl/publication/48604

A parameter trace for a Markov-Chain-Monte-Carlo OMP inference



Markov-chain Monte Carlo training – output

The MCMC “fit” yields a sample of the posterior distribution of potentials:

Potential 1: $r_{C0} = 1.21\,\text{fm}$, $V_{00} = 51\,\text{MeV}$, ...

Potential 2: $r_{C0} = 1.25\,\text{fm}$, $V_{00} = 46\,\text{MeV}$, ...

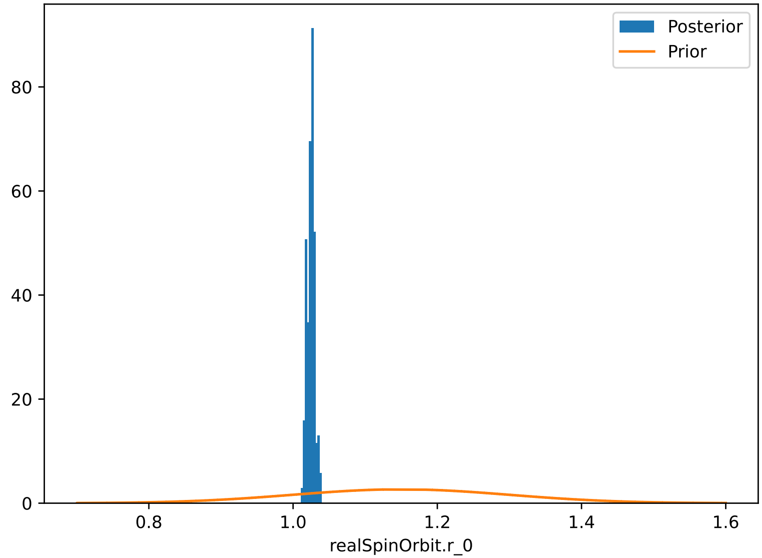
...

Potential 485: ...

From the sample, extract:

- Statistics on parameters
- Sample of distribution of predictions for any observable

Example of a posterior parameter distribution



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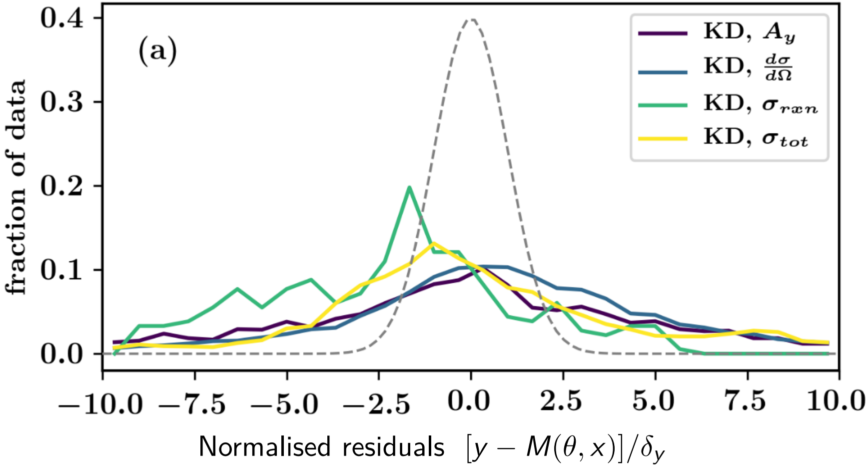
Koning-Delaroche training dataset, by observable type
(C. D. Pruitt et al. *Phys. Rev. C* 107.1 (2023))



...good uncertainty quantification is hard for this problem.

Limitations of OMP fitting

(C. D. Pruitt et al. *Phys. Rev. C* 107.1 (2023)
and e.g. A. J. Koning et al. *Nuclear Physics A* 713.3 (2003))

- There are outliers.
- Uncertainties (statistical and systematic) are underestimated.
- Errors due to experiment and model defects are not disentangled.
- Observations are not independent.
- $\chi^2 \gg 1$ and error estimation based on it is not meaningful

Unaccounted-for-uncertainties estimation

Covariance matrix in C. D. Pruitt et al. *Phys. Rev. C* 107.1 (2023)
(the expression was simplified for illustrative purposes):

$$\tilde{\Sigma} = \frac{k}{N}\,\mathrm{diag}(\vec{\Delta}) \quad , \quad \vec{\Delta} = \left\{ \delta_y^2 + \left(y\, \delta_{\hat{t}(y)} \right)^2 \right\}$$

δ_y reported data error, y observation, $M(x)$ model prediction,
$\hat{t}(y)$ "type" (proton elastic σ, neutron analyzing power, ...) of y,
$\delta_{\hat{t}}$ fitted parameters.

Likelihood (being $r = y - M(\vec{\theta}, x)$):

$$L = \left[(2\pi)^k \left| \tilde{\Sigma} \right| \right]^{-1/2} \exp\left[-\frac{1}{2} \frac{\vec{r}^2}{\left| \tilde{\Sigma} \right|} \right]$$

Outlier rejection

"Sigma clipping":

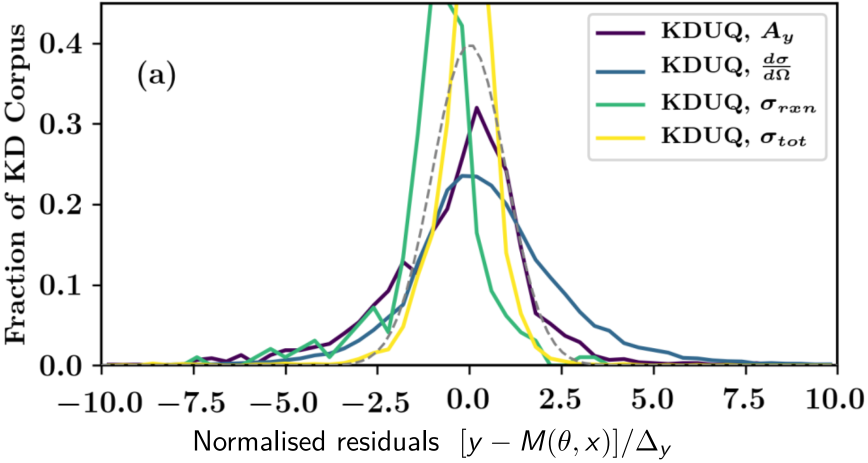
1. Converge fit on chosen data set (initially, all data).
2. Chose data set as points such that

$$y - M(\vec{\theta}, x) \leq 3\sqrt{\delta_y^2 + \mathrm{var}\left(M(\vec{\theta}, x)\right)}$$

   (discarded data can be recovered at a later step).
3. Repeat until convergent.

Past literature shows that...

Koning-Delaroche training dataset, by observable type
Uncertainty-quantified potential
(C. D. Pruitt et al. *Phys. Rev. C* 107.1 (2023))



...missing data- and model-uncertainties can be effectively estimated.

Contents

How much computing power do we need?

- Currently, $0.7\,\mathrm{s}$ for one Green's function, $0.04\,\mathrm{s}$ for one scattering energy. (Could be a great use case for emulators)
- 2×10^4 MCMC steps (at least, if fitted UAU and outlier rejection desired)
- 150 target nuclei (for a "global" fit).
- 2 projectiles (proton and neutron) per target.
- 400 MCMC walkers (~ 40 fit parameters)

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- Half walkers can run in parallel (stretch move): 200 cores, ~ 416 days.
- Each system can run in parallel: 6×10^4 cores, ~ 33 hours.

Quartz ($108\,648$ cores)

Contents

The currently-adopted potential

$$Z_1 Z_2 \,\text{Coulomb}\left(R_1, r_{C0}A^{1/3} + r_{C1}A^{-1/3} + r_{C2}A^{-4/3}\right) + \text{NLP}\cdot U$$

$$U = -\left(V_{v0} - V_{vA}A^{-1/3} \pm V_{vs}\frac{Z-N}{A}\right)\ \text{WS}(R, r_{v0}A^{1/3} - r_{v1}) +$$

$$+V_{SO}\vec{L}\cdot\vec{S}\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\text{WS} - iW(E, W_1, W_2, E_F, \dots)\text{WS} +$$

$$-\text{asymptotic imaginary volume correction}(E_a, \dots) +$$

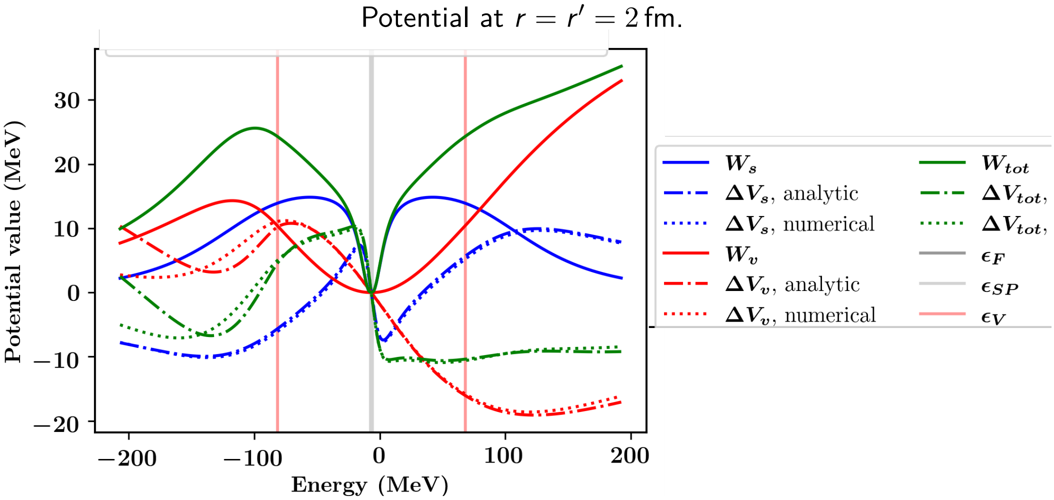
$$-\text{imaginary surface symmetric around } E_F + \sout{\text{imaginary spin-orbit}} +$$

$$+\text{dispersive correction}(E, W_1, \dots)$$

$$R = (R_1 + R_2)/2$$

$$\text{NLP} = \frac{2\sqrt{R_1 R_2}}{\beta^2}\exp\left(-\frac{R_1^2 R_2^2}{\beta^2}\right) J(L + 0.5, 2R_1 R_2/\beta^2)$$

Plot with current imaginary forms



Analytic dispersive correction at $E < E_F$ valid at all E only when E_a is big.

Present results

- Fit on ^{90}Zr, ^{112,124}Sn, ^{208}Pb: RCS, TCS, n_{nucleon}; fixed UAU, no rejections
- Fit on ^{40,48}Ca, ^{58,64}Ni, ^{90}Zr bound properties only; fit UAU, no rejections

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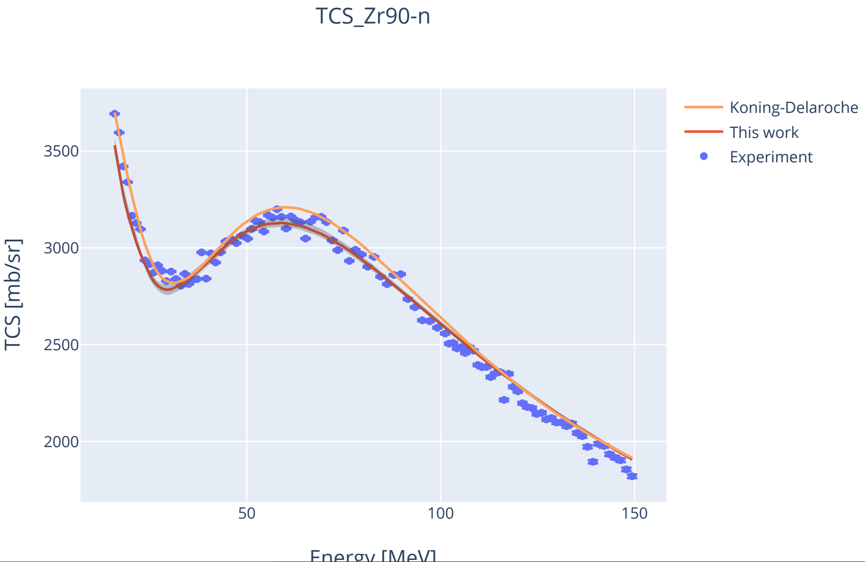

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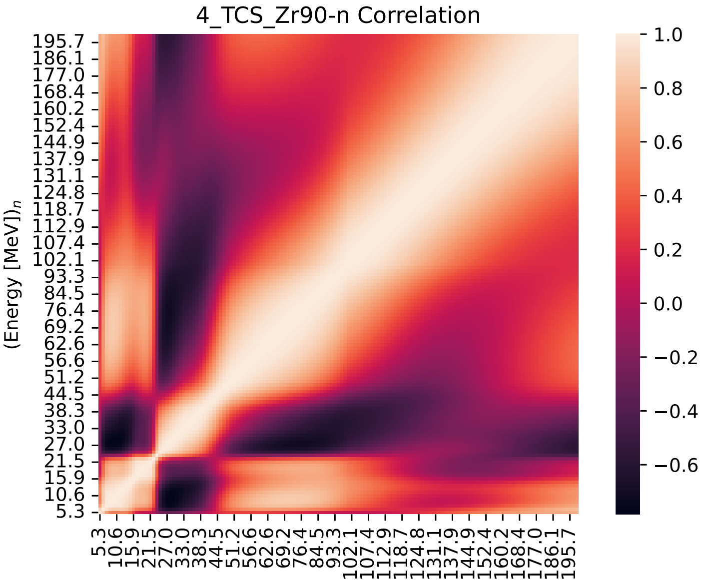

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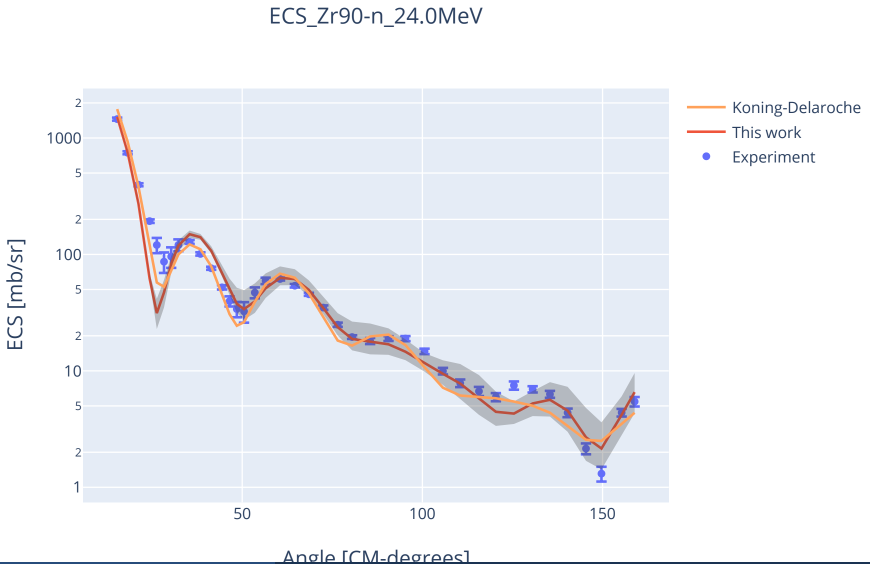

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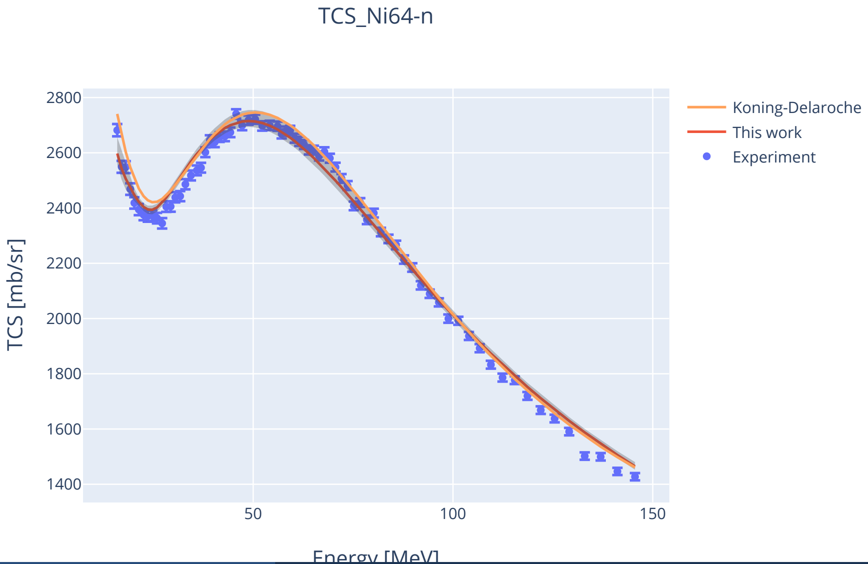

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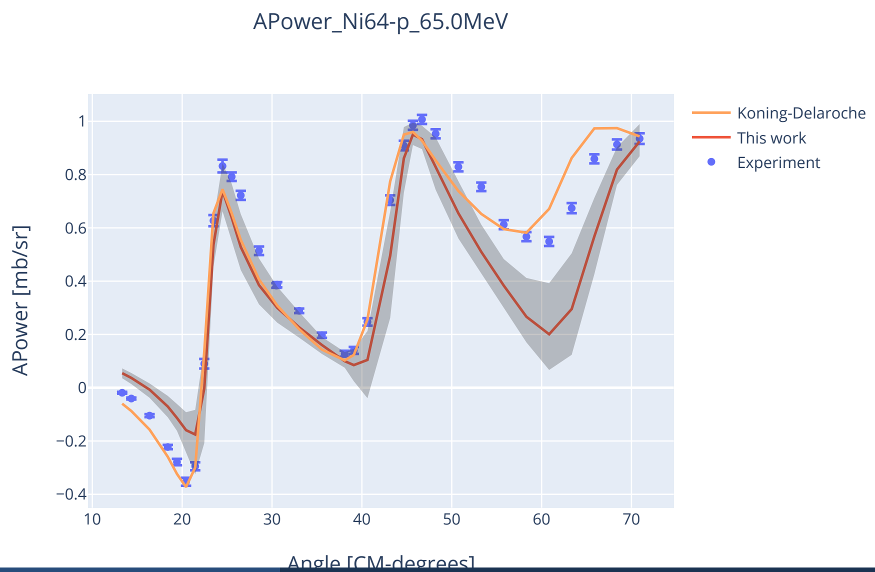

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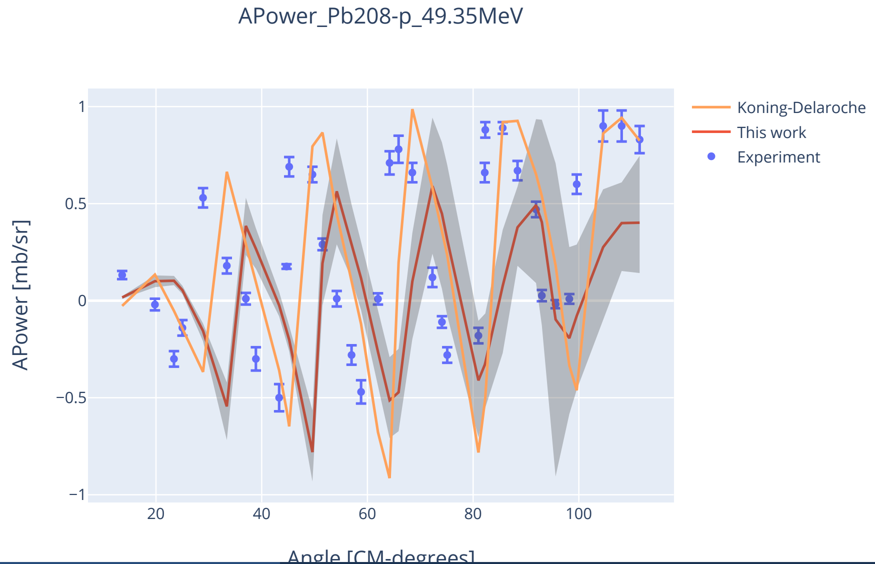

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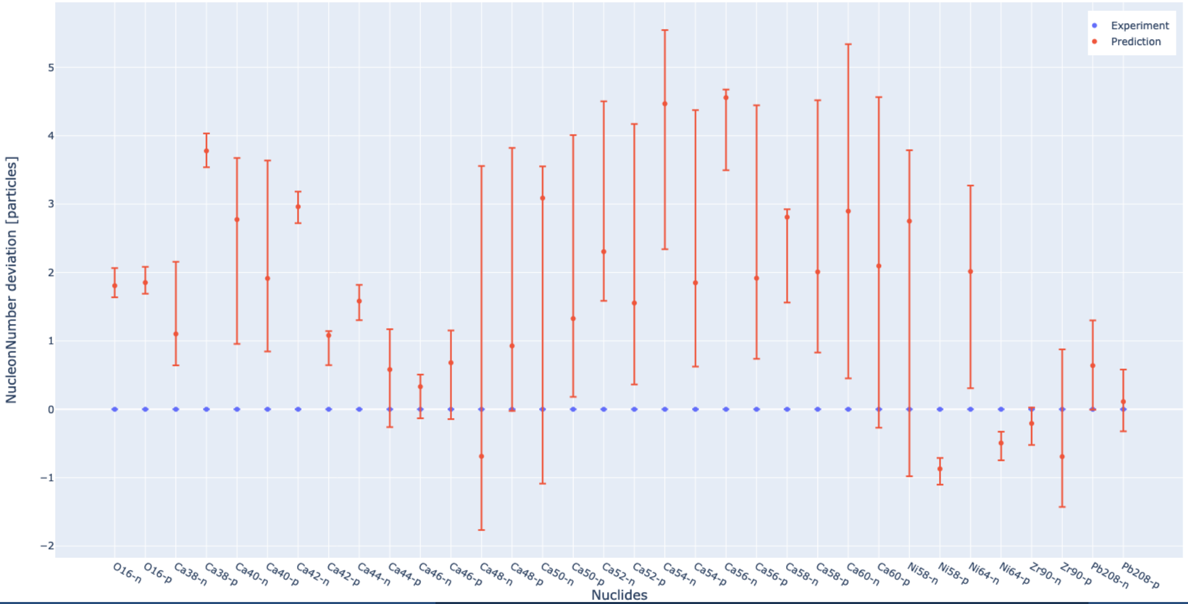

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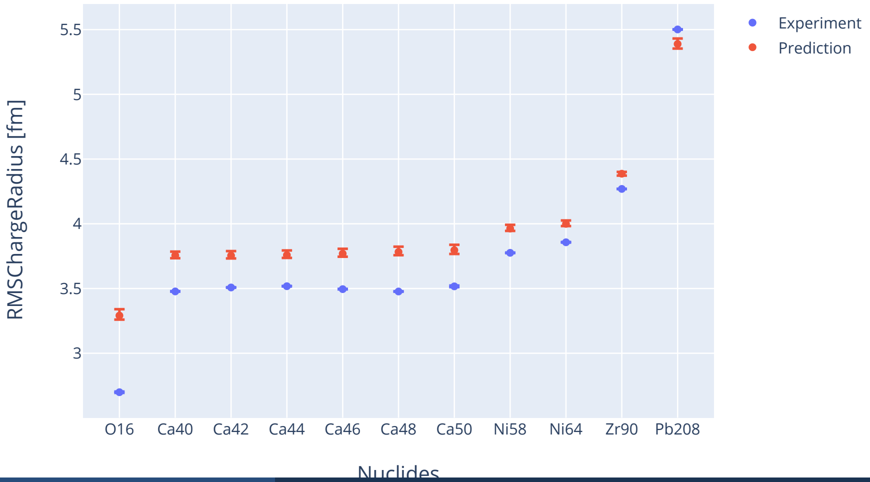

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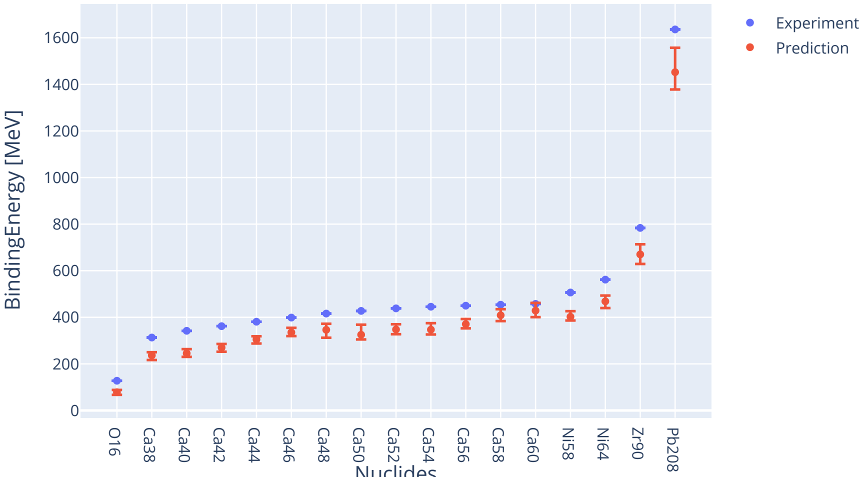

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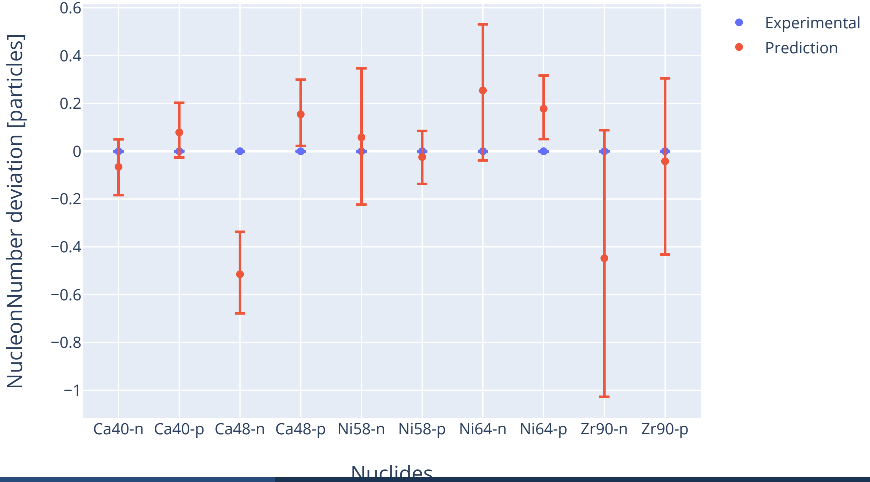

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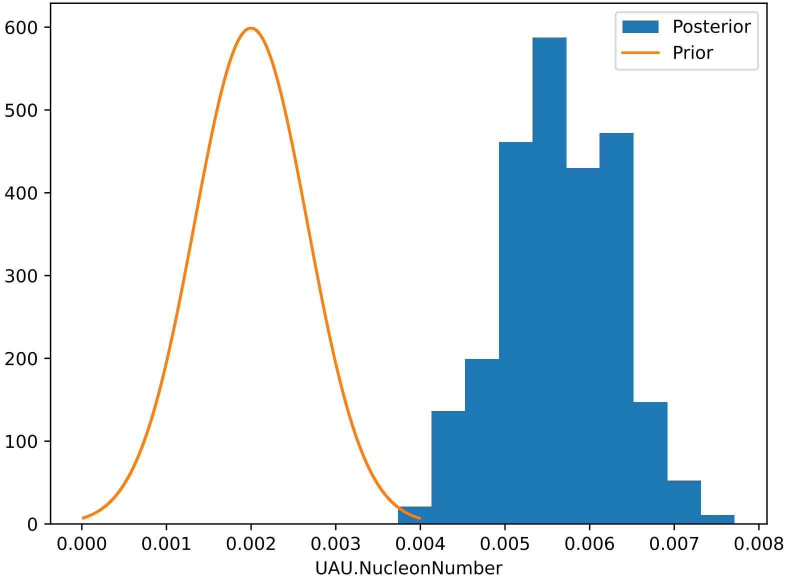

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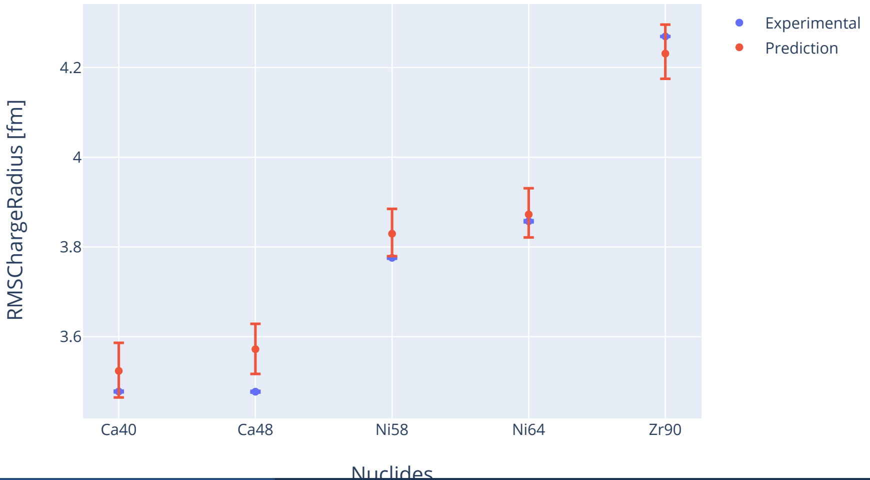

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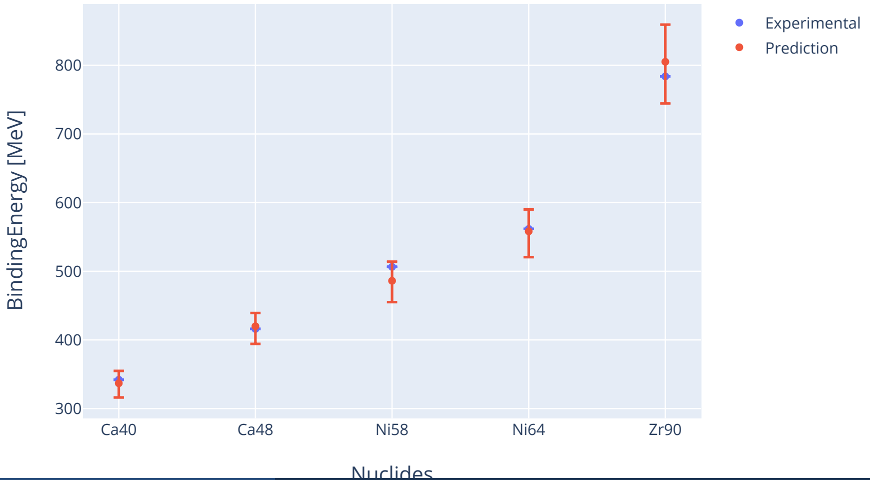

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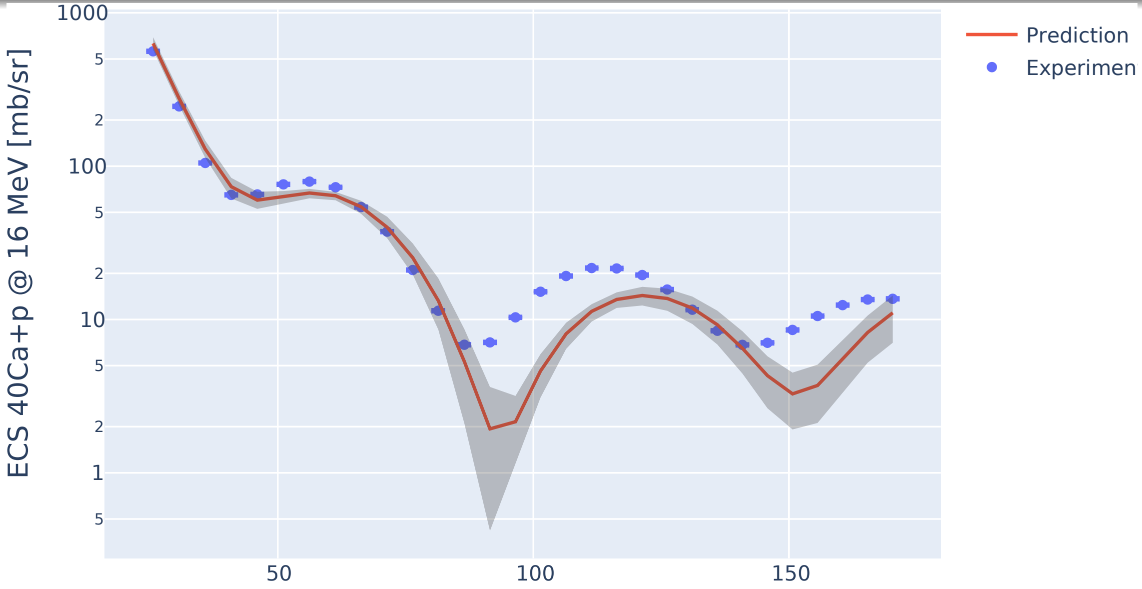

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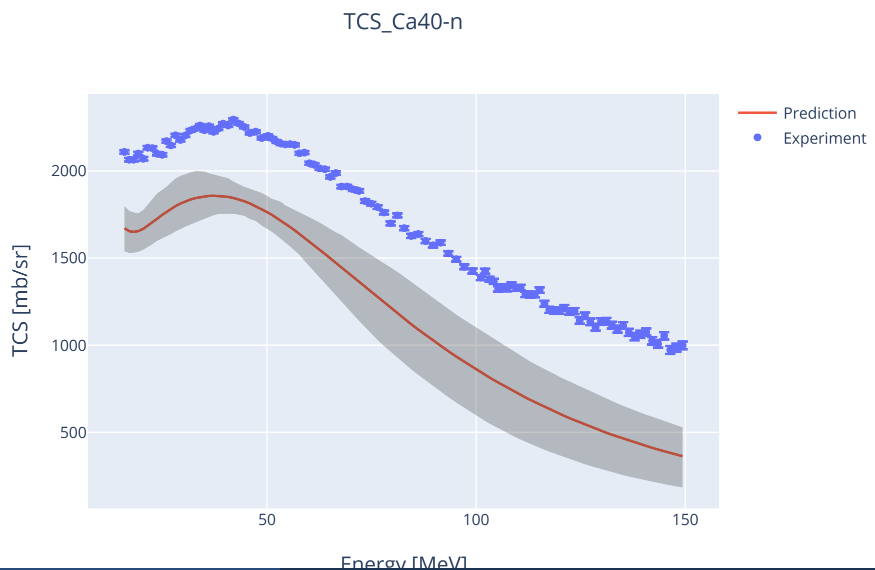


Contents

New potential form (under testing)

$$\text{Coulomb}\,(R_1,\dots) + \text{NLP} \cdot U$$

$$U = -\text{Real energy-independent volume}(R,\dots) + \text{spin-orbit}$$
$$-\text{only for } E > E_F\text{: Imaginary volume with asymptotic correction}$$
$$-\text{imaginary surface non-symmetric around } E_F$$
$$-\text{at } E < E_F\text{: im. volume with surface-like } E\text{-dependence (no asymptotic-corrected volume)}$$
$$+\text{dispersive correction}(E, W_1,\dots)$$

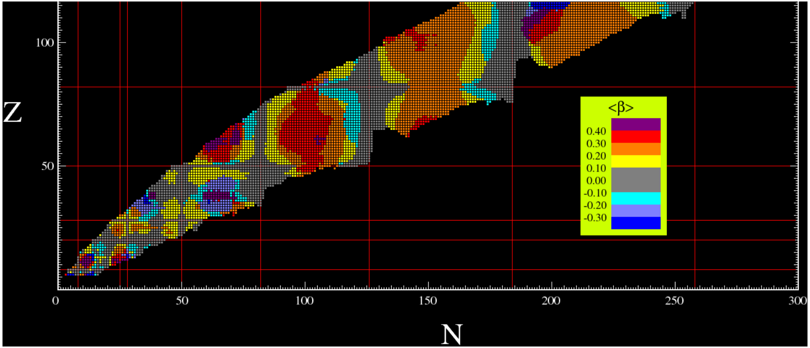
$$R = (R_1 + R_2)/2$$

$$\text{NLP} = \frac{2\sqrt{R_1 R_2}}{\beta^2} \exp\left(-\frac{R_1^2 R_2^2}{\beta^2}\right) J(L + 0.5, 2R_1 R_2/\beta^2)$$

- Preliminary testing look promising.

Perspectives: role of deformation

www-phynu.cea.fr/science_en_ligne/carte_potentiels_microscopiques/carte_potentiel_nucleaire_eng.htm



"Spherical" potentials perform worse for deformed nuclei [e.g. A. J. Koning et al. *Nuclear Physics A* 713.3 (2003)].

1. Take into account effects of deformation through models (e.g. coupled channels).
2. Extract equivalent OMP, minimal added complexity for e.g. elastic studies.

Summary

- Reliable global optical model, fully dispersive and non-local,
  trained on scattering and bound-state data,
  with sound uncertainty quantification, is within reach.
  (Nucleon numbers, binding energies, etc., available for very unstable systems).
- Changes to "traditional" potential form required for full dispersivity and good data reproduction (under testing now).
- User-friendly library handling such potentials (TOMFOOL) will be released.

To do:

- Test new form.
- Include more quantities (single-particle energies, charge exchange, skins, ...).
- Improve computational efficiency (more parallel, maybe emulators).

Thank you for your attention

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