The nucleon-nucleus scattering and structure

Markov-chain Monte Carlo parameter inference for a phenomenological dispersive optical-model potential

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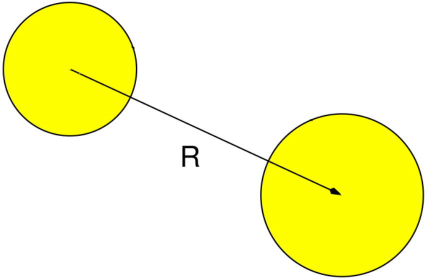
Optical-model potentials (a.k.a. irreducible self-energy)

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:

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

- Degrees of freedom: motion between reactants center-of-mass.
- A completely consistent U will be complex, non-local, and energy-dependent.
- Imaginary part: flux leaving the elastic channel.

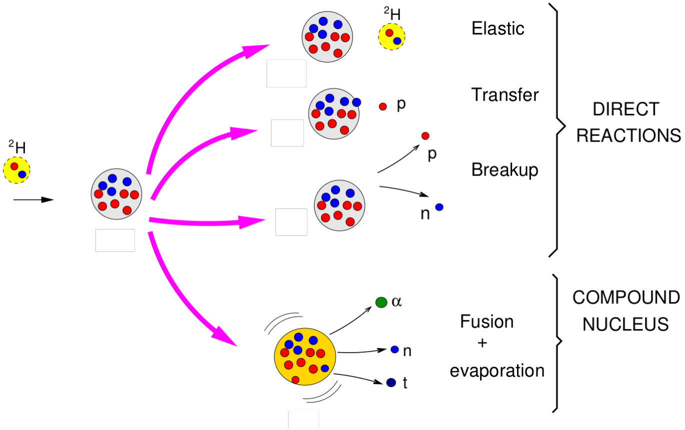
Exact framework (if detailed information on inelastic is not needed).

Optical potentials are a staple of current nuclear physics

Optical-model potentials (OMP) give a simple, concise description of the nuclear interaction.

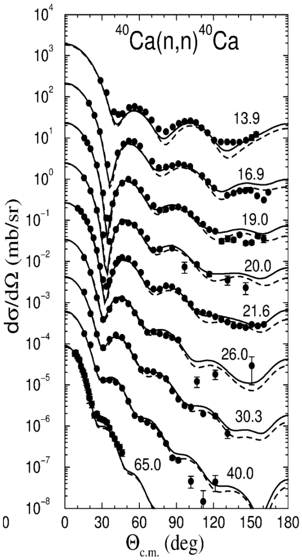
Countless applications… (fig. from A. Moro, 2019, `doi.org/10.3254/978-1-61499-957-7-129`)

Add in bound-state properties!



Traditional optical-model potentials

- Phenomenological: χ^2 fit on data.
- Only scattering (no structure).
- Local.
- "Error-propagation" superficial or absent.
- Extraordinarily successful!
  (in interpolation)
  [Fig. from A. J. Koning et al. *Nuclear Physics A* 713.3 (2003)].



This work

Goal

Design and train a (physics-informed) 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.
- Provides a good description on a wide area of the chart (global) and can be reliable in extrapolation.

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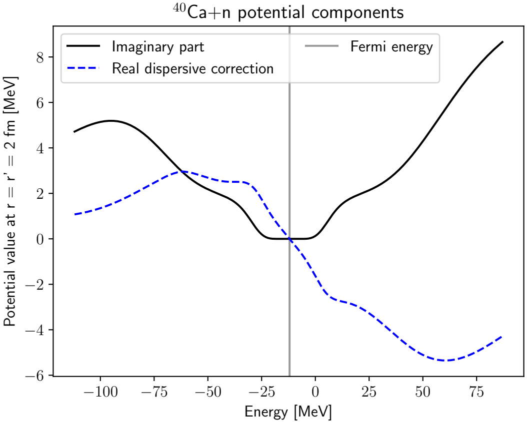
The dispersive optical model

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

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

Use forms analytic in E
whose dispersion integral is known
for faster calculations.



The adopted potential (as of June 2024)

Start by the "simplest possible" and add more only if data require it.

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

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

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

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

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

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

$$R = (R_1 + R_2)/2 \quad , \quad \text{NLP} = \frac{2\sqrt{R_1 R_2}}{\beta^2}\exp\left(-\frac{R_1^2 R_2^2}{\beta^2}\right) J(L + 0.5, 2R_1R_2/\beta^2)$$

How to compute observables from the optical potential

For scattering: solve (find the phase-shifts)

$$-\frac{\hbar^2 \nabla^2_{\vec{r}}}{2m}\chi(\vec{r}) + \int_{\mathbb{R}^3} U(\vec{r},\vec{r}')\chi(\vec{r}')\,\mathrm{d}^3\vec{r}' - E\chi(\vec{r}) = 0$$

For bound-state properties:

Given the Hamiltonian in a basis for the nucleus-nucleon motion $\{\alpha\}$, $H_{\alpha\beta}(E)$,

1. Compute the propagator (requires inverting H) and hole spectral functions

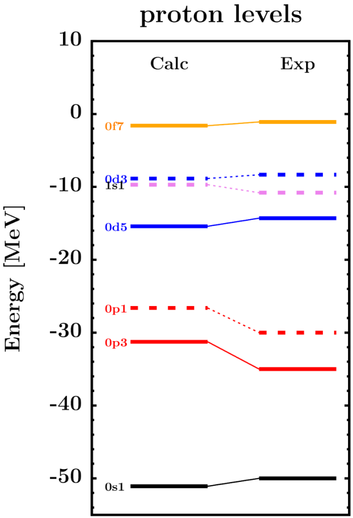
$$G_{\alpha\beta}(E) = \lim_{\eta\to 0} \frac{1}{E - H_{\alpha\beta}(E) + i\eta} \quad , \quad S^h_\alpha(E) = \frac{1}{\pi}\,\mathrm{Im}\, G_{\alpha\alpha}(E)$$

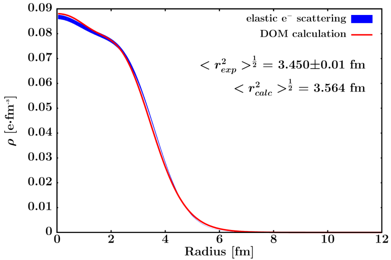
for all $E < E_F$ on a suitable finite grid.

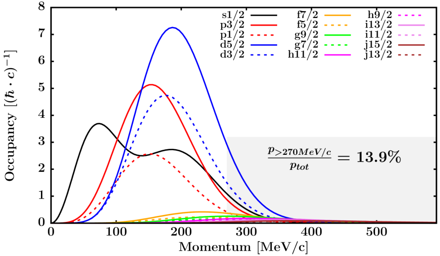
2. Derive one-body observables of interest, e.g.

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

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







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

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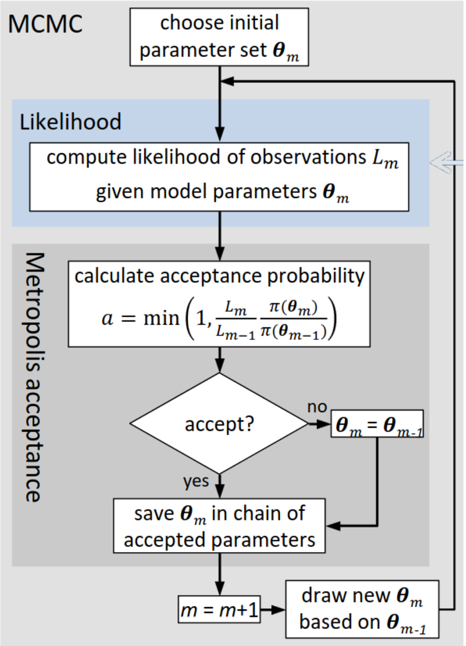
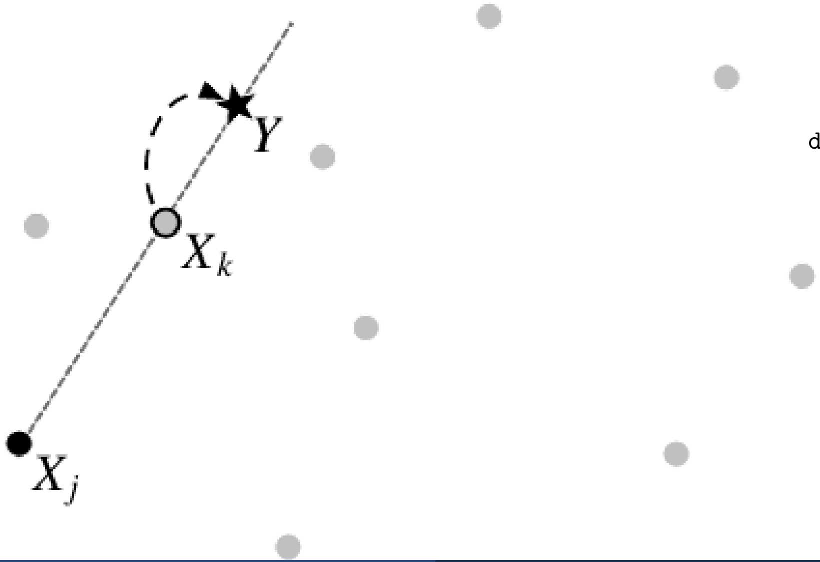


ebooks.iospress.nl/publication/48604

Stretch move



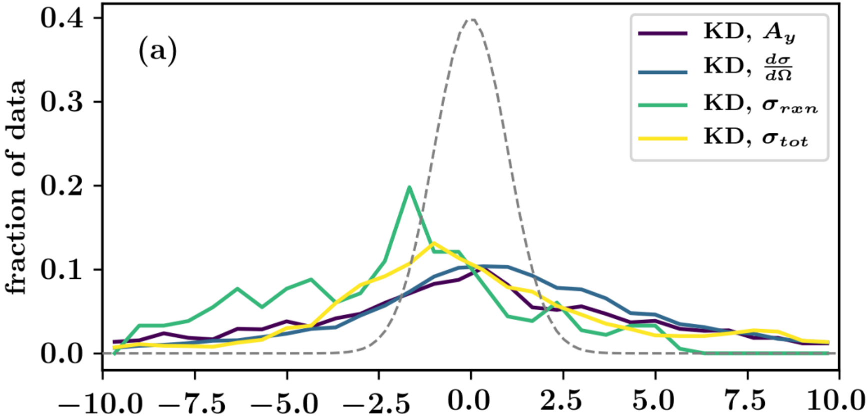
dx.doi.org/10.2140/camcos.2010.5-1

High-dimensional parameter space.

Posterior expected unimodal.

Limitations of OMP fitting: past literature shows that...

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



Normalised residuals $[y - M(\theta, x)]/\delta_y$

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

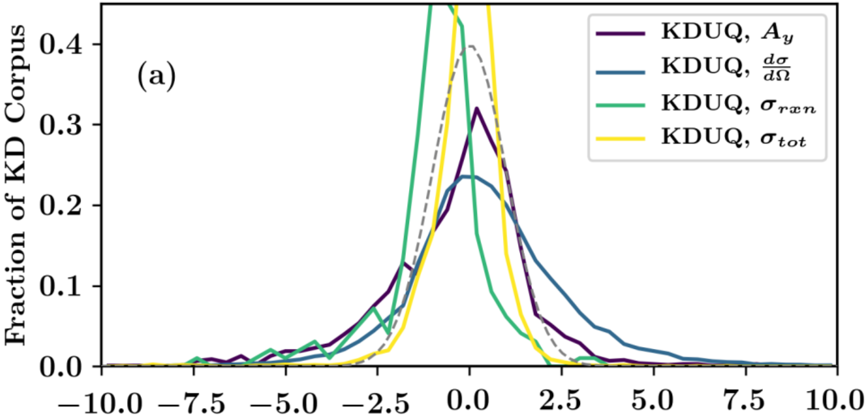
Limitations of optical potentials fitting

(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))

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

Past literature shows that...

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



Normalised residuals $[y - M(\theta, x)]/\Delta_y$

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

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.
$\hat{t}(y)$ "type" of y (proton elastic σ, neutron analyzing power, ...),
$\delta_{\hat{t}}$ 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 capping":
Residuals are capped at $r_{\mathrm{max}} = \Delta_y \cdot R_{\hat{t}(y)}$ ("R standard deviations")
$R_{\hat{t}(y)}$ chosen manually, different for each data "type"
(3 for ECS, ∞ for particle number, ...)

Suspect outliers add constant penalty
$\Rightarrow$ don't affect the fit unless they can be reasonably reproduced by the model.

How to weight different datasets?

E.g., a $\mathrm{d}\sigma/\mathrm{d}\Omega$ with 100 data points, and a single point for the binding energy.

Case 1: data are independent (up to the model's k degrees of freedom),

$$\tilde{\Sigma} = \frac{k}{N}\,\mathrm{diag}(\Delta_1, \ldots, \Delta_N)$$

Case 2: data in a dataset are fully correlated,

$$\tilde{\Sigma} = \frac{k}{n_s}\,\mathrm{diag}\left(\frac{1}{N_1}\Delta_1, \ldots, \frac{1}{N_1}\Delta_{N_1}, \frac{1}{N_2}\Delta_{N_1+1}, \ldots \frac{1}{N_{n_s}}\Delta_N\right)$$

In reality, data points for a given measurement
are not fully independent, neither fully correlated.

Contents

How much computing power do we need?

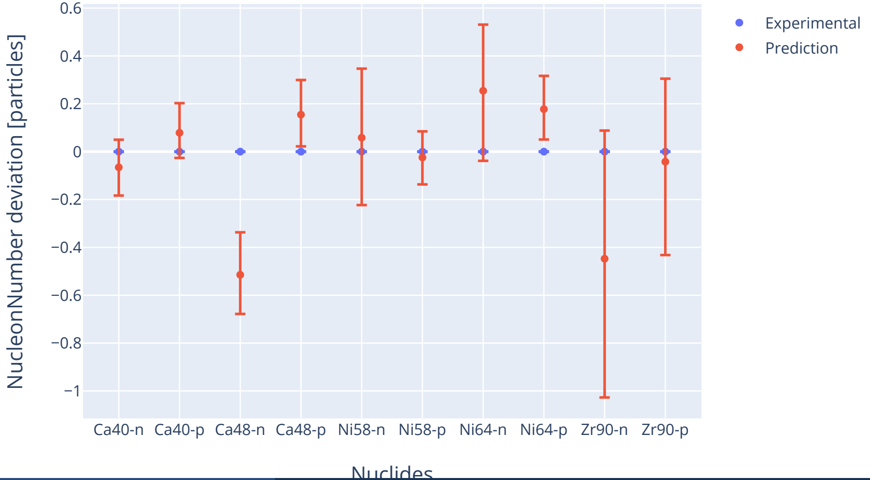
- Currently, $0.7\,$s for one Green's function, $0.04\,$s for one scattering energy.
- 10^4 MCMC steps (at least, if fitted UAU and outlier rejection desired)
- 150 target nuclei (for a "global" fit).
- 2 projectiles (proton and neutron) per target.
- 400 MCMC walkers (~ 40 fit parameters)

~ 114 years in serial.

- Half walkers can run in parallel (stretch move): 200 cores, ~ 208 days.
- Each system can run in parallel: 6×10^4 cores, ~ 17 hours.

Contents

Fit on ^{40,48}Ca, ^{58,64}Ni, ^{90}Zr bound properties only; fit UAU, no rejections



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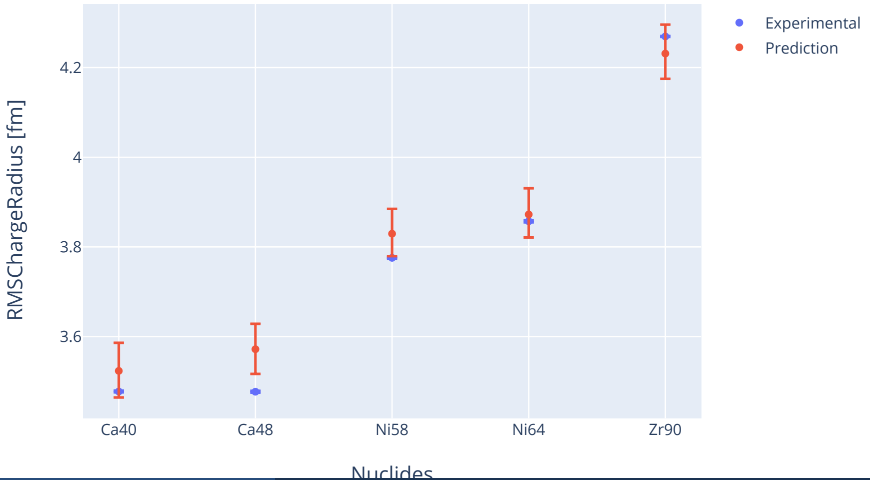

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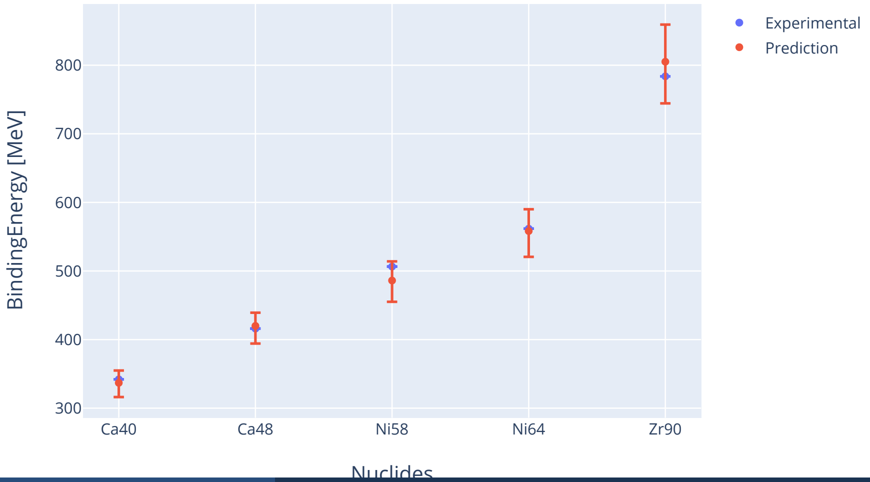

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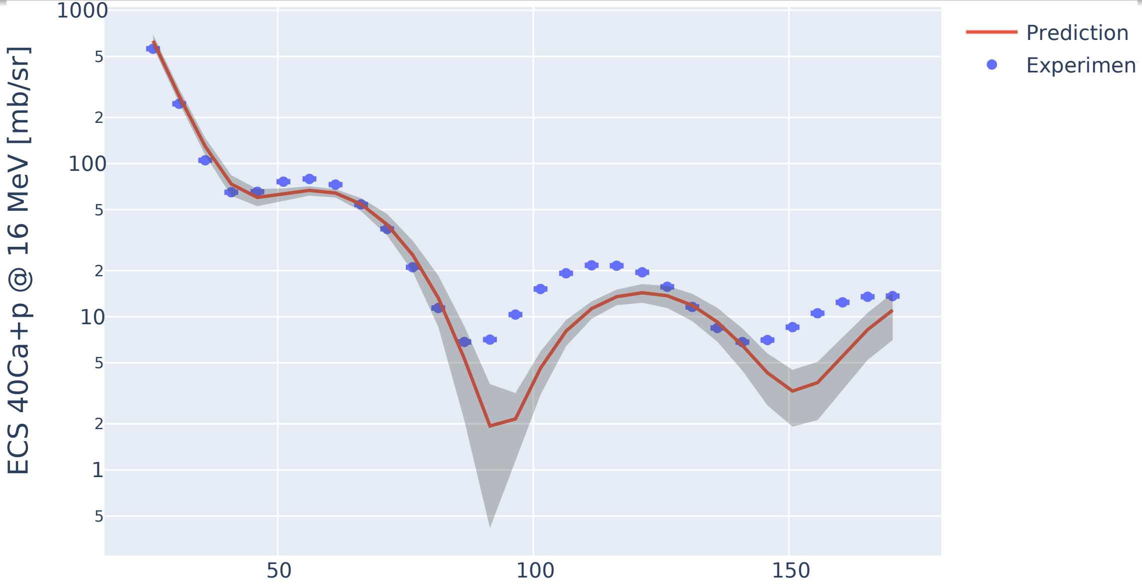

Summary

- 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).
- User-friendly library handling such potentials (TOMFOOL) will be released.
- Careful choice of likelihood function required for the problem at hand.

To do:

- Include more quantities (single-particle energies, charge exchange, skins, ...).
- Improve computational efficiency (parallelization, emulators).

Thank you for your attention

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