Microscopic optical potentials for the FRIB era

Jeremy Holt*
Texas A&M University, College Station

*Collaborators: Taylor Whitehead, Yeunhwan Lim, Pengsheng Wen

FRIB TA Topical Program: Theoretical Justifications and Motivations for Early High-Profile FRIB Experiments, 5/18/23

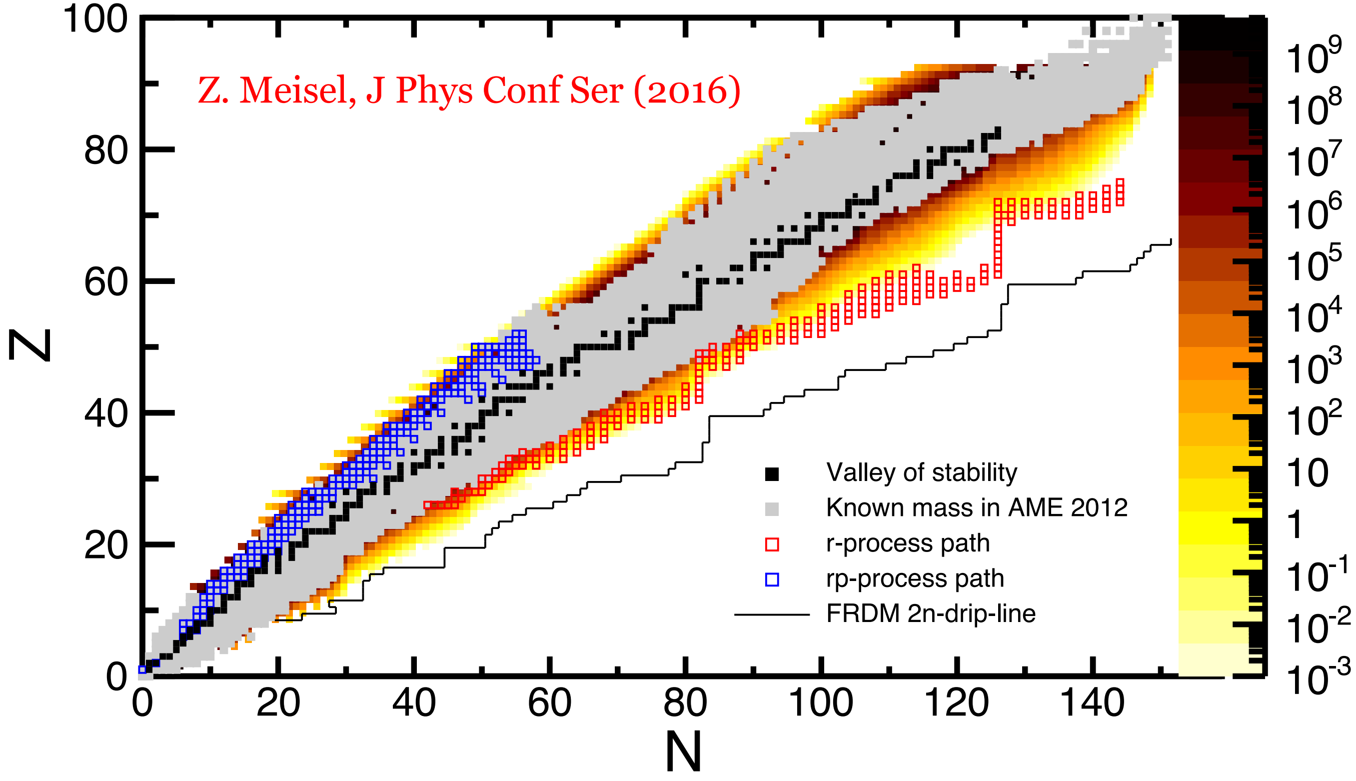
Motivation: Nuclear reactions with unstable isotopes

- Interpretation of rare isotope beam experiments (neutron skins, nuclear properties near the dripline, capture rates in astrophysical environments)

- Challenges:
  - Ab initio nuclear reaction theory available for light systems at low energies
  - *Optical potentials* are a necessary ingredient in most reaction models, including transport analysis of heavy-ion collisions
  - *Global* optical potentials are needed for a consistent reaction theory over a wide range of unstable isotopes
  - Commonly used global optical potentials are phenomenological and fitted around nuclear stability

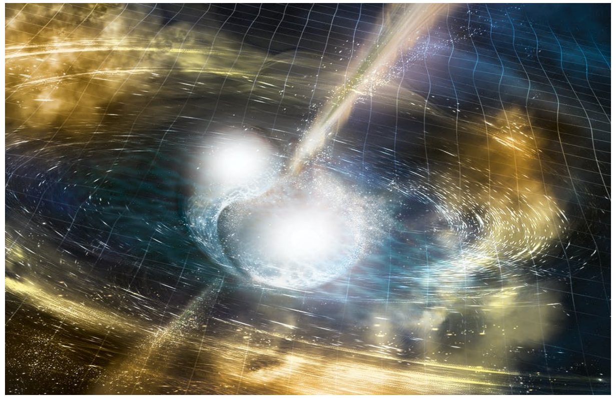
- Advantages of *microscopic approaches*
  - Start from the same many-body principles governing ab initio nuclear structure theory
  - Can reveal more efficient parameterizations for phenomenological optical potentials
  - Can provide a suitable *prior* as part of a more comprehensive Bayesian uncertainty analysis that incorporates scattering data

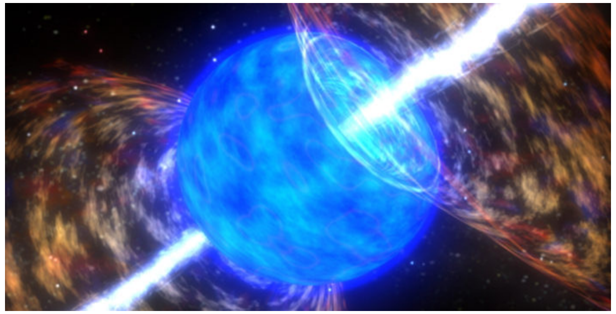
Application: R-process nucleosynthesis



Astrophysical site?

Neutron star mergers



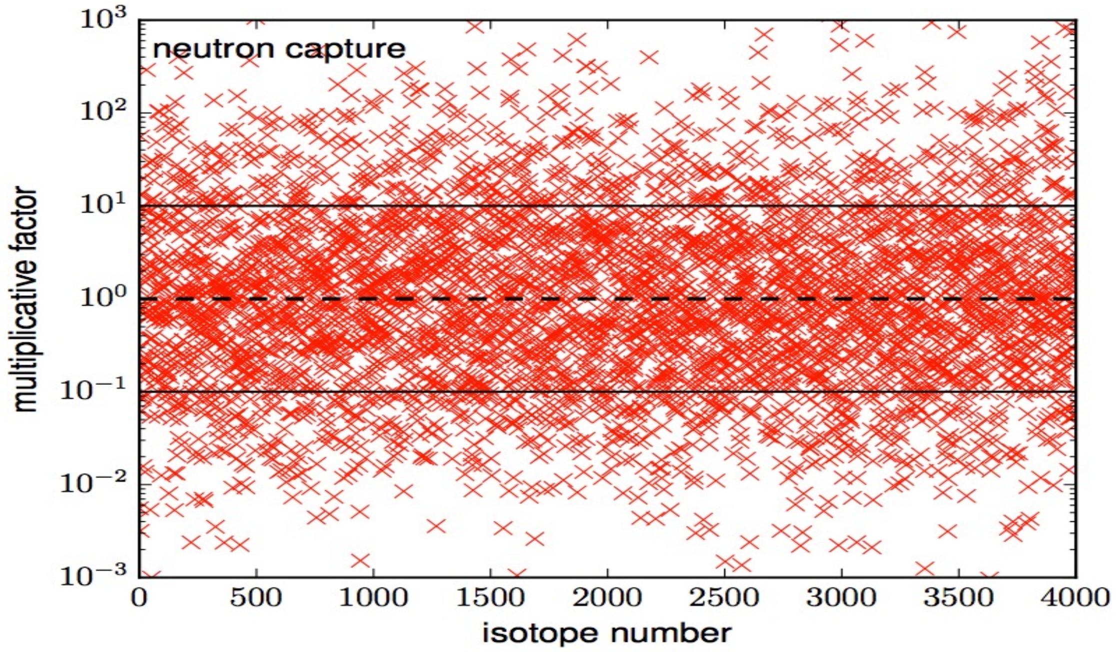


Collapsars

Neutron capture sensitivity studies

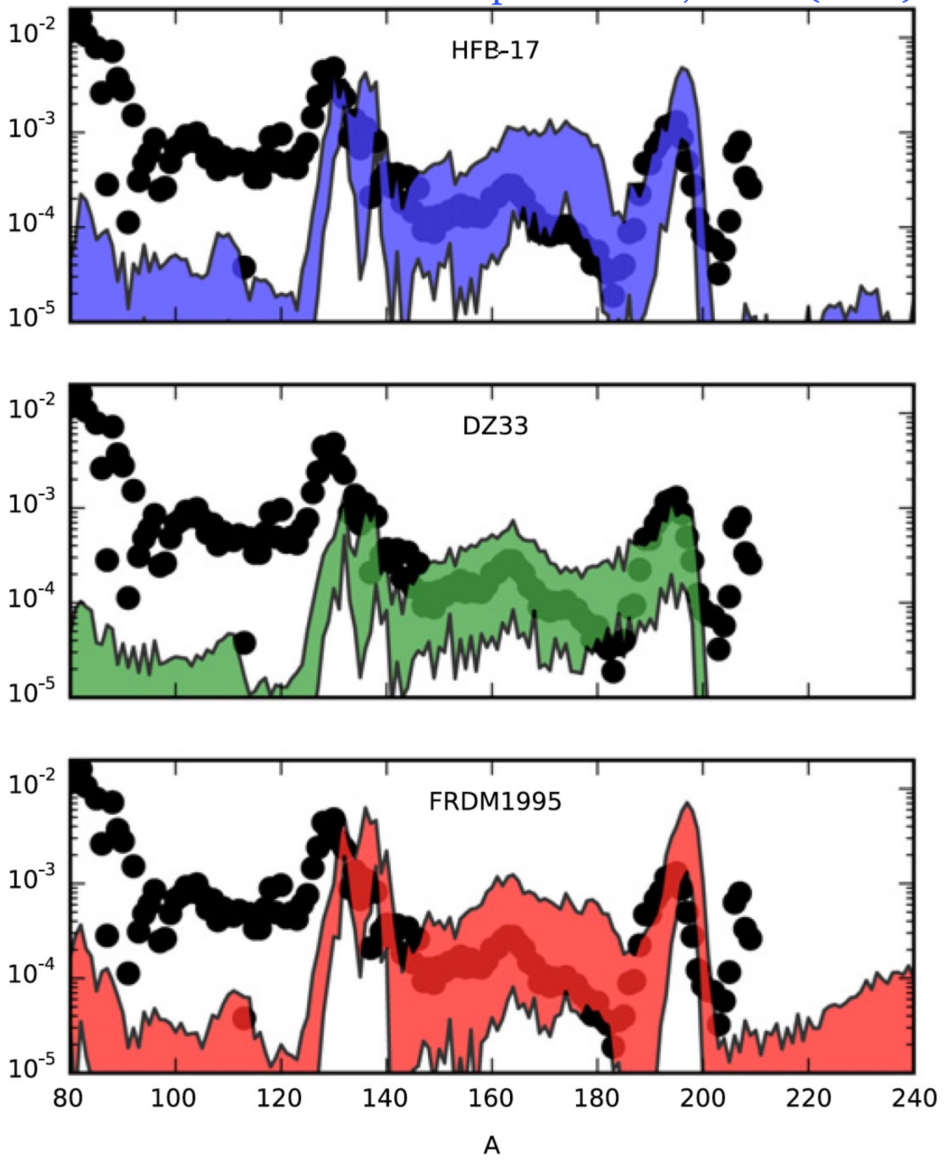
Uncertainties coming from:

- Neutron-nucleus optical potentials
- Nuclear level densities for Hauser-Feshbach
- γ strength functions



Mumpower et al., JPCF (2015)

Mumpower et al., PPNP (2016)



Neutron capture sensitivity studies

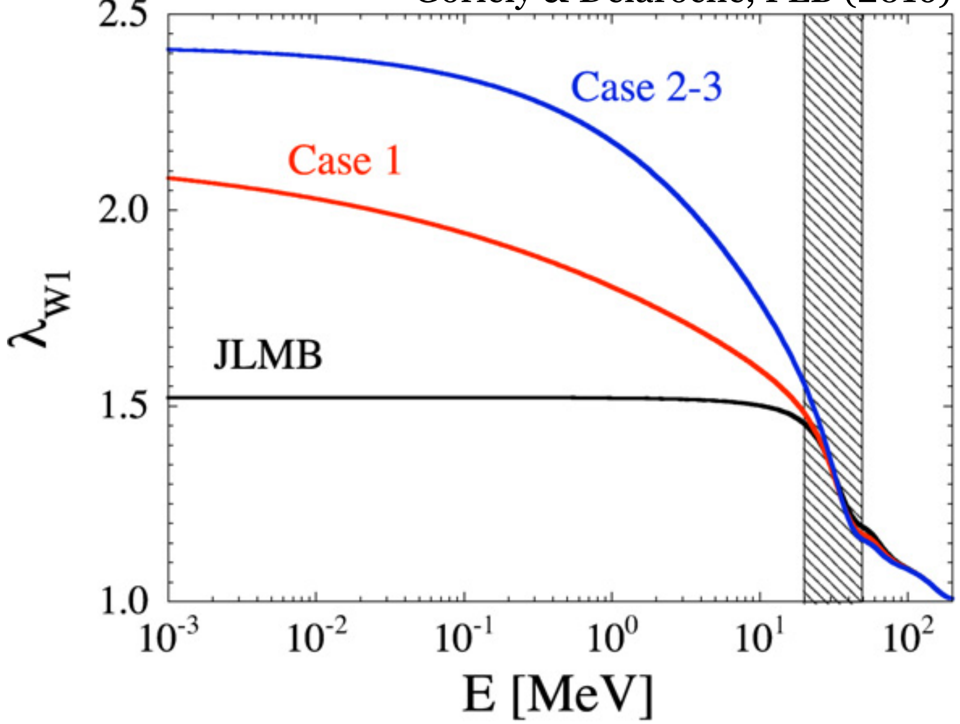
Uncertainties coming from:

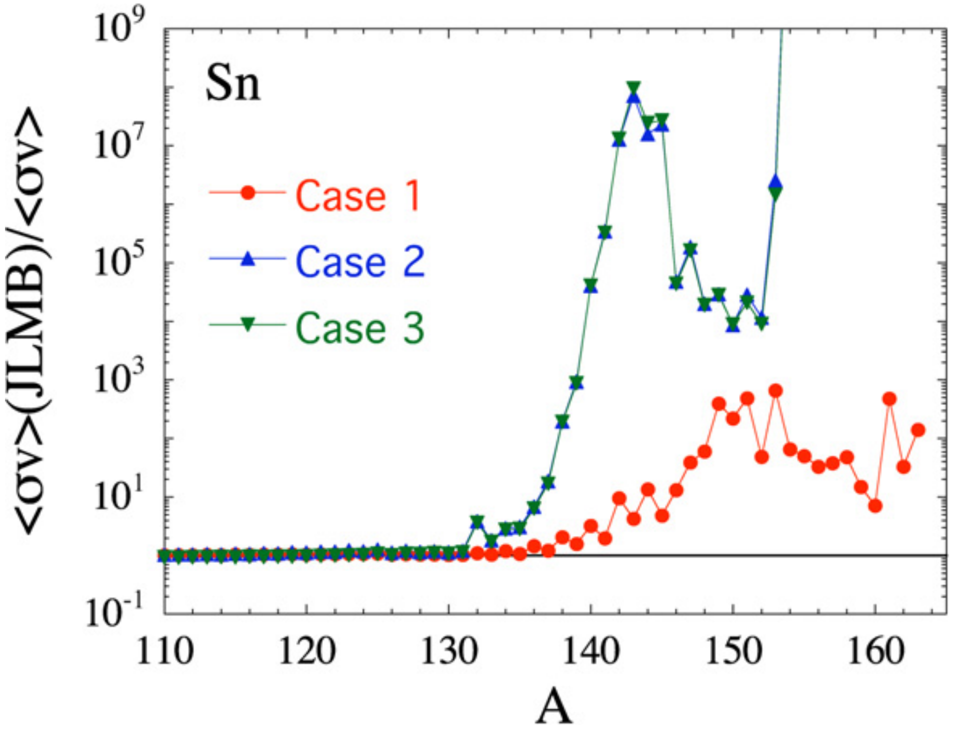
- Neutron-nucleus optical potentials

$$U(E) = \lambda_V(E)\left[V_0(E) + \lambda_{V_1}(E)\alpha V_1(E)\right] + i\lambda_W(E)\left[W_0(E) + \lambda_{W_1}(E)\alpha W_1(E)\right]$$

$$\alpha = (\rho_n - \rho_p)/\rho$$

Goriely & Delaroche, PLB (2016)



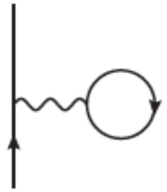


Global microscopic optical potential: start from nucleon optical potential in infinite nuclear matter

- Identified with the on-shell nucleon self-energy $\Sigma(\vec{r}_1, \vec{r}_2, \omega)$

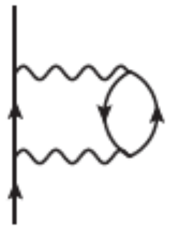
- First-order (Hartree-Fock) contribution (real & energy independent):

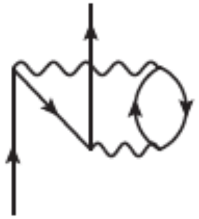
$$\Sigma_{2N}^{(1)}(q; k_f) = \sum_1 \langle \vec{q}\vec{h}_1 s s_1 t t_1 | \bar{V}_{2N} | \vec{q}\vec{h}_1 s s_1 t t_1 \rangle n_1$$



- Second-order perturbative contribution (complex & energy dependent):

$$\Sigma_{2N}^{(2a)}(q, \omega; k_f) = \frac{1}{2} \sum_{123} \frac{|\langle \vec{p}_1 \vec{p}_3 s_1 s_3 t_1 t_3 | \bar{V} | \vec{q}\vec{h}_2 s s_2 t t_2 \rangle|^2}{\omega + \epsilon_2 - \epsilon_1 - \epsilon_3 + i\eta} \bar{n}_1 n_2 \bar{n}_3$$



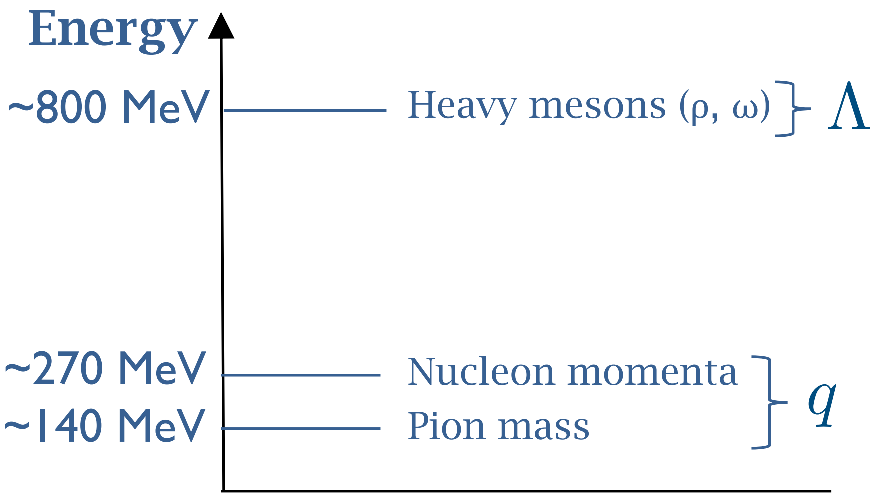


- Self consistency: $\epsilon(q) = \dfrac{q^2}{2M} + \mathrm{Re}\,\Sigma(q, \epsilon(q))$

- Derived from high-precision chiral two- and three-body forces

Chiral effective field theory (EFT) for nuclear forces

1. Natural Separation of Scales

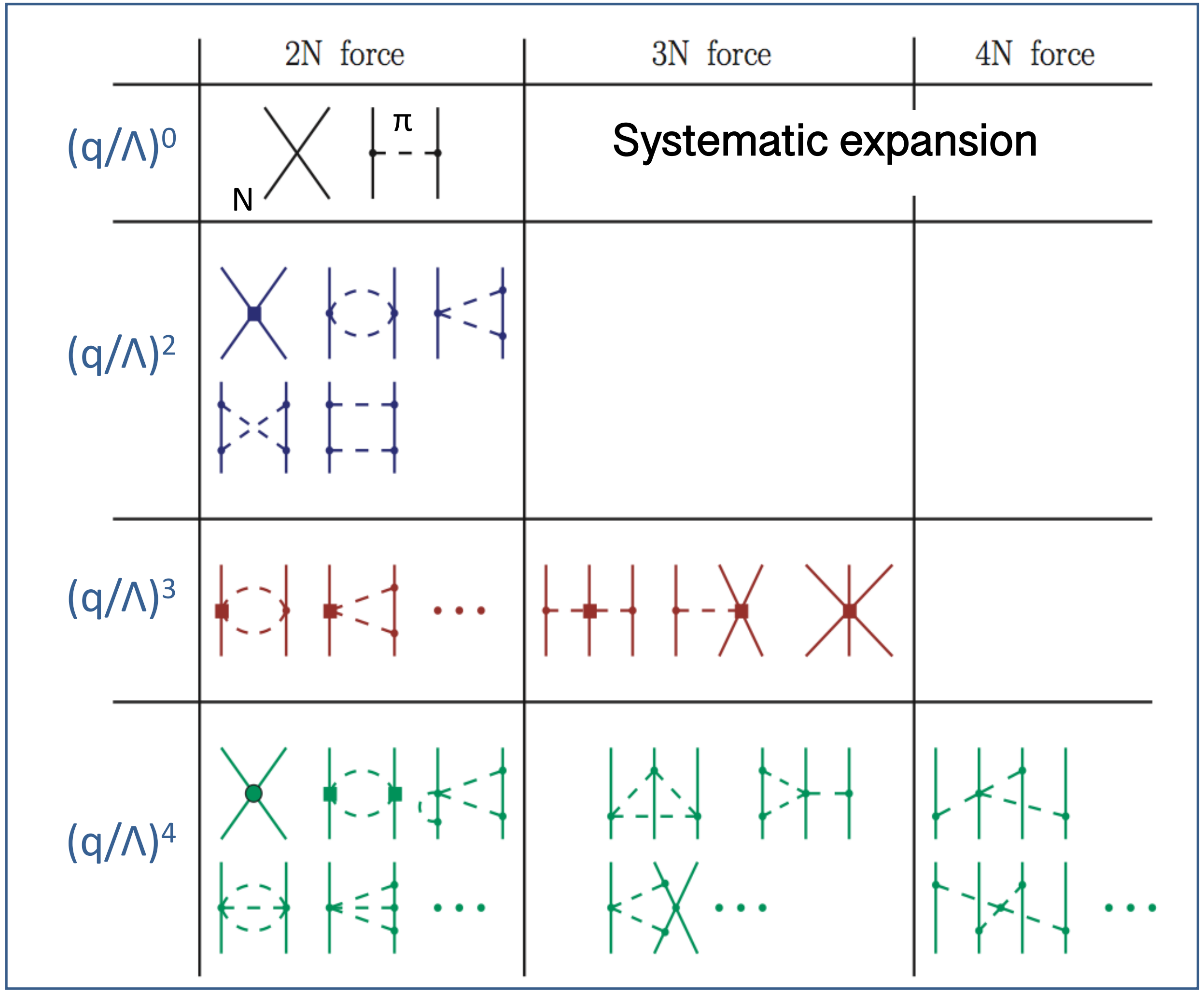


2. Goldstone bosons (pions) weakly-coupled at low momenta

$$\mathcal{L}_{\pi\pi}^{(2)} = \frac{1}{2}\partial_\mu \vec{\pi}\cdot\partial^\mu\vec{\pi} + \frac{1}{2f_\pi^2}(\partial_\mu\vec{\pi}\cdot\vec{\pi})^2$$

$$\mathcal{L}_{\pi N}^{(1)} = \bar{N}\left(i\gamma^\mu D_\mu - m - \frac{g_A}{2f_\pi}\gamma^\mu\gamma_5\vec{\tau}\cdot\partial_\mu\vec{\pi}\right)N$$

Nuclear forces from chiral EFT



Enables uncertainty quantification

Chiral effective field theory (EFT) for nuclear forces

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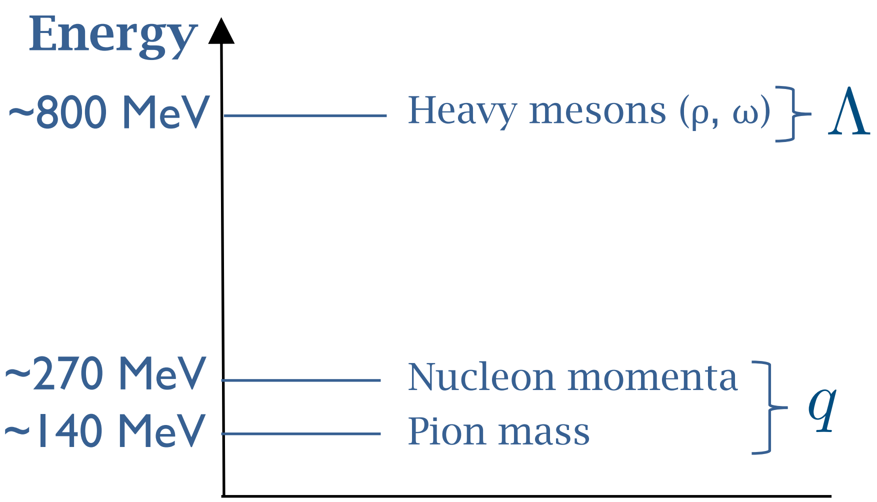

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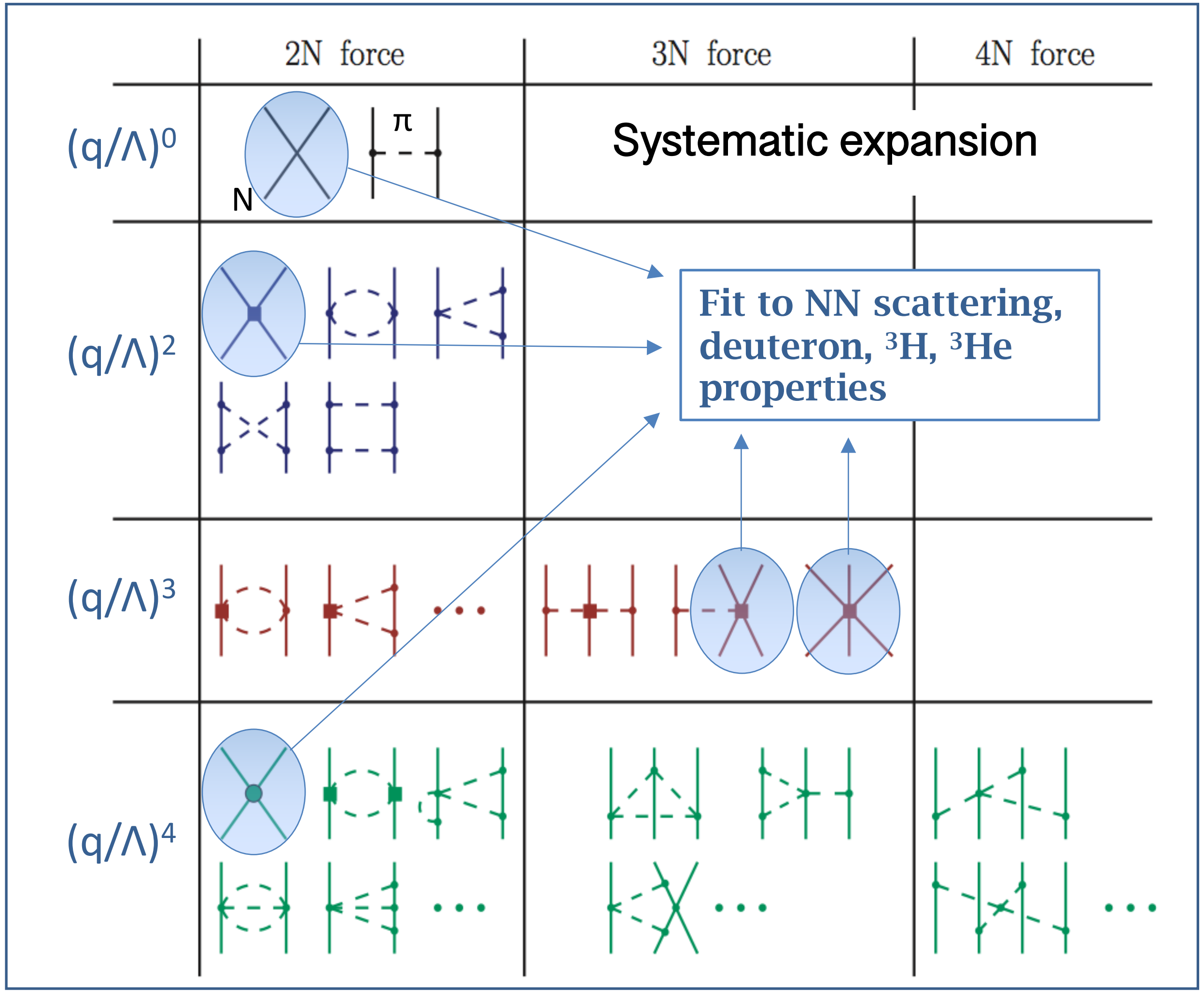
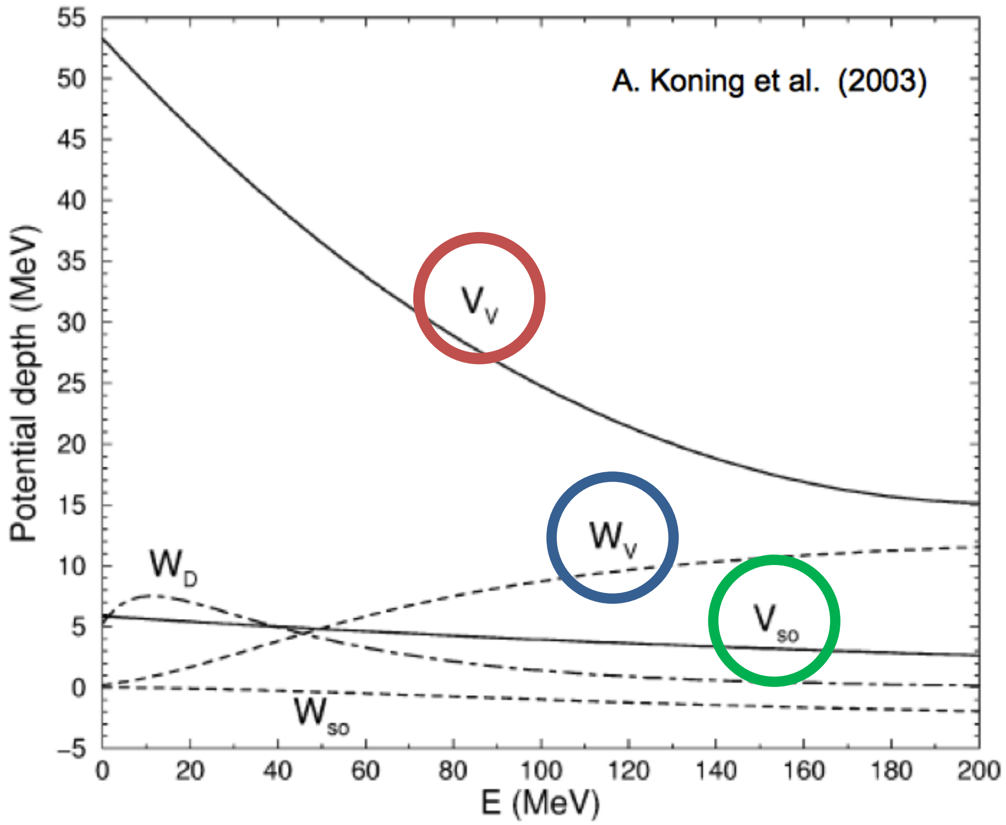


Enables uncertainty quantification

Global optical potential parameterization

$$\mathcal{U}(r,E) = -\mathcal{V}_V(r,E) - i\mathcal{W}_V(r,E) - i\mathcal{W}_D(r,E) + \mathcal{V}_{SO}(r,E).\mathbf{l}.\sigma + i\mathcal{W}_{SO}(r,E).\mathbf{l}.\sigma + \mathcal{V}_C(r).$$



Woods-Saxon shape: $f(r, R_i, a_i) = \left(1 + \exp\left[(r - R_i)/a_i\right]\right)^{-1}$

$$\mathcal{V}_V(r,E) = V_V(E) f(r, R_V, a_V),$$

$$\mathcal{W}_V(r,E) = W_V(E) f(r, R_V, a_V),$$

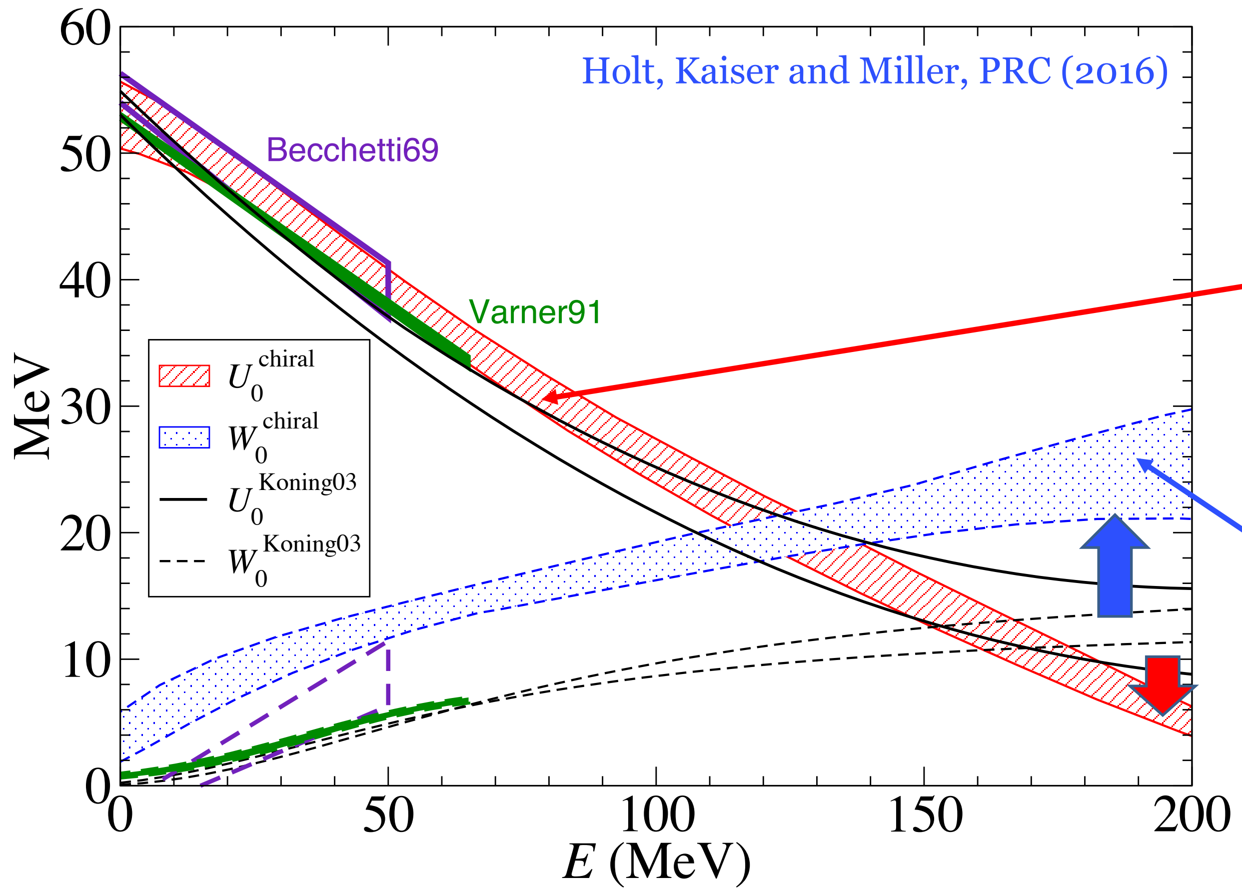
$$\mathcal{W}_D(r,E) = -4a_D W_D(E) \frac{d}{dr} f(r, R_D, a_D),$$

$$\mathcal{V}_{SO}(r,E) = V_{SO}(E) \left(\frac{\hbar}{m_\pi c}\right)^2 \frac{1}{r} \frac{d}{dr} f(r, R_{SO}, a_{SO}),$$

$$\mathcal{W}_{SO}(r,E) = W_{SO}(E) \left(\frac{\hbar}{m_\pi c}\right)^2 \frac{1}{r} \frac{d}{dr} f(r, R_{SO}, a_{SO}).$$

Global optical potential parameterization: *volume terms*

$$\mathcal{U}(r,E) = -\mathcal{V}_V(r,E) - i\mathcal{W}_V(r,E) - i\mathcal{W}_D(r,E) + \mathcal{V}_{SO}(r,E).\mathbf{l}.\sigma + i\mathcal{W}_{SO}(r,E).\mathbf{l}.\sigma + \mathcal{V}_C(r),$$



$$\mathcal{V}_V(r,E) = V_V(E) f(r, R_V, a_V),$$

Real volume strength function:

Very good agreement with phenomenology

$$\mathcal{W}_V(r,E) = W_V(E) f(r, R_V, a_V)$$

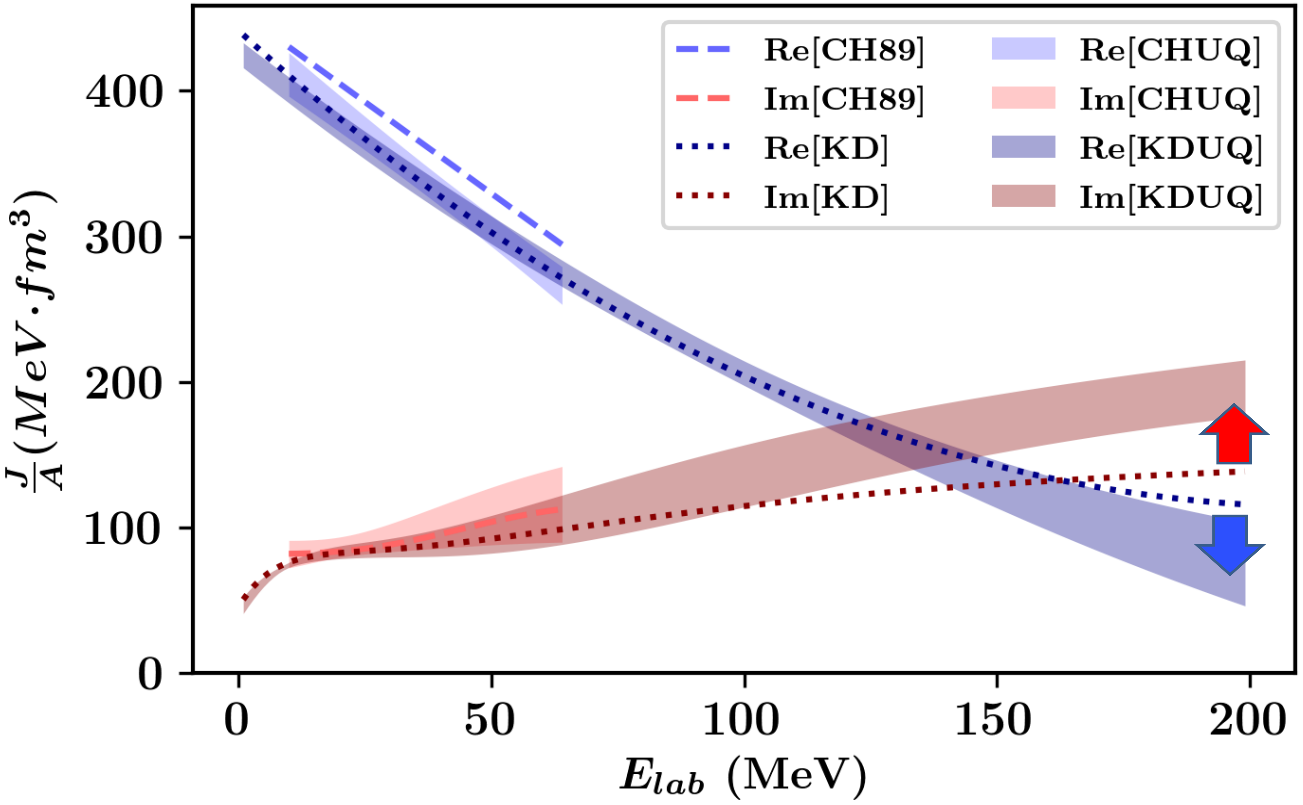
Imaginary volume strength function:

Too strongly absorptive

Global optical potential parameterization: *volume terms*

$$\mathcal{U}(r,E) = -\mathcal{V}_V(r,E) - i\mathcal{W}_V(r,E) - i\mathcal{W}_D(r,E) + \mathcal{V}_{SO}(r,E).\mathbf{l}.\sigma + i\mathcal{W}_{SO}(r,E).\mathbf{l}.\sigma + \mathcal{V}_C(r),$$

Pruitt, Escher and Rahman, PRC (2023)



$$\mathcal{W}_V(r,E) = W_V(E) f(r, R_V, a_V)$$

Imaginary volume strength increases

$$\mathcal{V}_V(r,E) = V_V(E) f(r, R_V, a_V),$$

Real volume strength decreases

Optical potentials in neutron-rich infinite matter

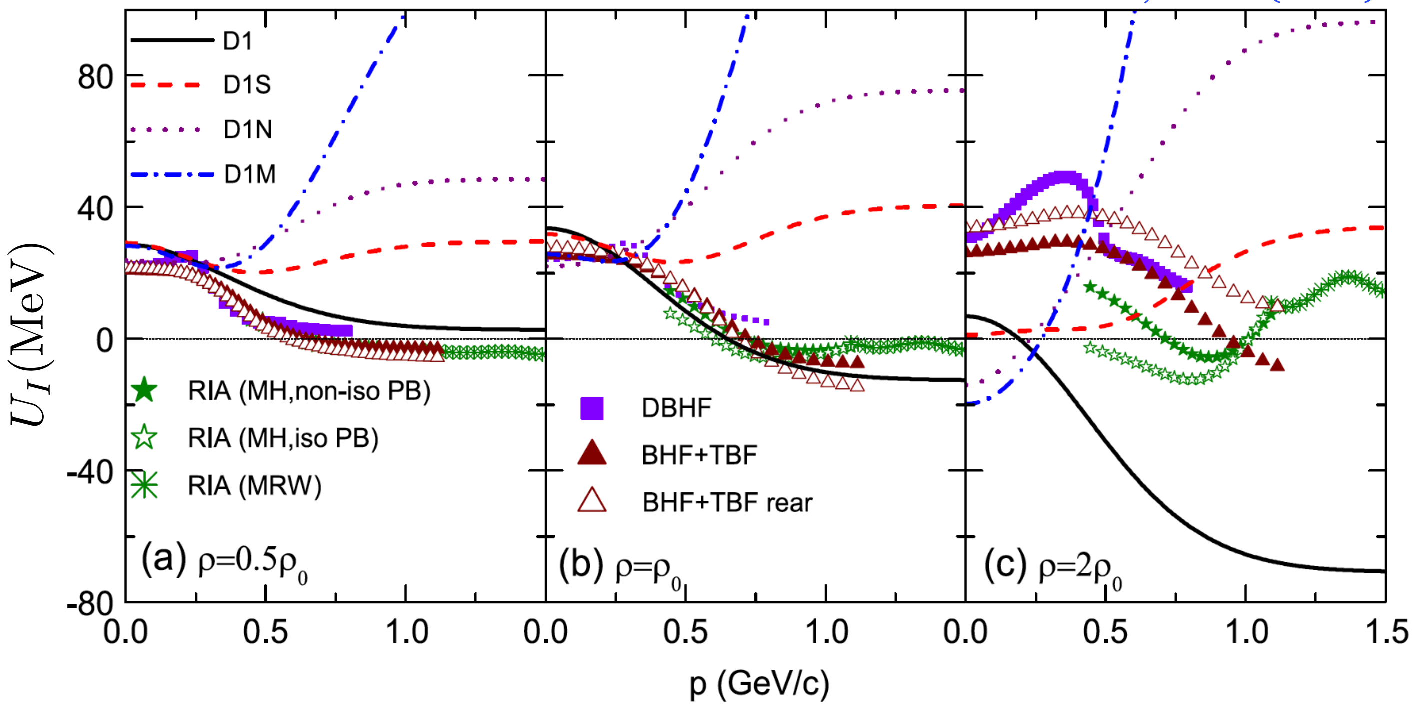
- Isovector optical potential obeys “Lane form”:

$$U_V = U_0 - U_I \delta_{np} \tau_z$$

- Much larger uncertainties for the isovector optical potential

- Isospin inversion $(U_p > U_n)$ at high energies present in only some models

B.-A. Li et al., PPNP (2018)



- Isovector Lane form above not obeyed at high energy in phenomenological Koning-Delaroche optical potential

Optical potentials in neutron-rich infinite matter

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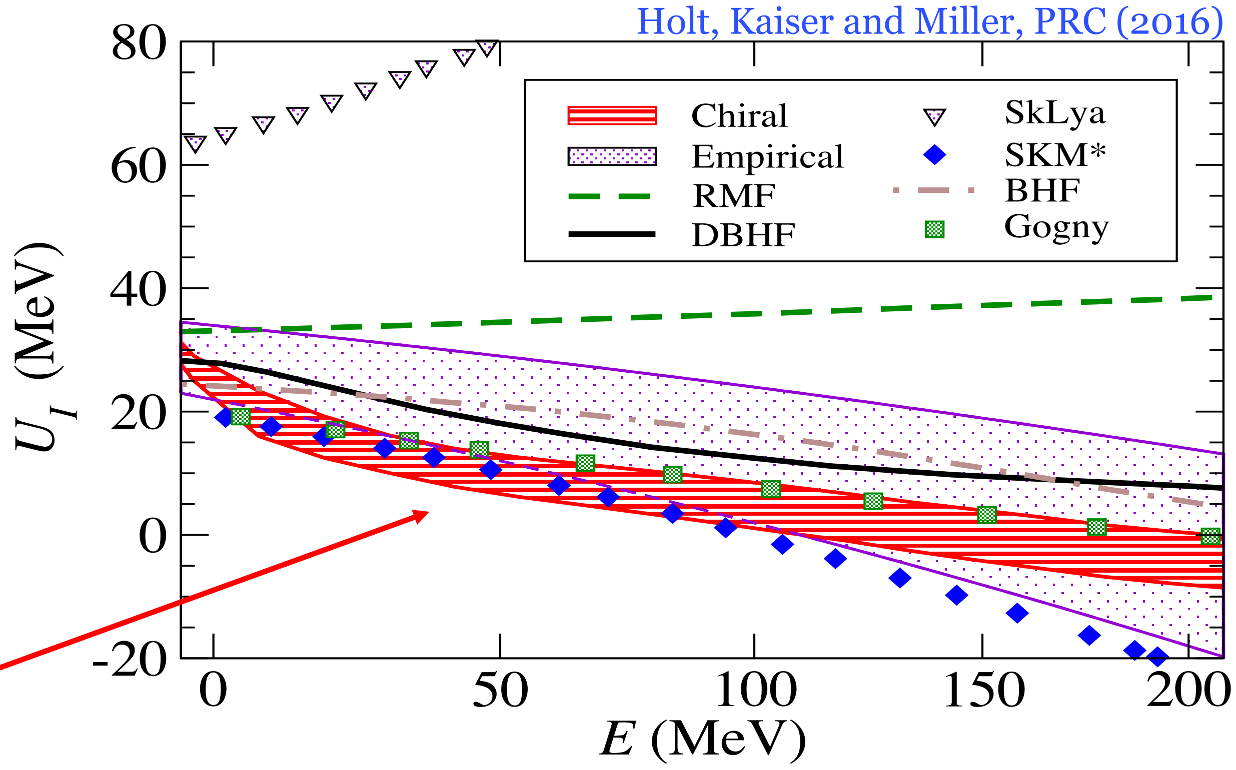


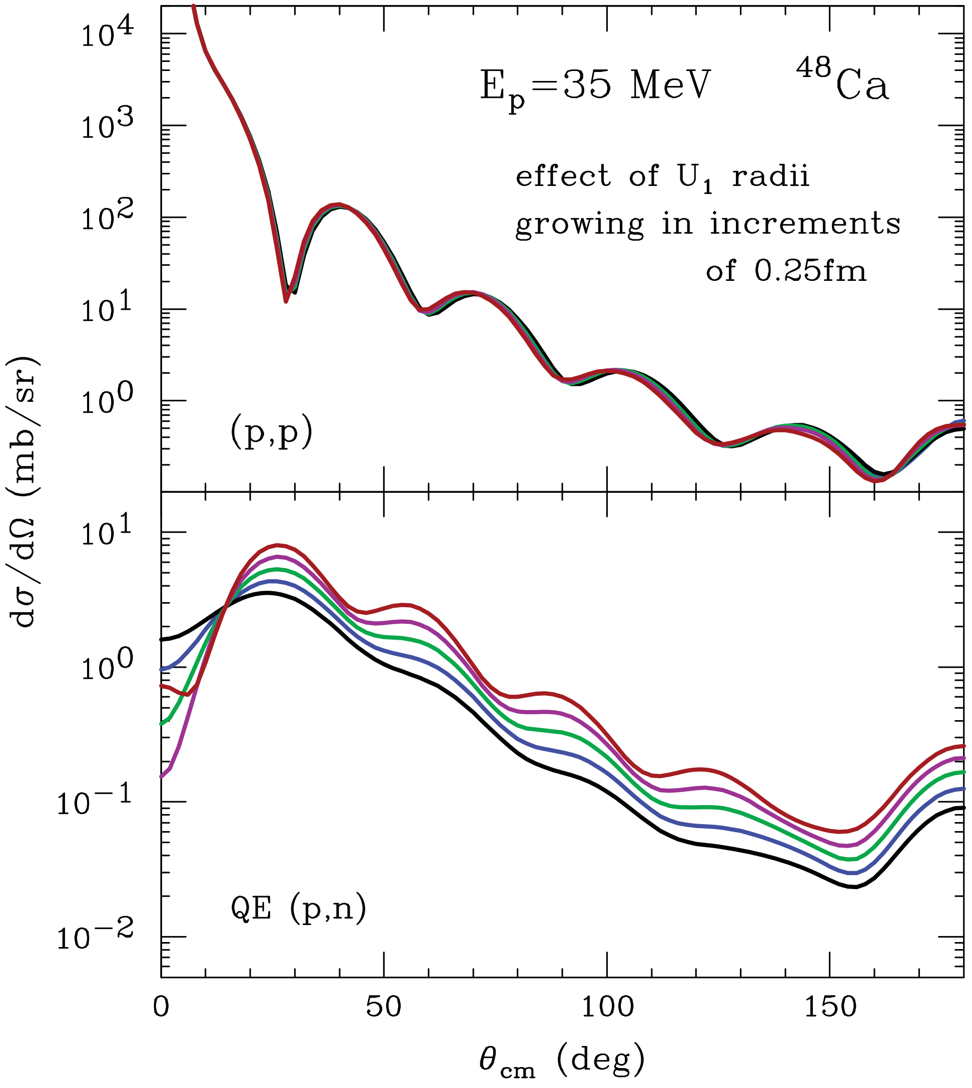
- Chiral effective field theory:
  - Matches energy dependence of phenomenological potentials well
  - Predicts isospin inversion around $E \approx 150 - 200$ MeV

Robust prediction that in general

$$m_n^* > m_p^*$$

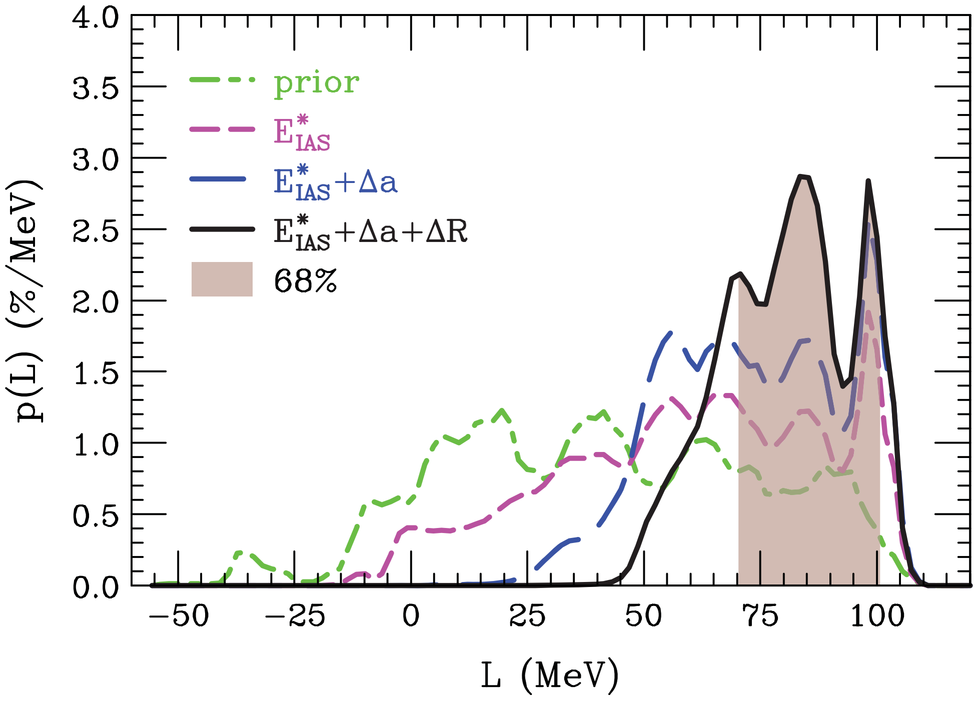
Isovector optical potential and quasielastic charged-current reactions

Danielewicz, Singh & Lee, NPA (2017)



- Charged-current reactions probe isovector part of optical potential

$$\langle n, Z+1|U(\boldsymbol{r})|p, Z\rangle = 2\frac{\sqrt{|N-Z|}}{A} U_1(\boldsymbol{r})$$



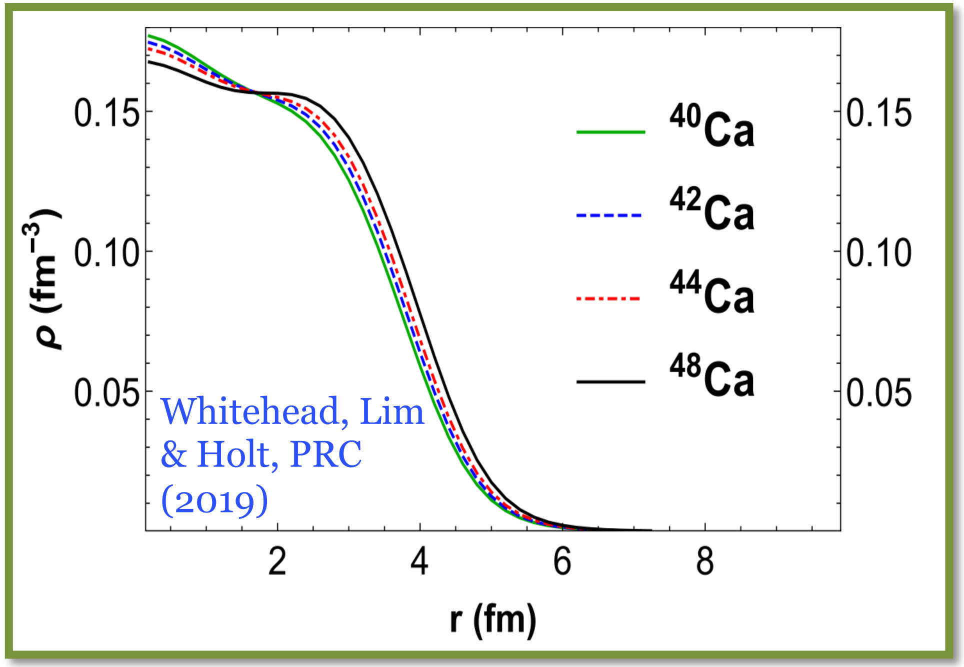
From nuclear matter to *finite nuclei:* Local density approximation (LDA)

$$V(E;r)+iW(E;r)=V(E;k_f^p(r),k_f^n(r))$$
$$+iW(E;k_f^p(r),k_f^n(r))$$

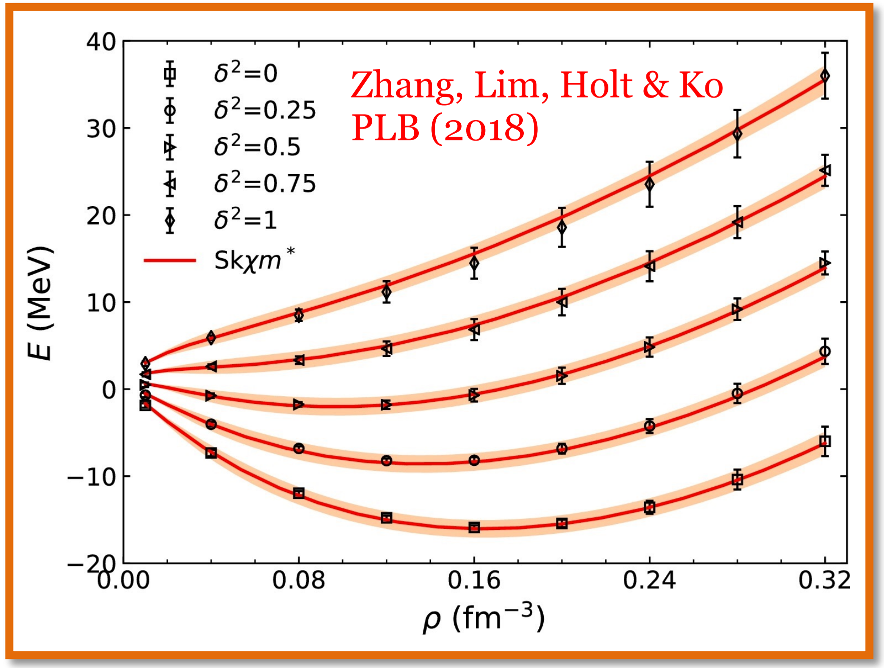
Local density approximation:

Optical potential in a finite nucleus matched to that of infinite matter at same isoscalar/isovector density

Density distributions from Skχ450 effective interaction



Skχ450 fitted to equation of state and effective mass



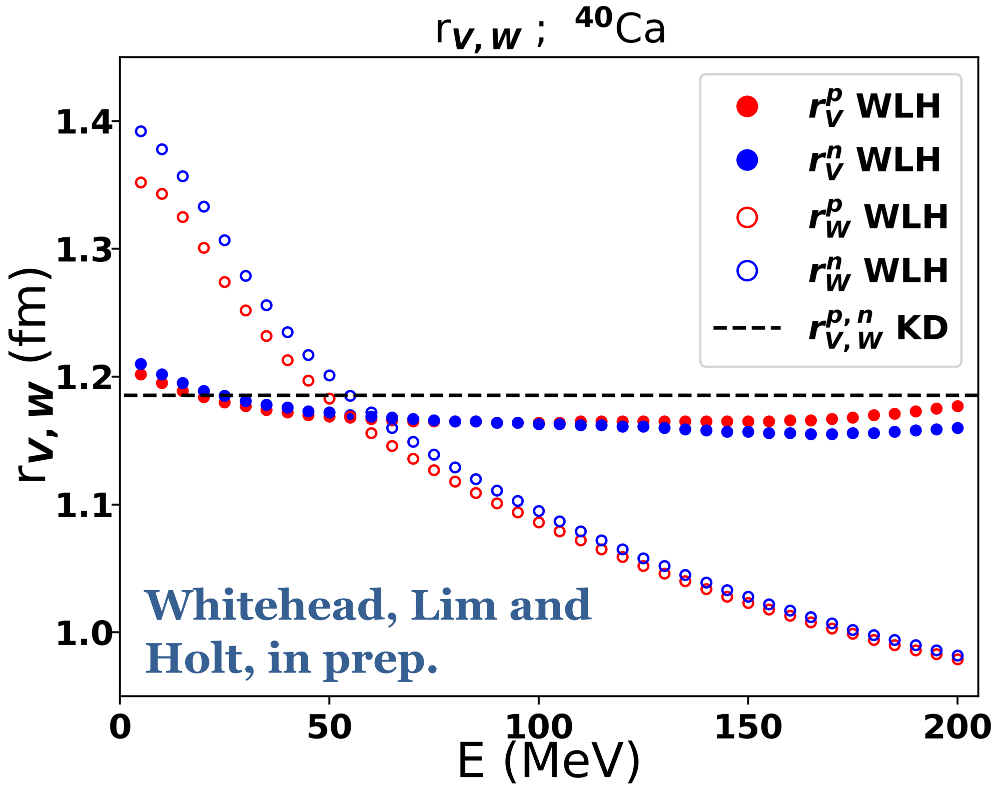
Comparison to phenomenology: radius parameter

New insights from microscopic calculations

- Phenomenological optical potentials make (necessary) assumptions in the parameterization
- Global analysis from microscopic calculations can inform phenomenological parameterizations
- Example: Energy-dependent Woods-Saxon shape parameters

$$\mathcal{V}(r,E) = V(E)\frac{1}{1+e^{(r-r_0)/a}}$$

radius



Comparison to phenomenology: diffuseness parameter

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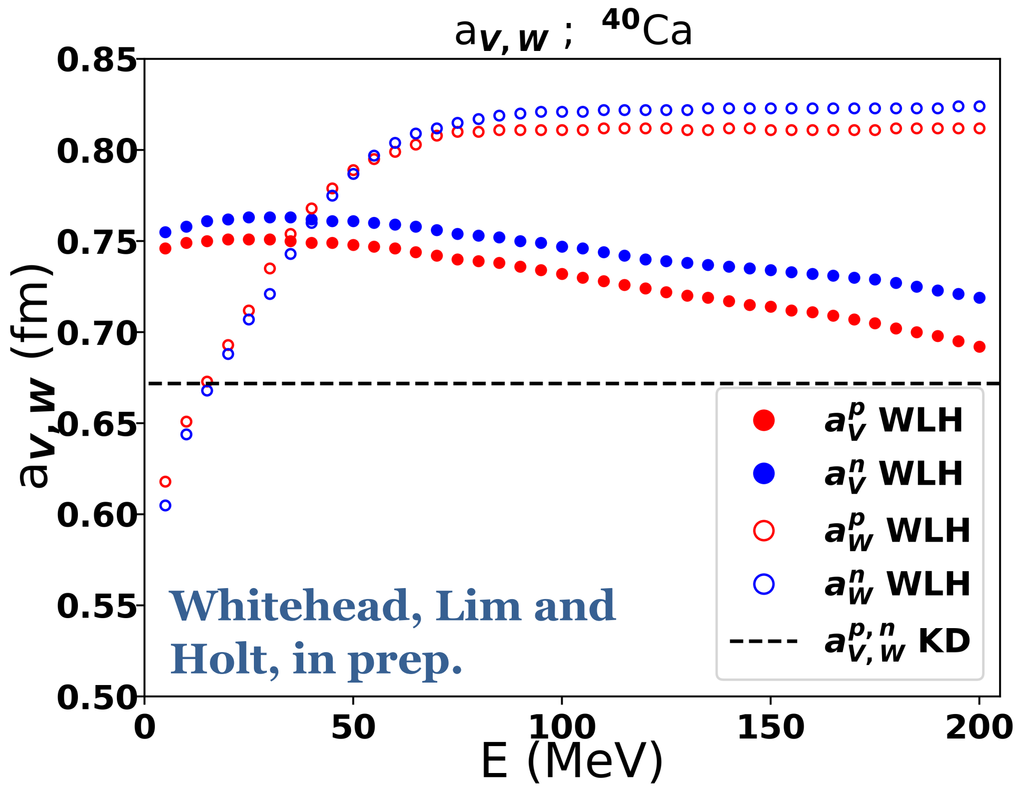
diffuseness

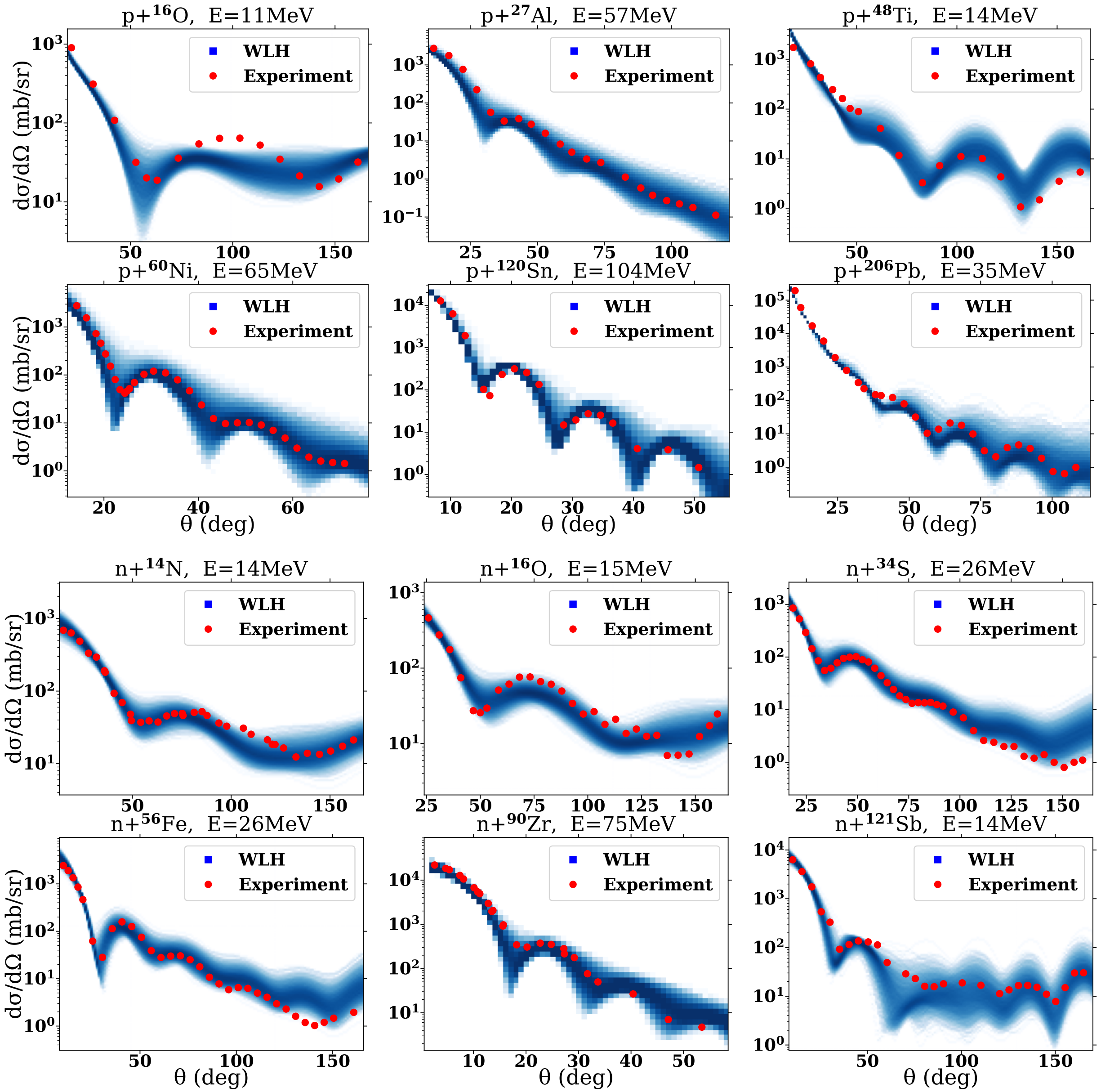


Uncertainty quantification: differential elastic scattering cross sections

Whitehead, Lim & Holt, PRL (2021)

<u>New global “WLH” microscopic global optical potential with uncertainties</u>

- Proton/neutron optical potentials for 1800 target nuclei
- Projectile energies $E < 200\,\mathrm{MeV}$
- Microscopic results motivate **<u>new directions for phenomenology</u>**
  - Different Woods-Saxon geometry parameters for real and imaginary parts
  - Energy dependence of Woods-Saxon geometry parameters
- Uncertainties obtained using **5000 sampled global optical potentials** from covariance analysis of 5 chiral optical potentials



Uncertainty quantification: vector analyzing powers

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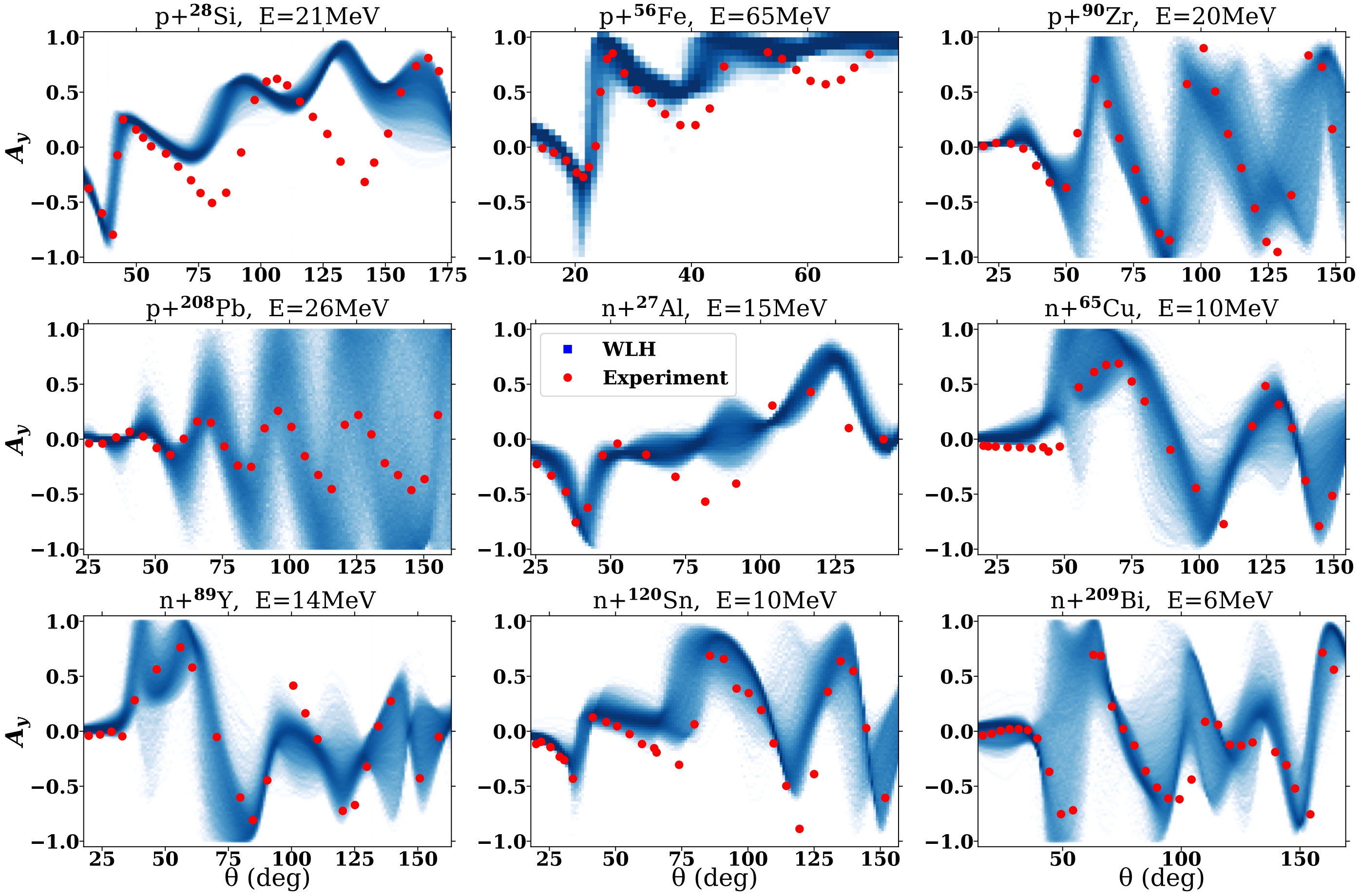
Whitehead, Lim & Holt (2021)

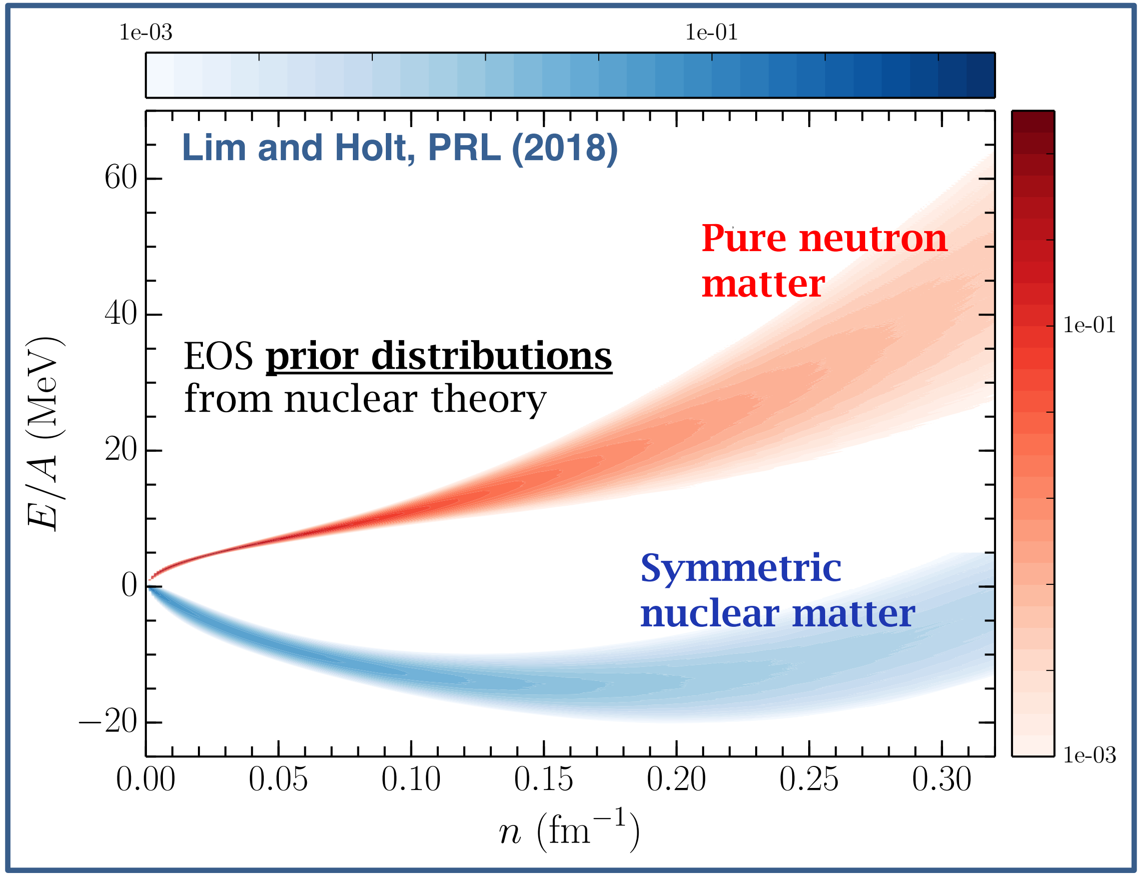


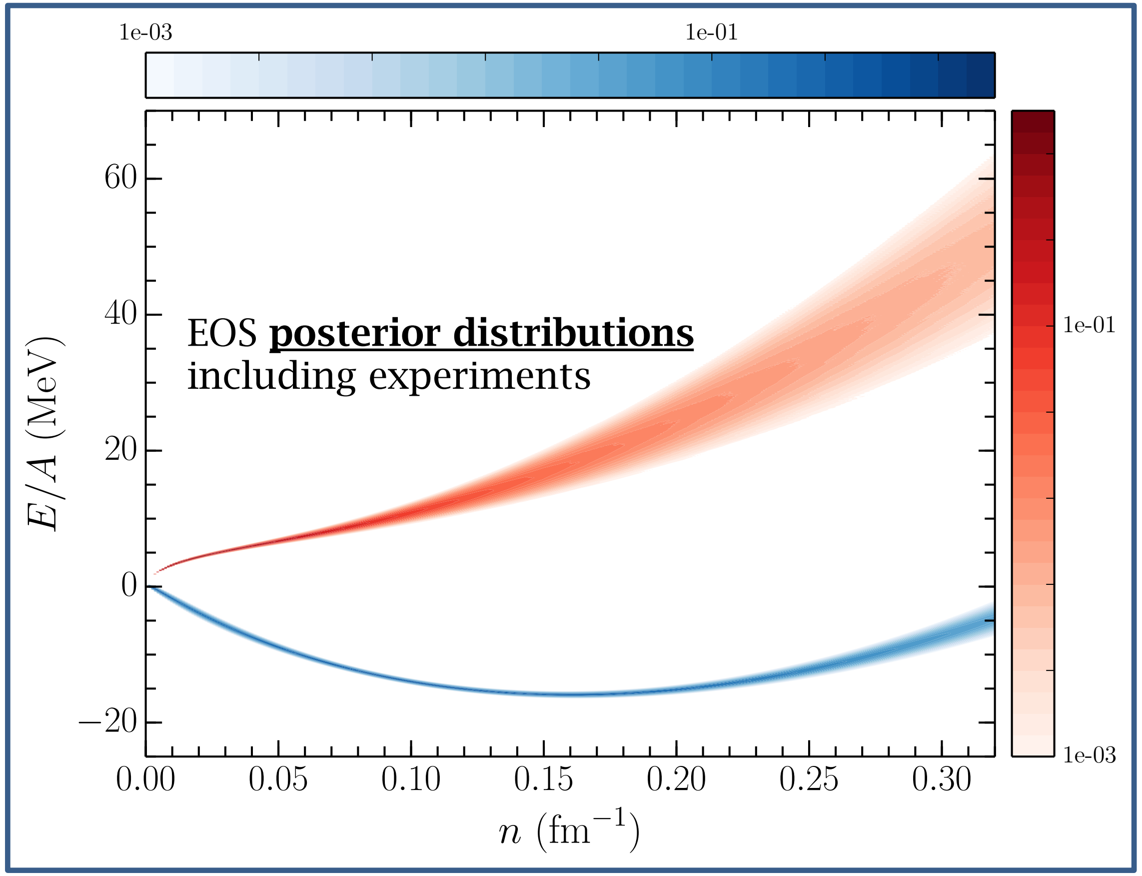
<u>Codes to generate optical potentials</u>
https://www.trwhitehead.com/WLH

Consistency with the nuclear EOS

- Order in the chiral expansion
- Scale dependence of nuclear force
- Quantum many-body method

- Nuclear binding energies
- Experimental constraints on isospin-asymmetry energy





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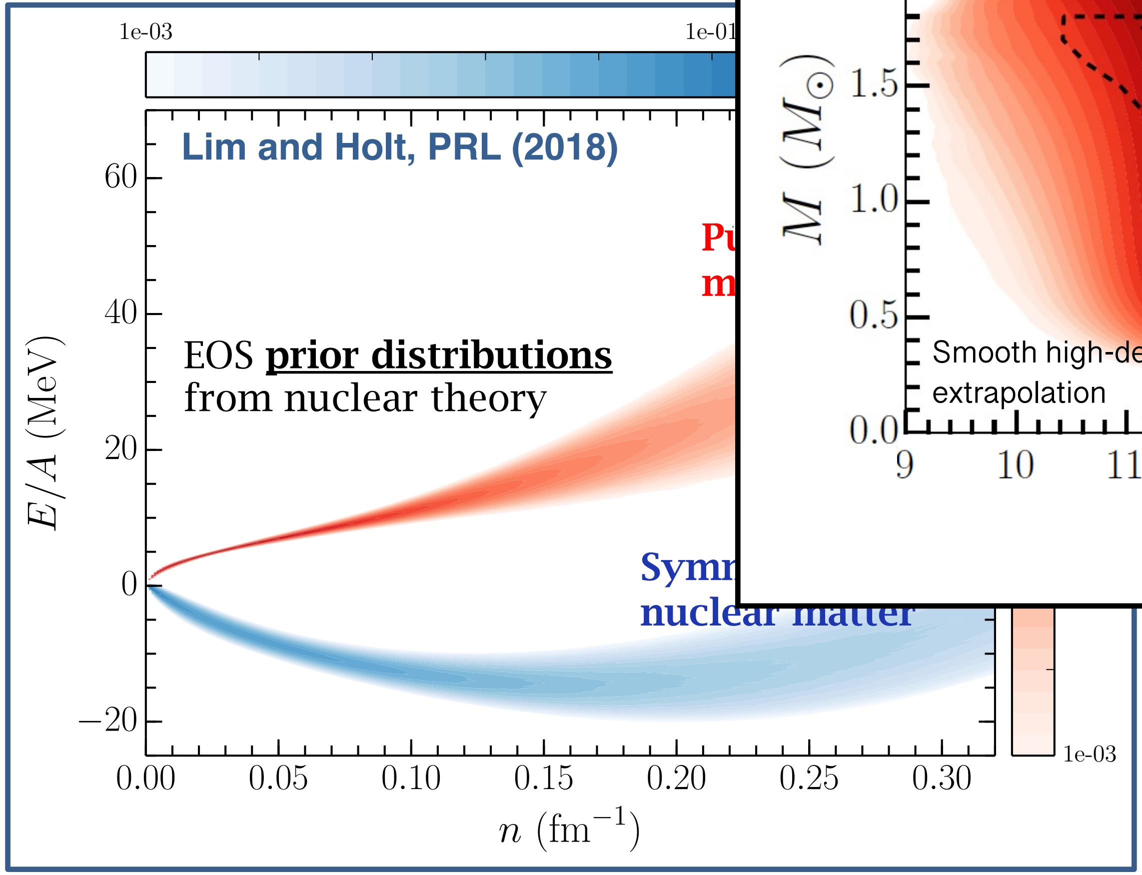
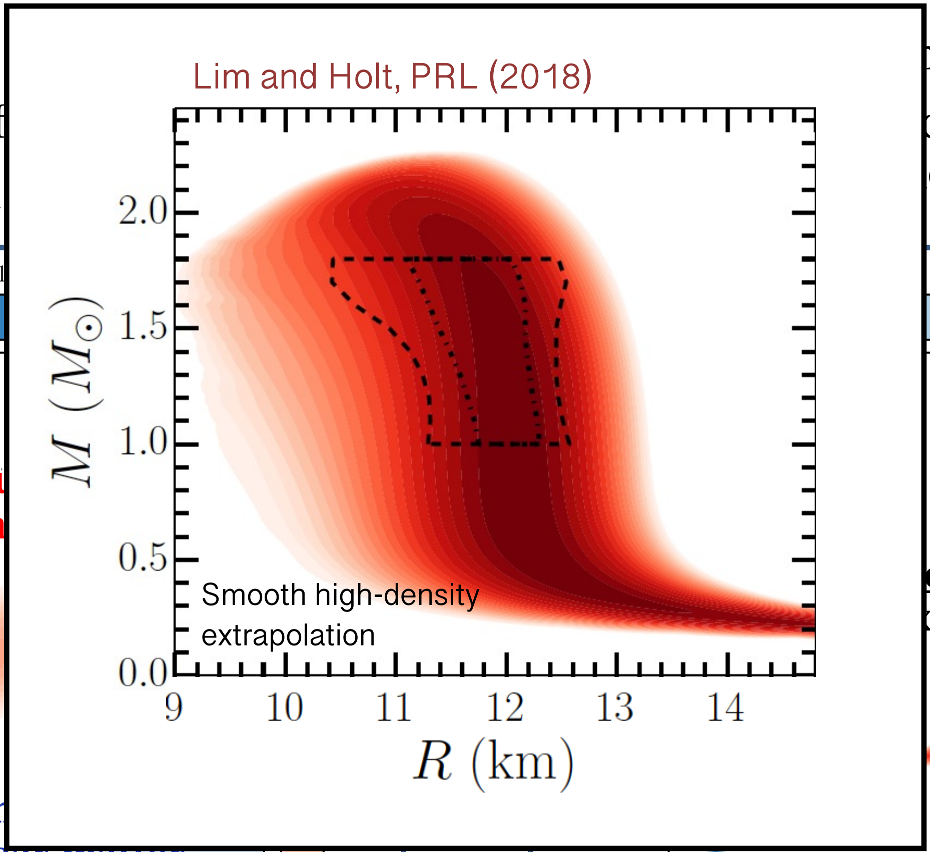
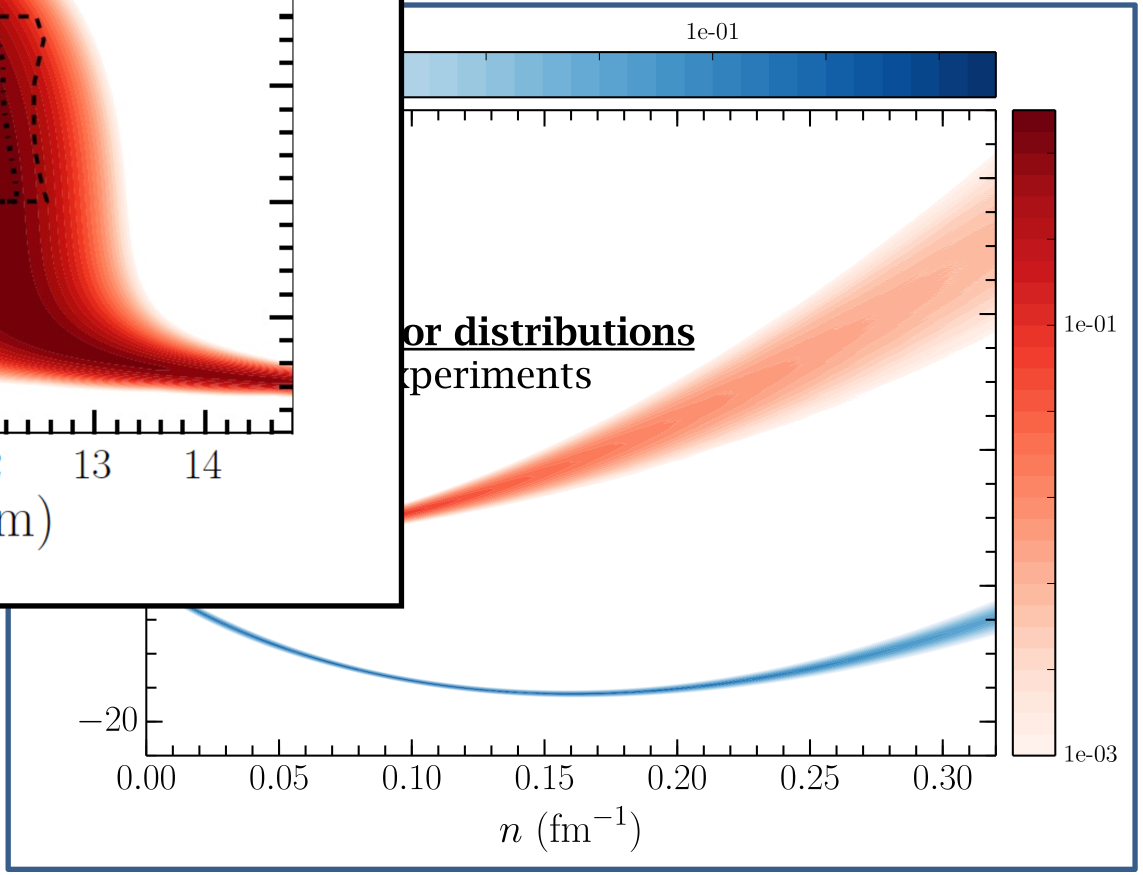




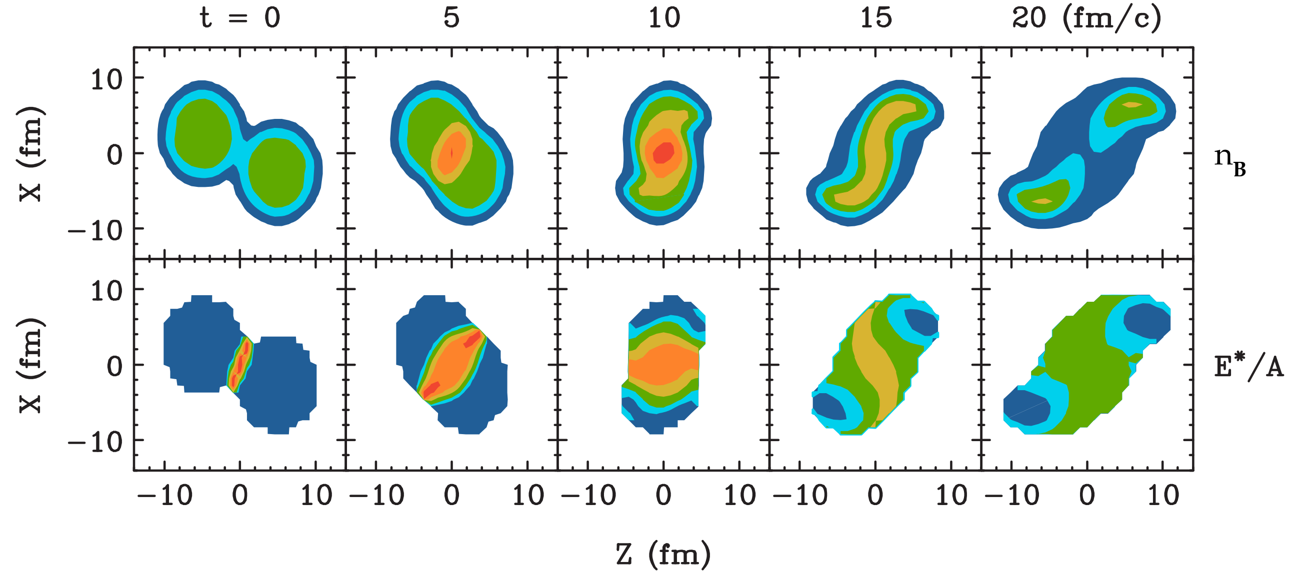


Transport simulations of heavy-ion collisions and the EOS

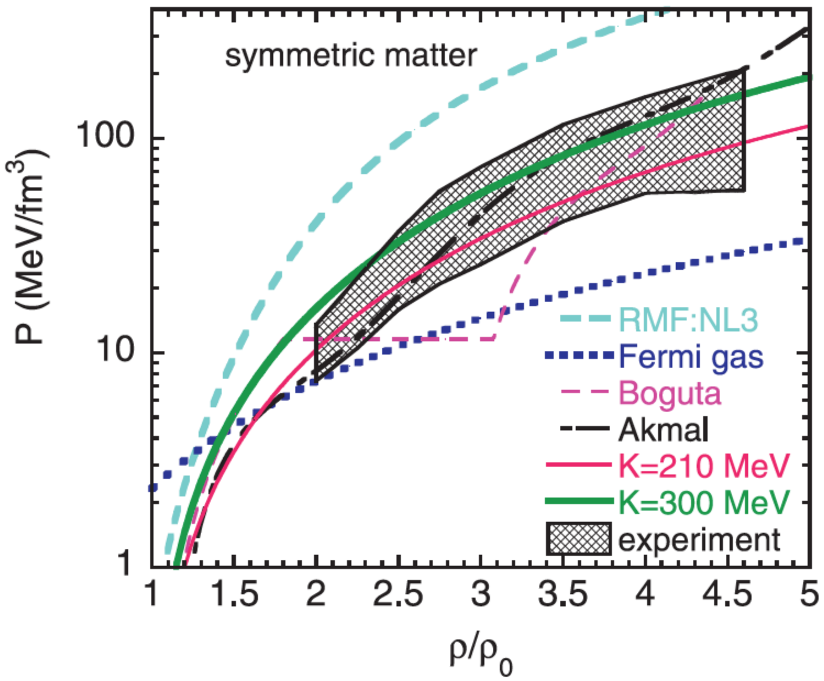
Dense Nuclear Matter Equation of State from Heavy-Ion Collisions *

Agnieszka Sorensen[1], Kshitij Agarwal[2], Kyle W. Brown[3,4], Zbigniew Chajecki[5], Paweł Danielewicz[3,6], Christian Drischler[7], Stefano Gandolfi[8], Jeremy W. Holt[9,10], Matthias Kaminski[11], Che-Ming Ko[9,10], Rohit Kumar[3], Bao-An Li[12], William G. Lynch[3,6], Alan B. McIntosh[10], William G. Newton[12], Scott Pratt[3,6], Oleh Savchuk[3,13], Maria Stefaniak[14], Ingo Tews[8], ManYee Betty Tsang[3,6], Ramona Vogt[15,16], Hermann Wolter[17], Hanna Zbroszczyk[18]

arXiv:2301.13253



Danielewicz et al., Science (2002)



- Analysis requires molecular dynamics or transport models

$$\frac{\partial f}{\partial t} + \nabla_p \varepsilon \cdot \nabla_r f - \nabla_r \varepsilon \cdot \nabla_p f = I$$

- **Observables**: transverse and elliptic flow, fragment yields, charged pion ratios

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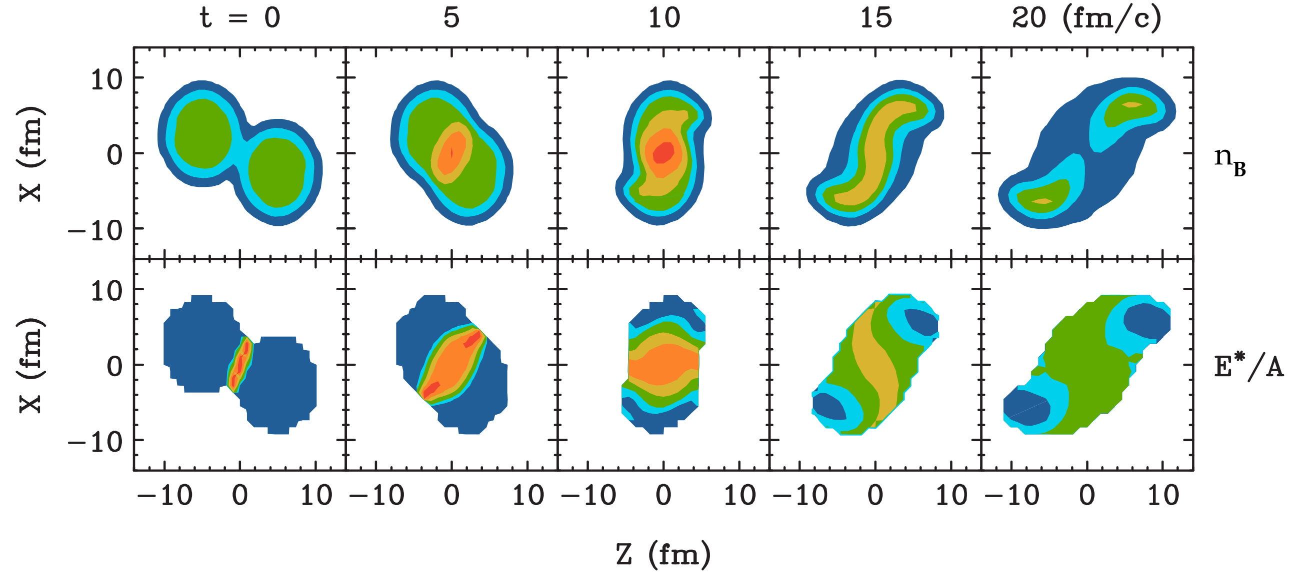
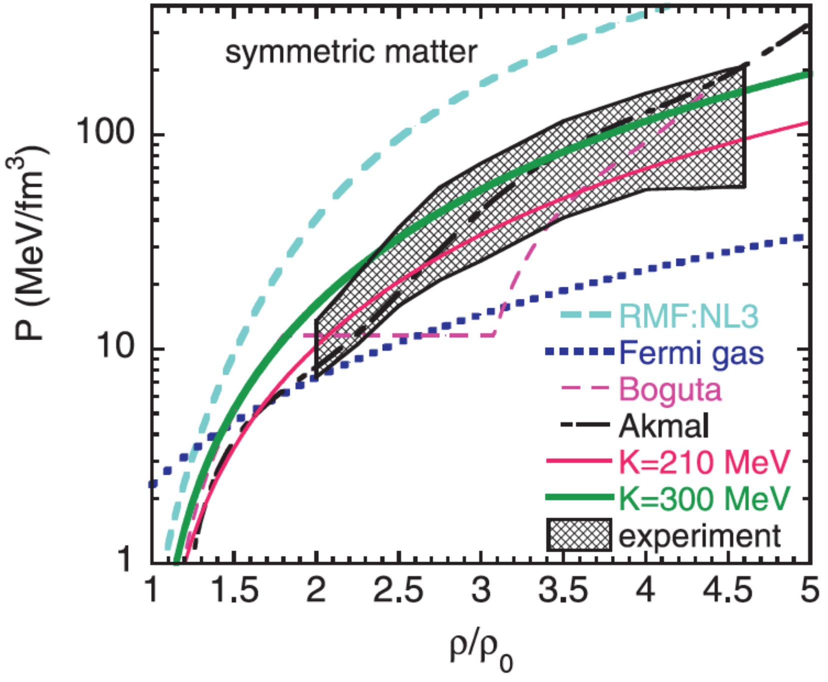


Danielewicz et al., Science (2002)



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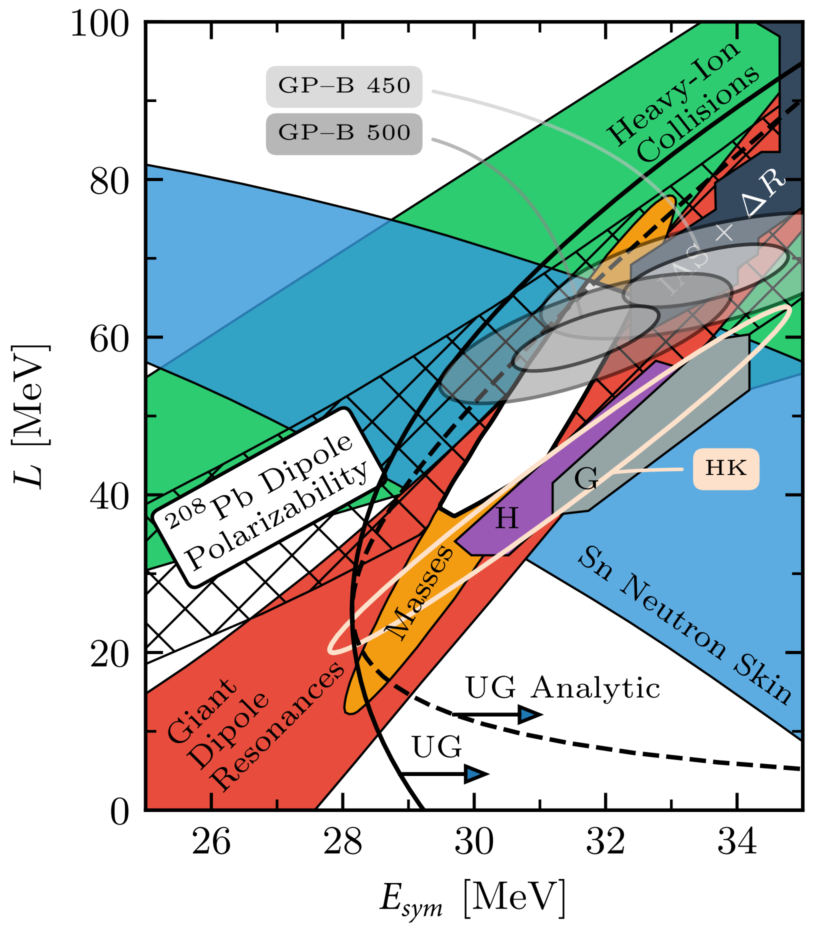
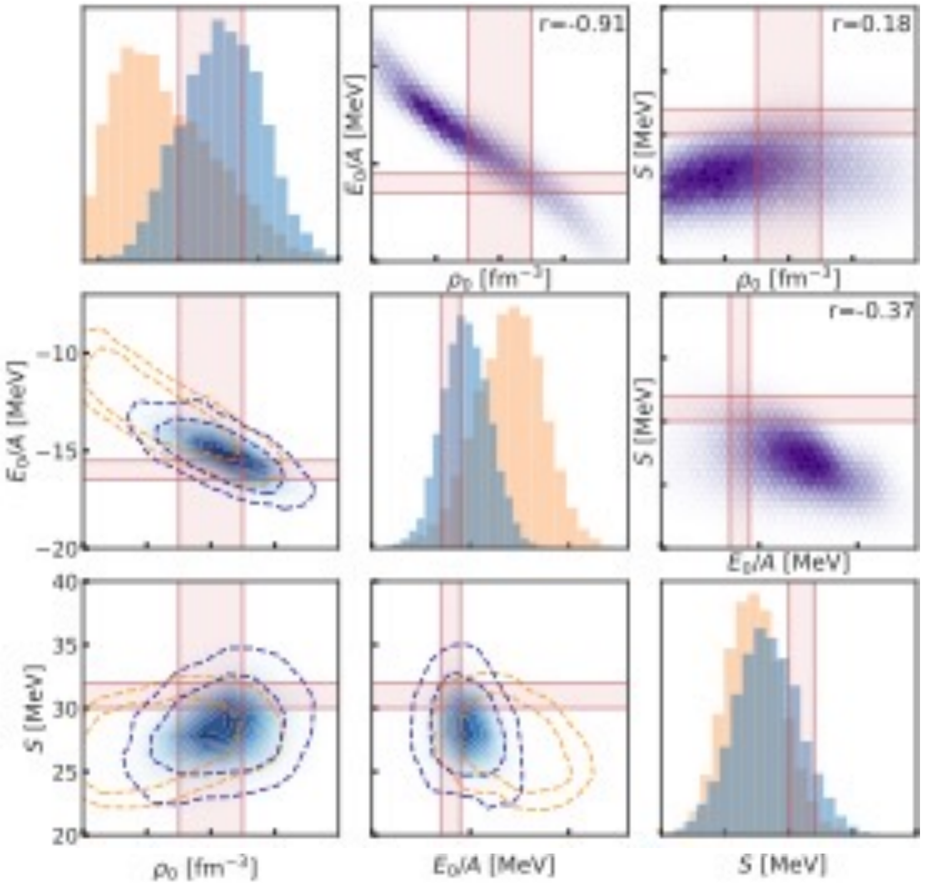
Improved uncertainty quantification

Drischler, Furnstahl, Melendez & Phillips, PRL (2020)

Drischler, Holt & Wellenhofer, ARNPS (2021)



Jiang, Forssen, Djarv & Hagen, arXiv2212.13203



- EFT truncation errors
- Probability distributions for EFT low-energy constants

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Drischler, Furnstahl, Melendez & Phillips, PRL (2020)

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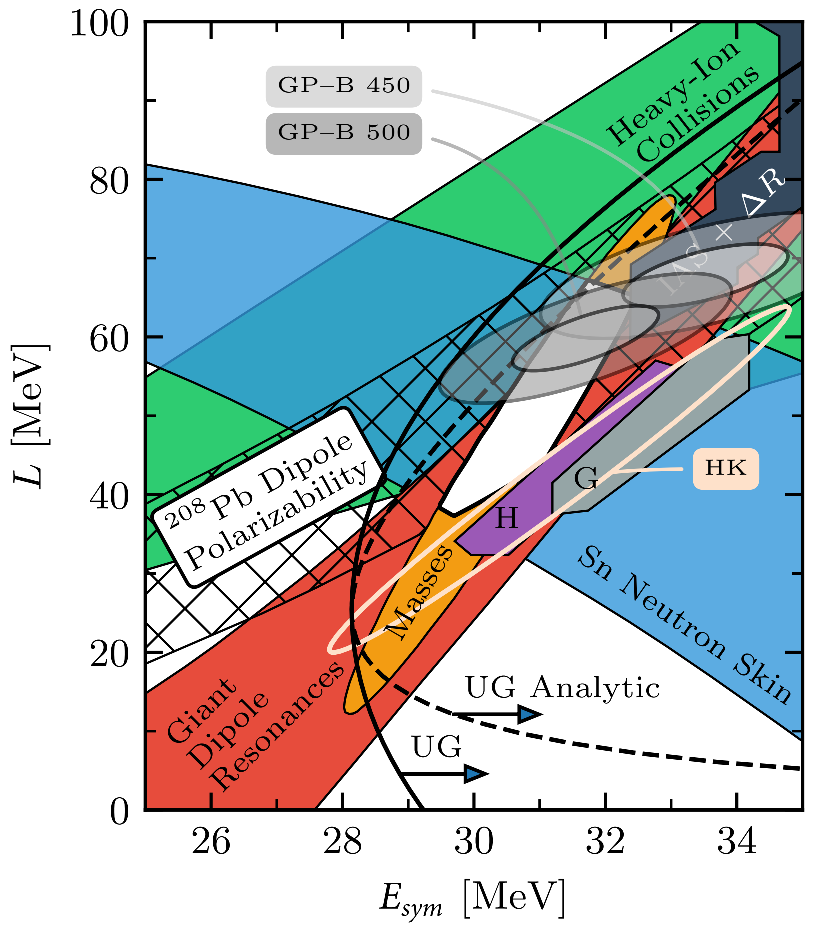
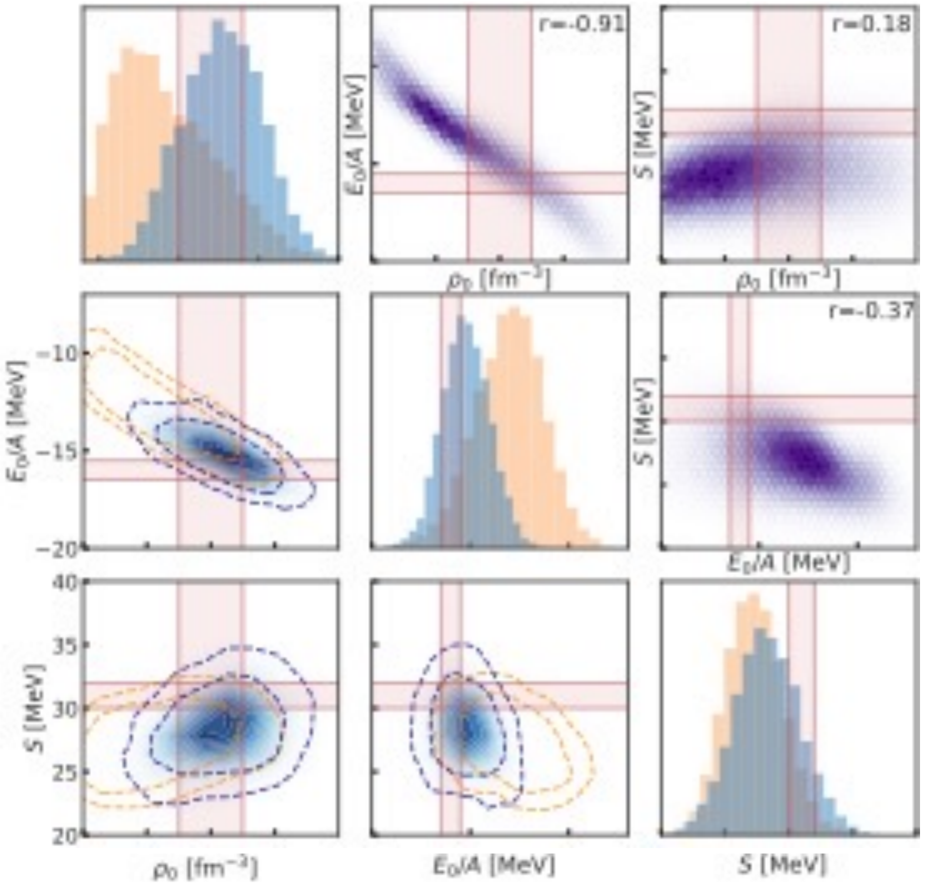


Jiang, Forssen, Djarv & Hagen, arXiv2212.13203



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Goal: use generative machine learning models to create new chiral potentials

Generative modeling for nucleon-nucleon interactions

Glow: generate realistic faces

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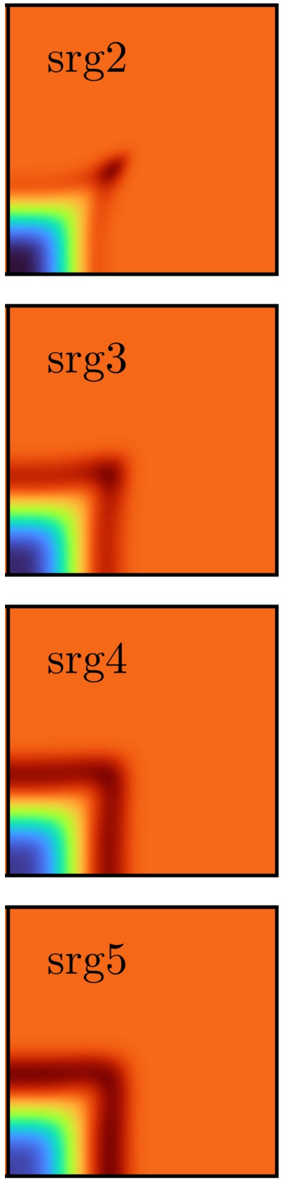


Generative modeling for nucleon-nucleon interactions

Glow: Manipulate attributes of a ~~face~~ **Nuclear Potentials**

Original face

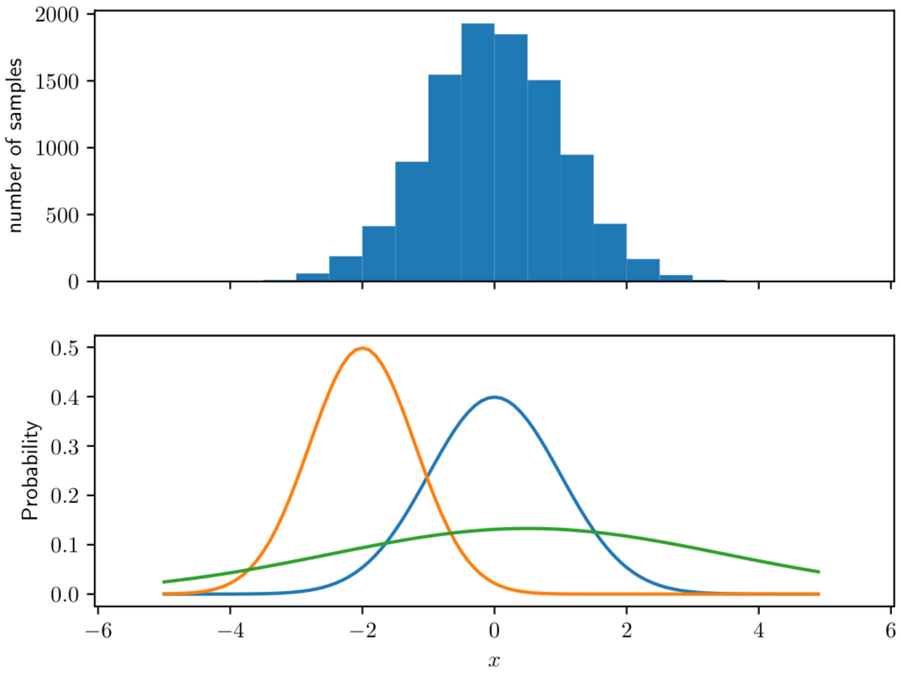
Glow

Age

Beard

Blonde Hair

Basic Algorithm



Maximize likelihood: optimize the estimation of density

Example: $x \sim \mathcal{N}(\mu = 0, \sigma = 0.1)$

$$\mathcal{L}_1 = \prod_i \mathcal{N}(X_i|\mu = 0, \sigma = 0.1)$$

$$\mathcal{L}_2 = \prod_i \mathcal{N}(X_i|\mu = -2, \sigma = 0.8)$$

$$\mathcal{L}_3 = \prod_i \mathcal{N}(X_i|\mu = 0.5, \sigma = 3)$$

A proper probability distribution model $\mathcal{N}(\mu, \sigma) \rightarrow$ the maximum likelihood $\mathcal{L}$

If $X =$ potential V, how to find $p(V) \rightarrow$ maximum $\mathcal{L}\,(V)$?

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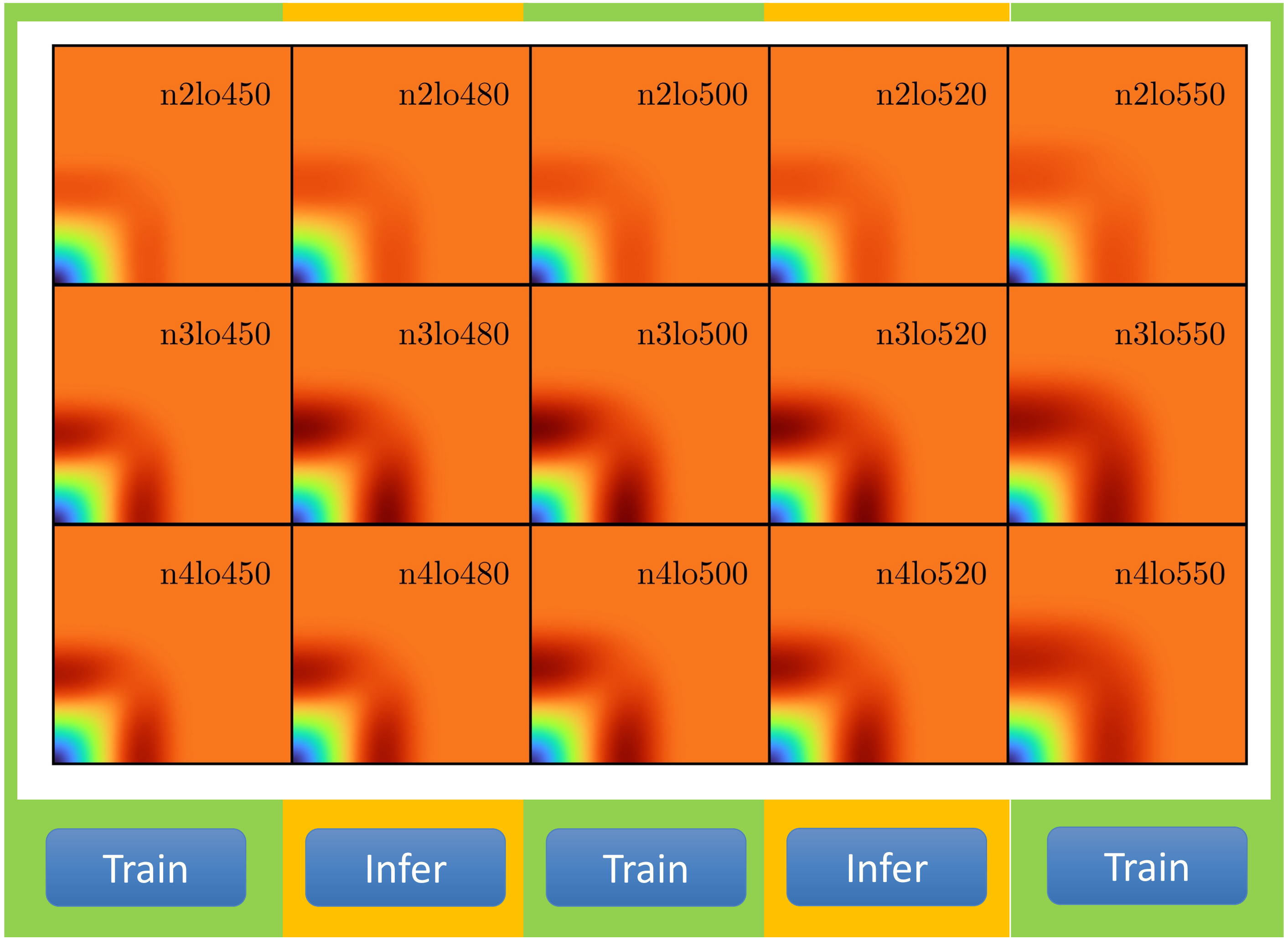

1. Distinguish truncation orders in ChEFT
2. Predict how the chiral potentials evolve with cutoff

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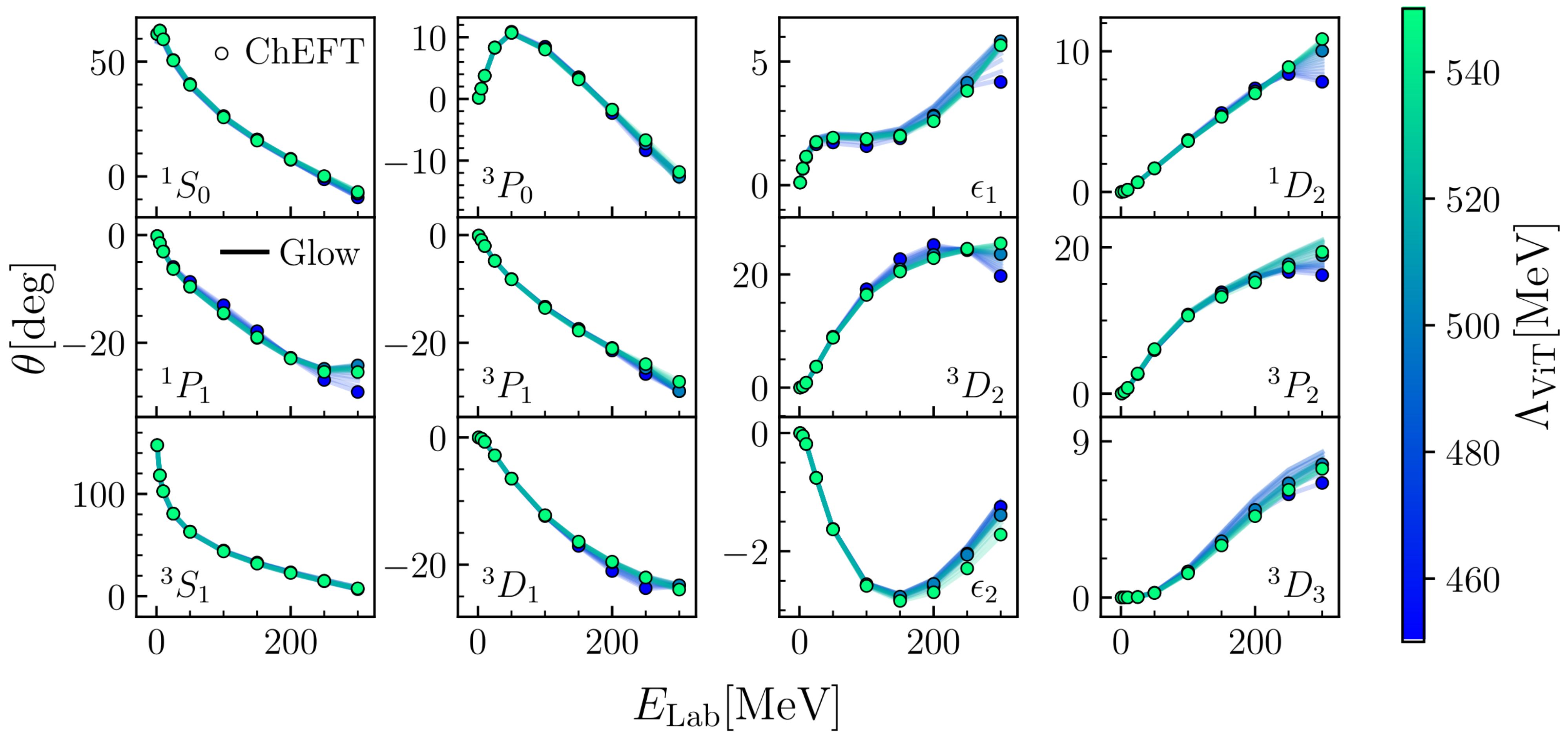

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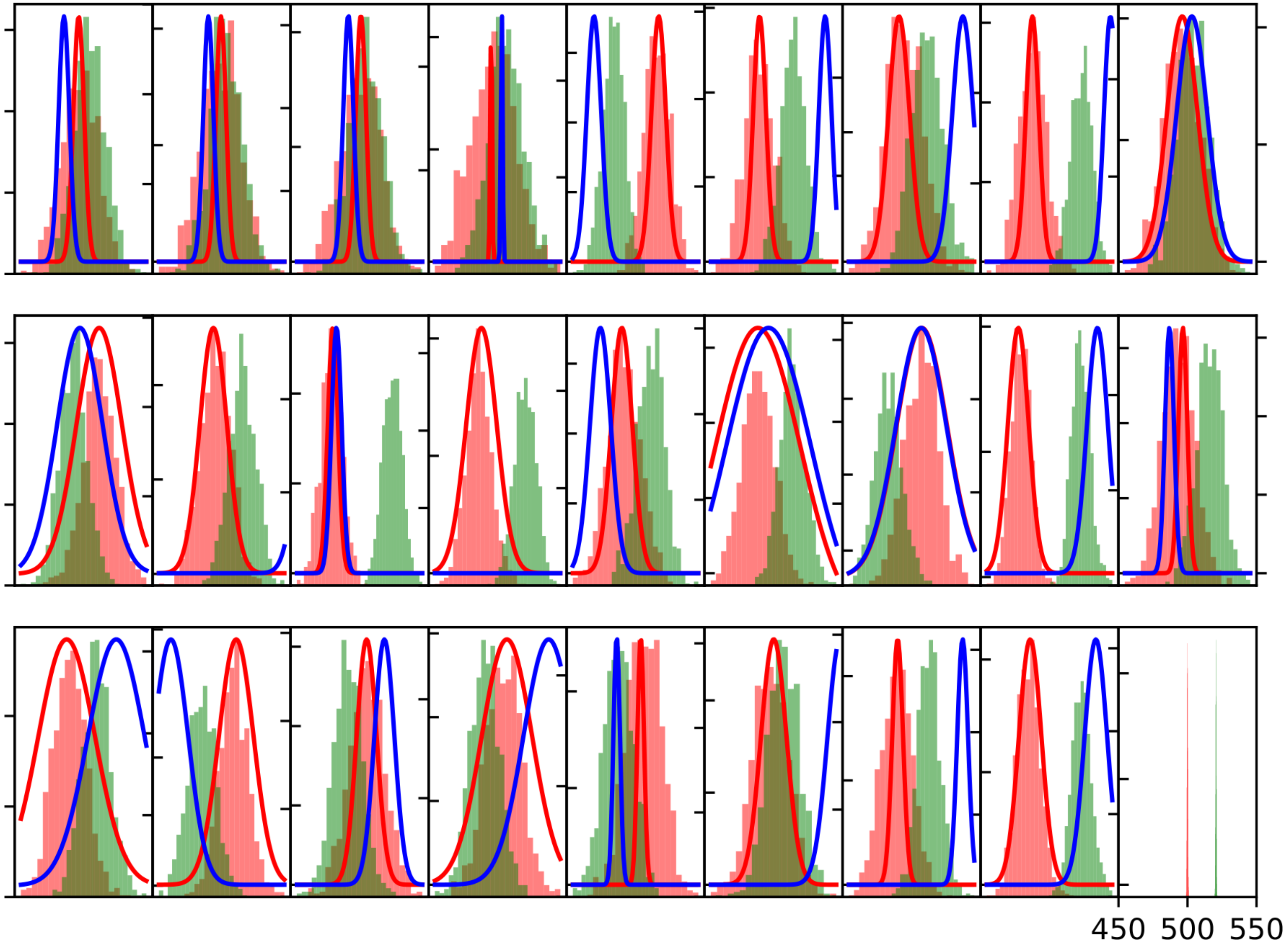
Low energy constant distributions



1. Can extract LECs from generated chiral potentials
2. Input LEC distributions can also be propagated to

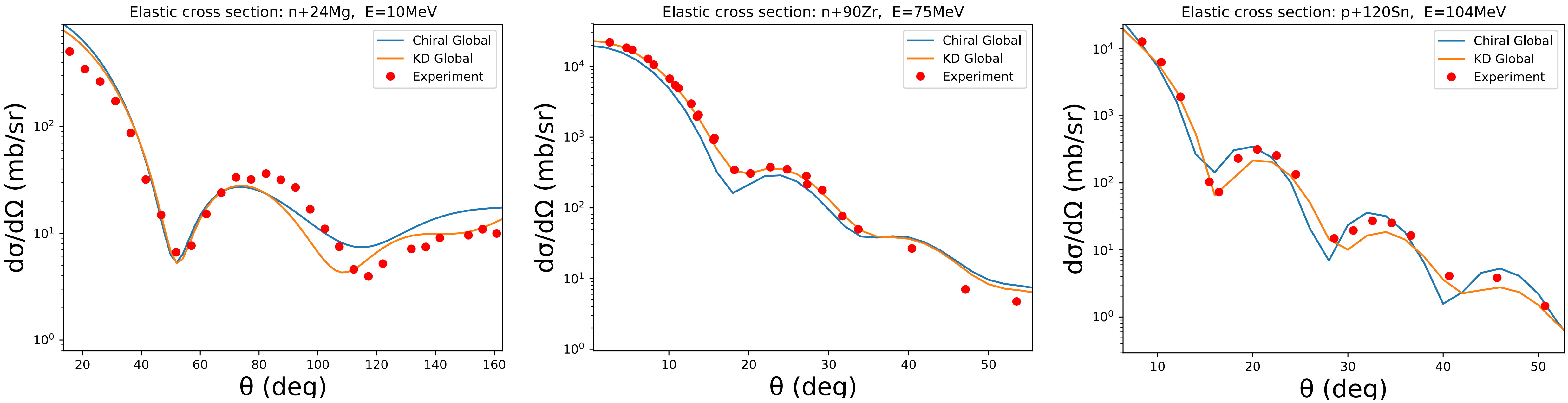
Summary and future directions

- First microscopic global optical potential with quantified uncertainties
  - Good description of differential nucleon-nucleus elastic scattering cross sections within uncertainties
  - Analyzing powers have larger uncertainties but also compare well to experiment

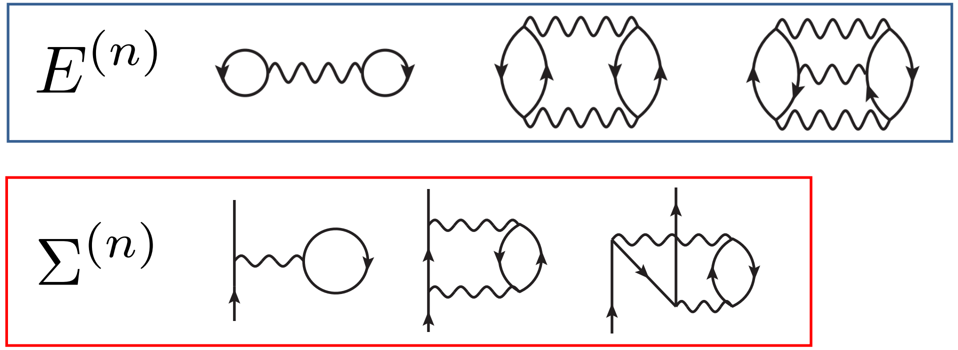
- <u>Improved uncertainty quantification possible</u>: variations in chiral low-energy constants, more sophisticated treatments of EFT truncation errors and choice of resolution scale

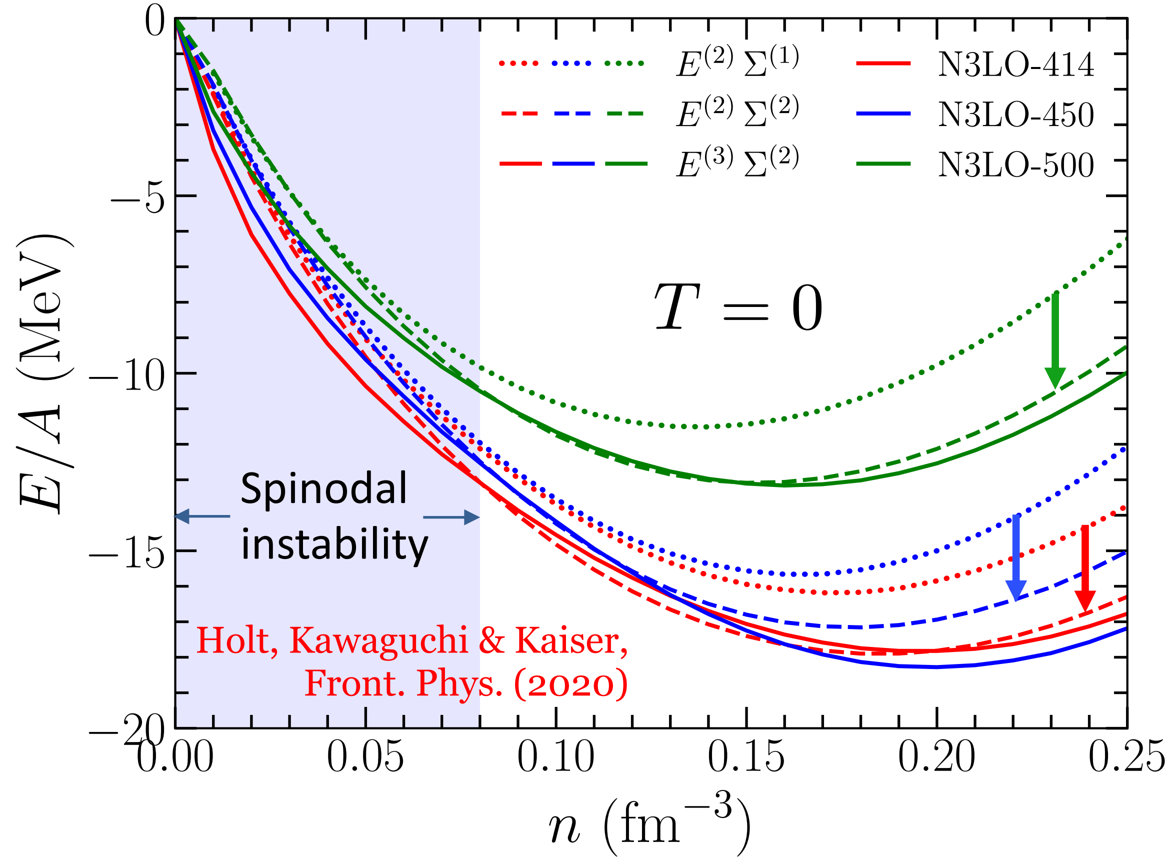
- Work in progress to interface new optical potentials with nuclear reaction codes for rare-isotope beam experiments

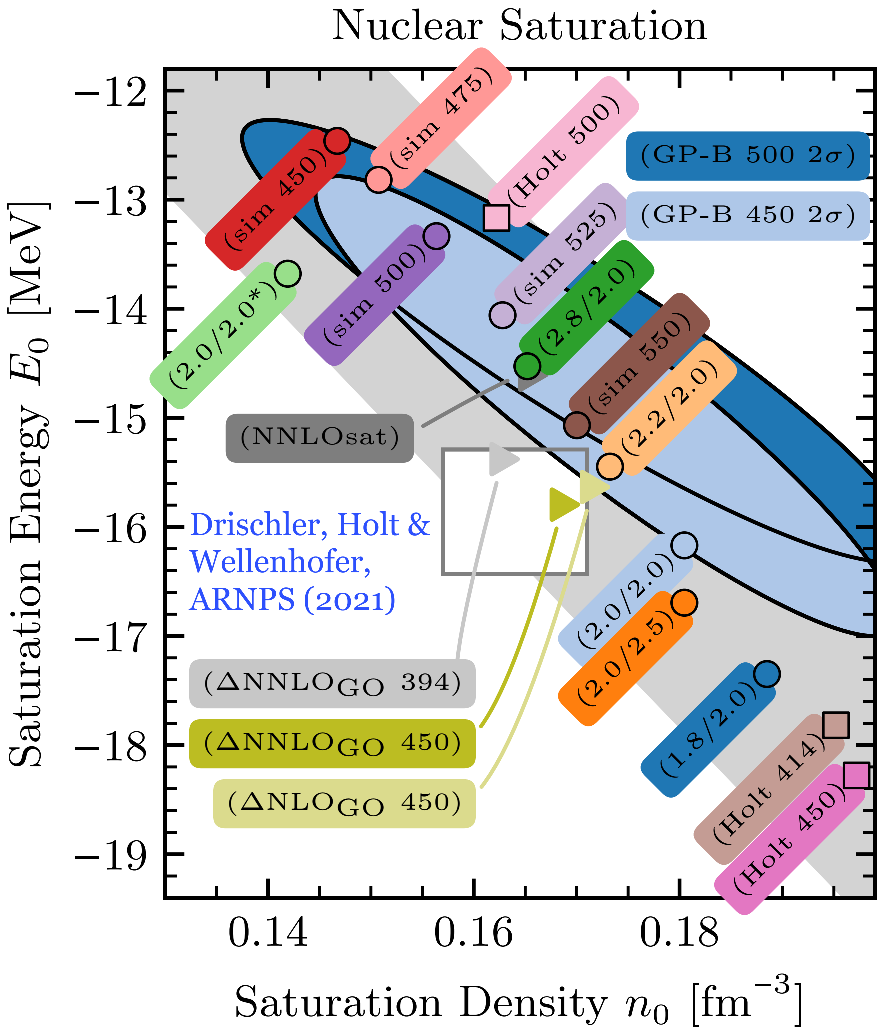
Comparison to phenomenology and data: selected results



Nuclear matter uncertainties







- **Saturation point is a fine-tuned quantity**

From nuclear matter to *finite nuclei:* spin-orbit interactions

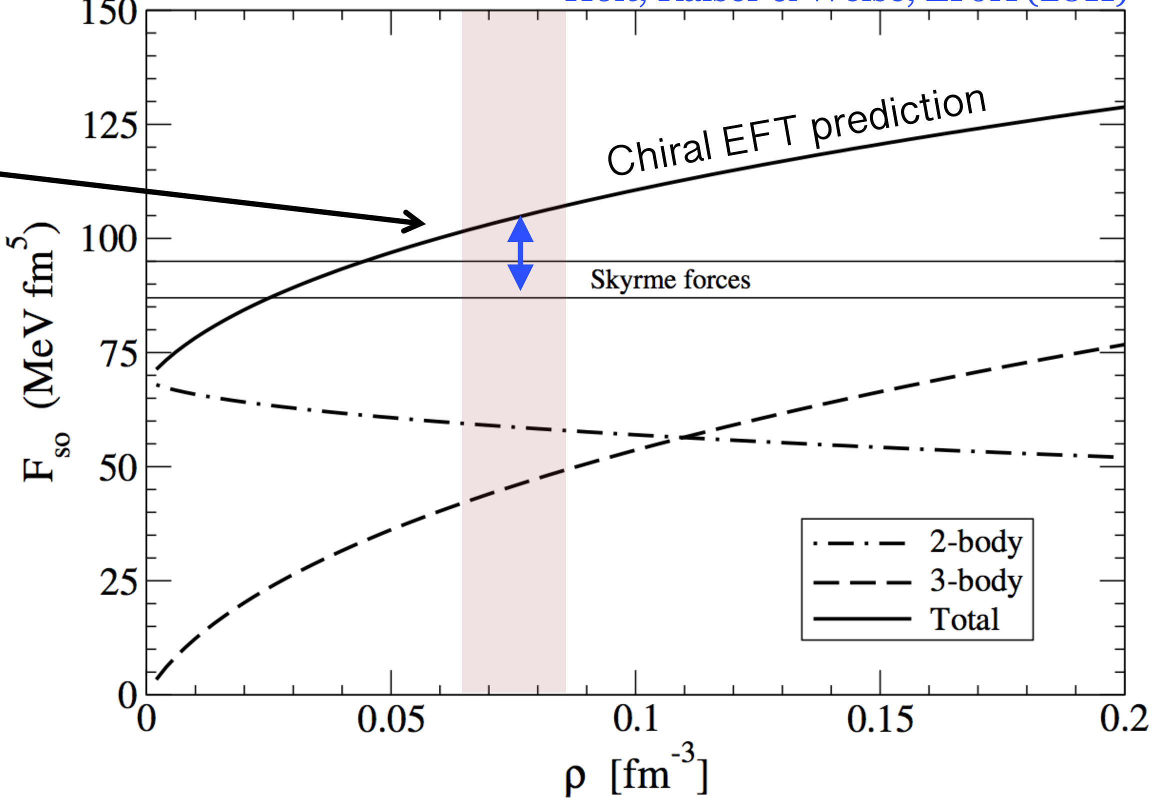
- Spin orbit interaction vanishes in infinite homogeneous nuclear matter

Density matrix expansion (Negele & Vautherin, PRC 1972)

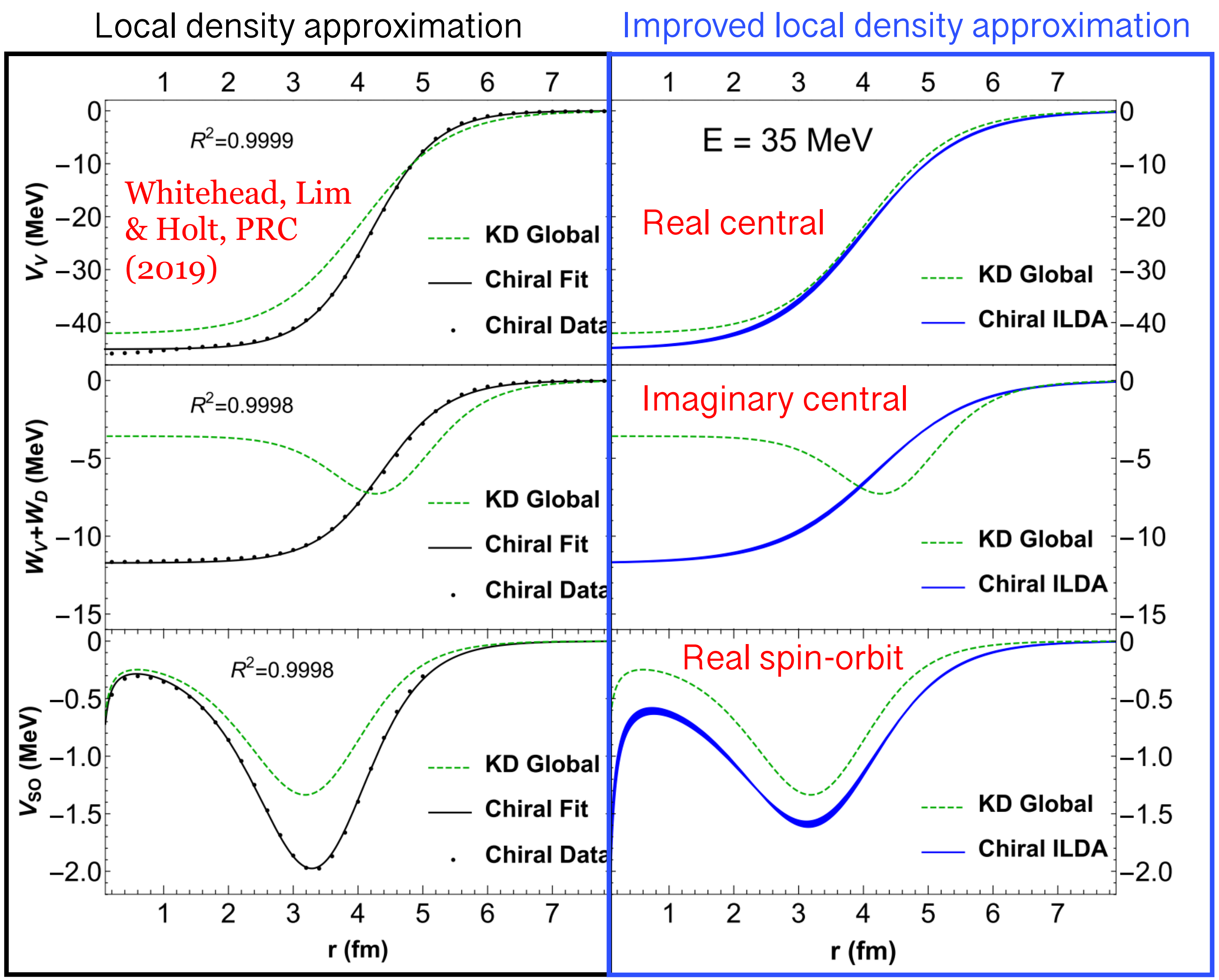
$$E_{\rm HF} = \frac{1}{2}{\rm Tr}_1{\rm Tr}_2 \int d\vec{r}_1 \cdots d\vec{r}_4 \langle \vec{r}_1\vec{r}_2|V(1-P_{12})|\vec{r}_3\vec{r}_4\rangle \rho(\vec{r}_3,\vec{r}_1)\rho(\vec{r}_4,\vec{r}_2)$$

- 20% too large at density region of interest
- 2nd-order perturbative contributions known to reduce spin-orbit strength

Holt, Kaiser & Weise, EPJA (2011)



From nuclear matter to *finite nuclei:* Improved LDA



$$V(E;r)_{ILDA} = \frac{1}{(t\sqrt{\pi})^3}\int V(E;r')e^{\frac{-|\vec{r}-\vec{r}'|^2}{t^2}}d^3r'$$

- Finite range of nuclear force must be accounted for
- Introduce Gaussian smearing function with range parameter t
- Increases the Woods-Saxon diffuseness parameter in agreement with phenomenology