Eigenvector Continuation for scattering with local chiral NN and optical potentials

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Christian Drischler

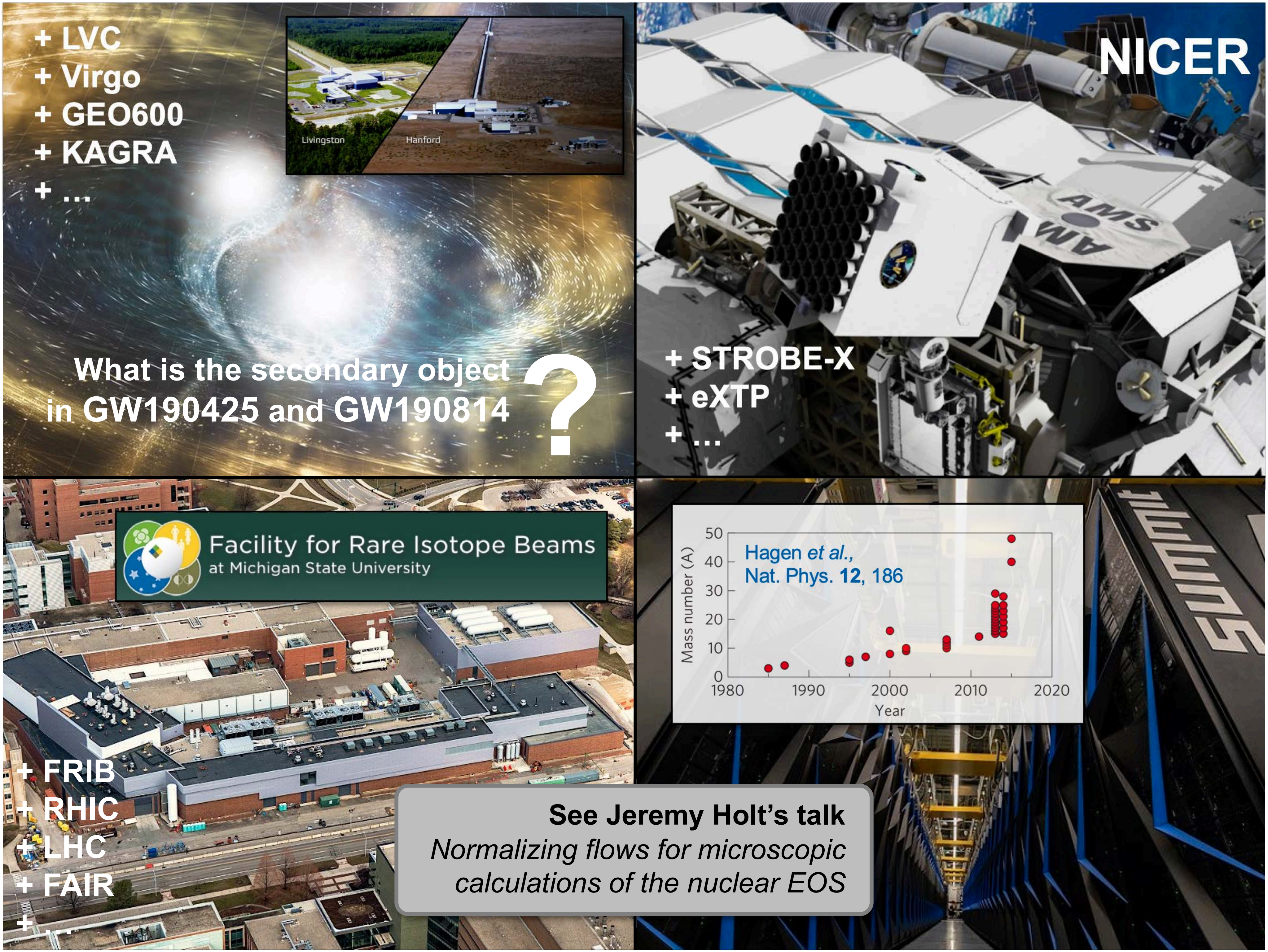
April 26, 2021 | INT 21-1b: Nuclear Forces for Precision Nuclear Physics

This week's topic:
Improving nuclear forces with *novel fitting strategies* and higher orders in chiral EFT

1. using EC as an efficient emulator for scattering with local chiral interactions and optical potentials
2. statistical quantification and propagation of EFT truncation errors in nuclear matter calculations

Keywords:

+ ChEFT + scattering
+ Variational principles
+ Eigenvector Continuation
+ Bayesian UQ
+ infinite nuclear matter
+ EFT truncation errors
+ …



+ LVC
+ Virgo
+ GEO600
+ KAGRA
+ ...
Livingston
Hanford
What is the secondary object
in GW190425 and GW190814
?
NICER
AMS
+ STROBE-X
+ eXTP
+ ...
Facility for Rare Isotope Beams
at Michigan State University
+ FRIB
+ RHIC
+ LHC
+ FAIR
+ ...
Hagen et al.,
Nat. Phys. 12, 186
Mass number (A)
Year
0
10
20
30
40
50
1980
1990
2000
2010
2020
SUMMIT
See Jeremy Holt's talk
Normalizing flows for microscopic
calculations of the nuclear EOS

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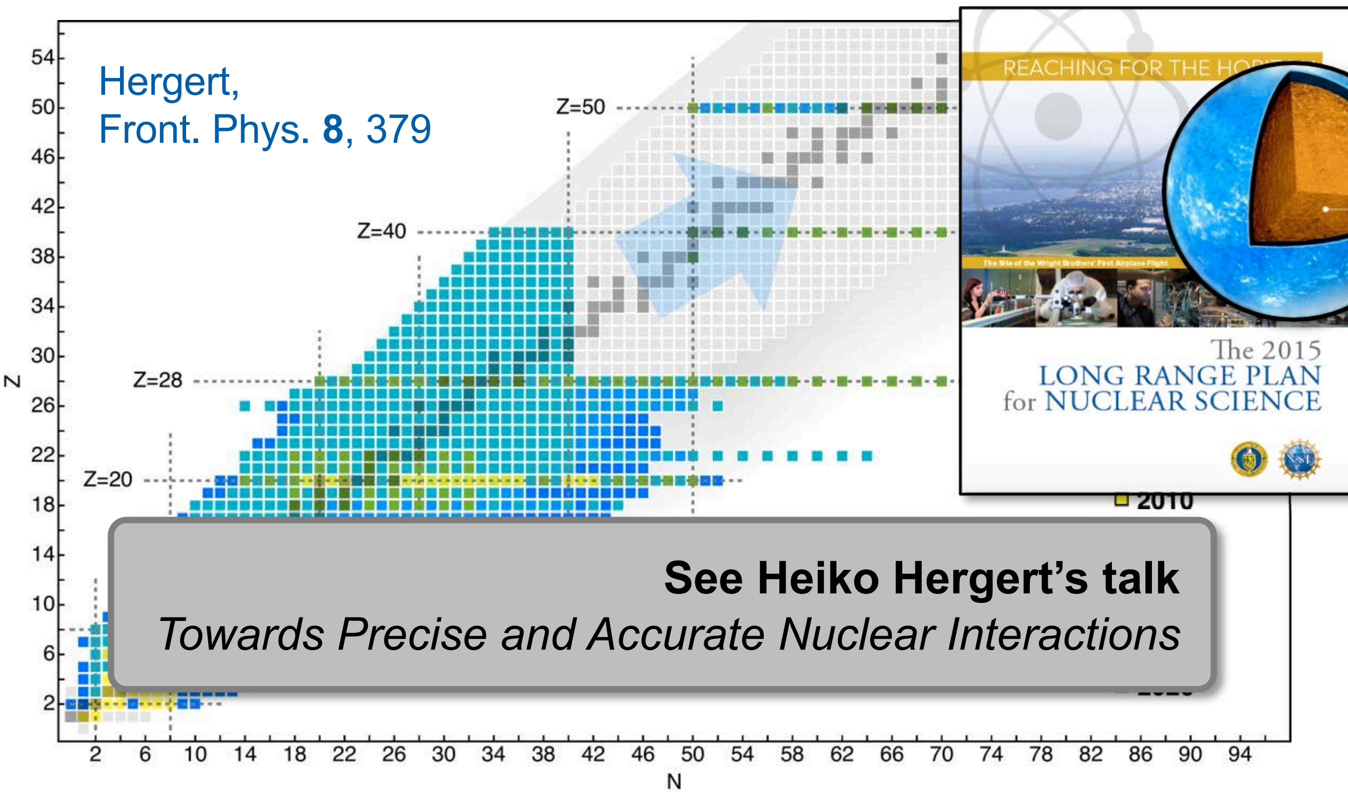
CD, Haxton, McElvain *et al.*, arXiv:1910.07961 (PPNP in press)

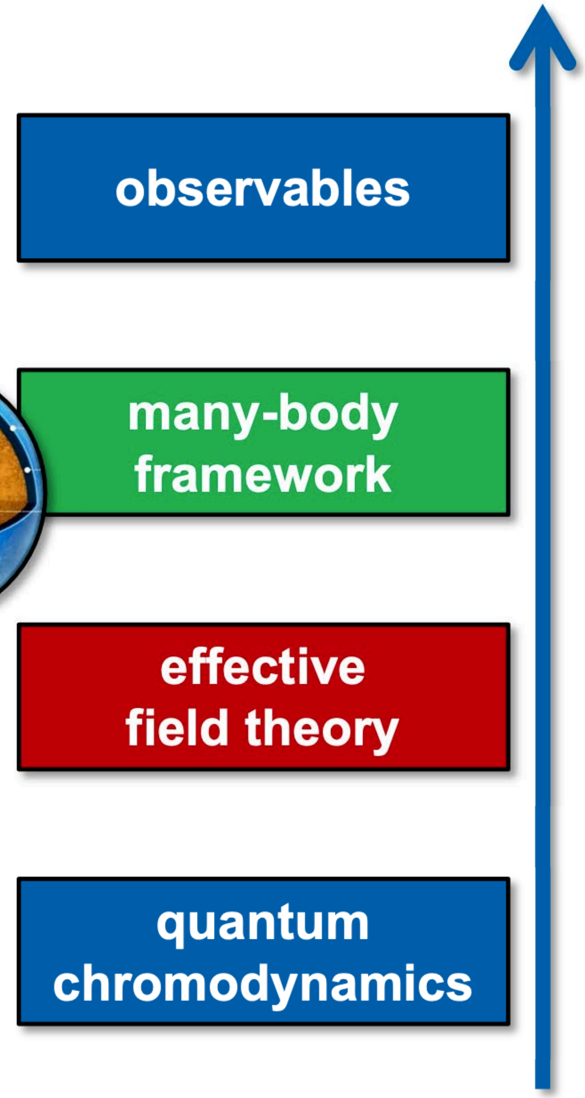
How does the nuclear chart emerge from QCD?

Where do heavy elements come from?

How does subatomic matter organize itself?



See Heiko Hergert's talk
Towards Precise and Accurate Nuclear Interactions



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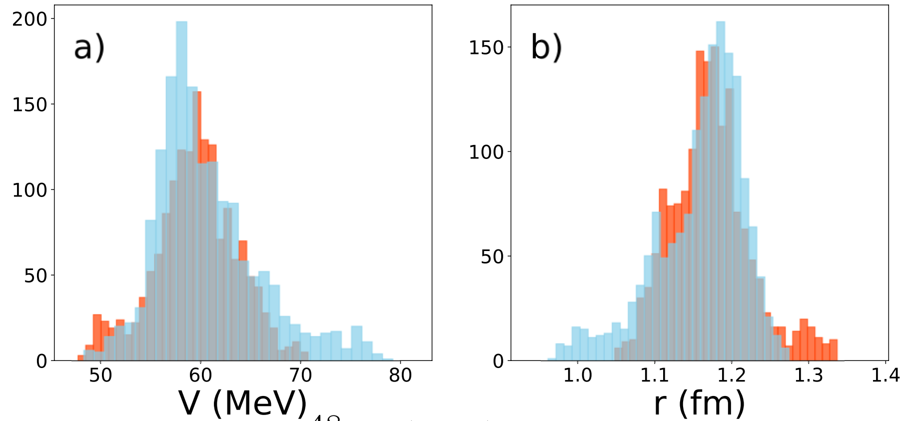
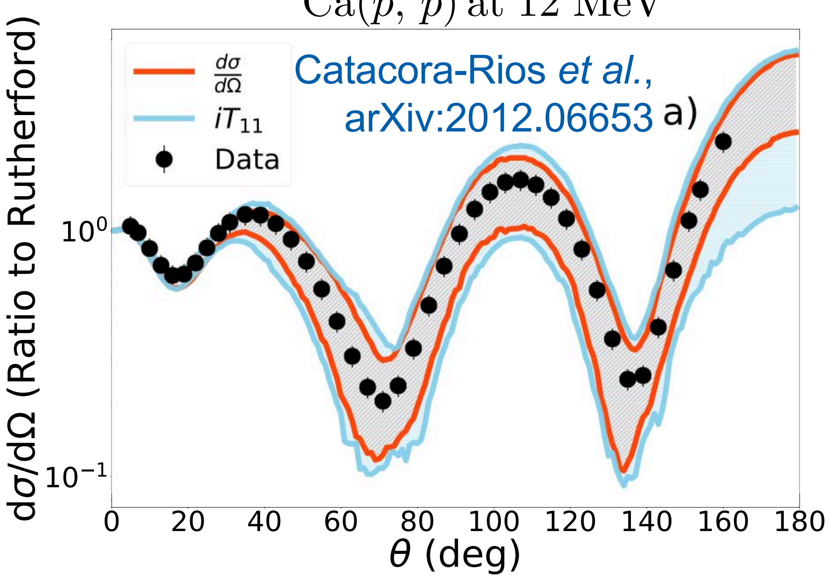
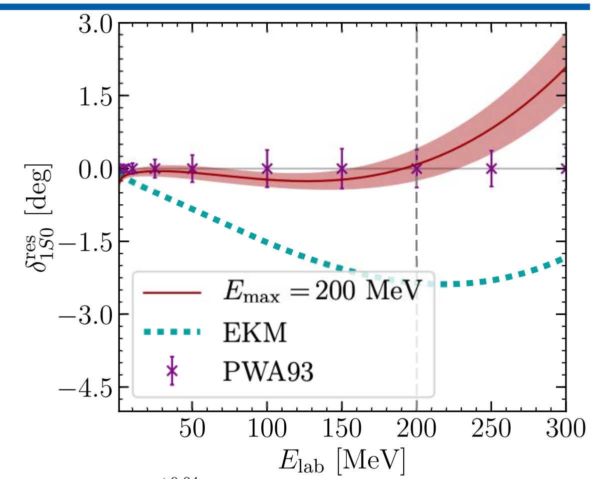
Bayesian uncertainty quantification

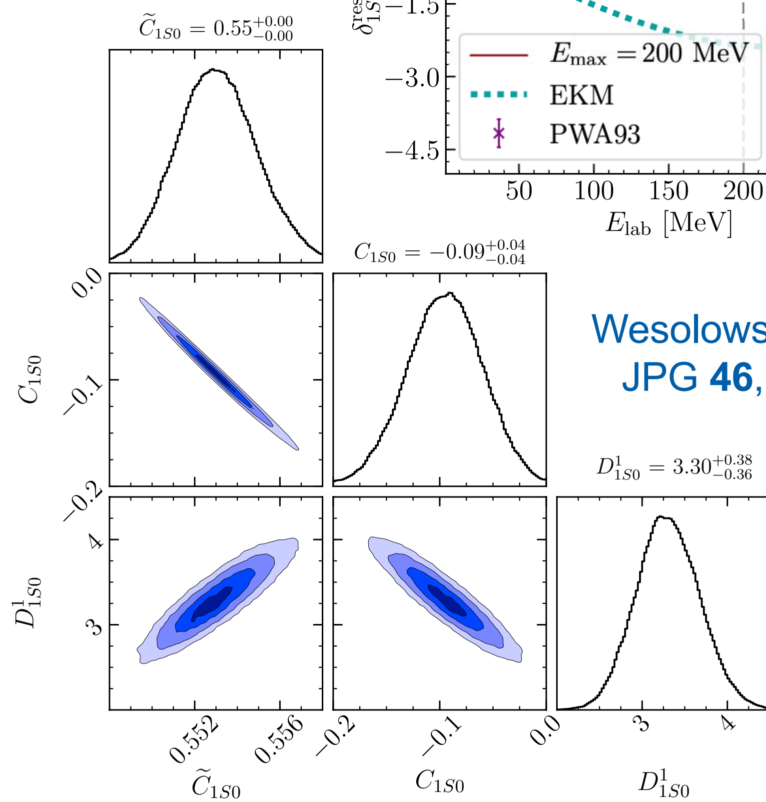




Optical potentials

Chiral potentials





Wesolowski *et al.*,
JPG **46**, 045102

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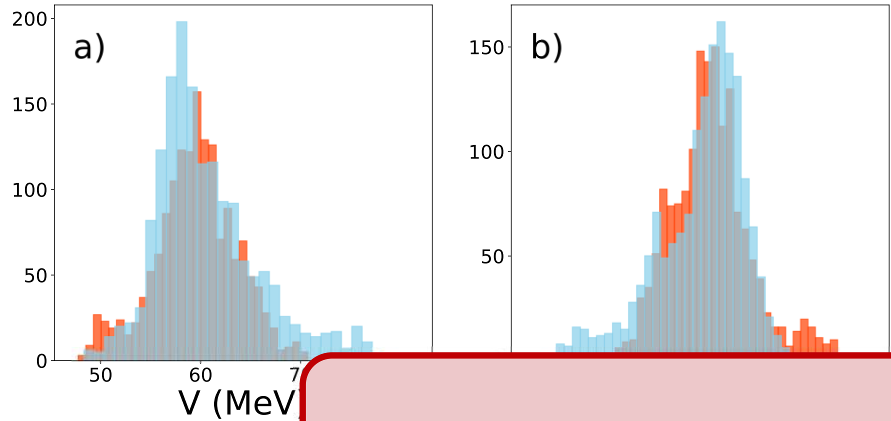
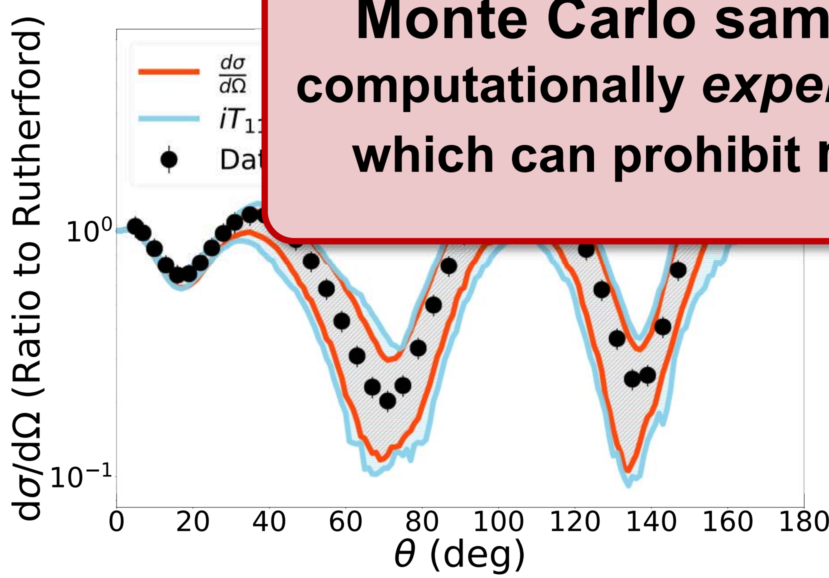
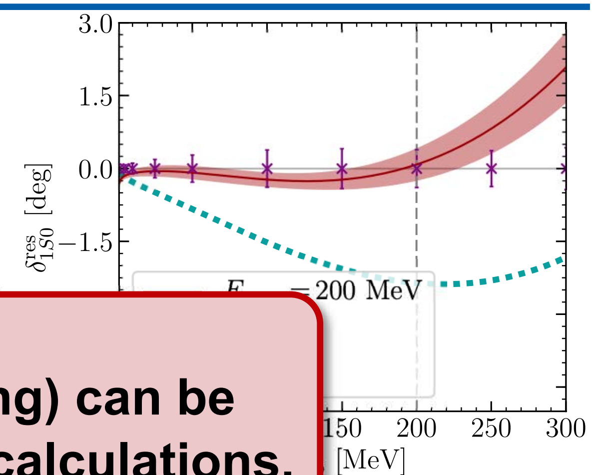
Bayesian uncertainty quantification

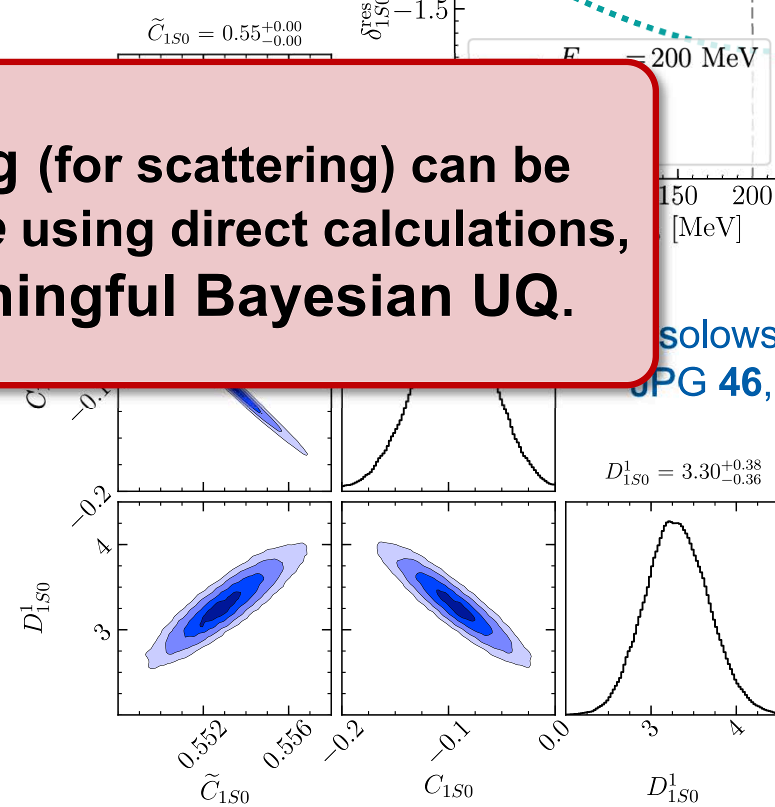




Optical potentials

Chiral potentials





...solowski *et al.*, ...JPG **46**, 045102

Monte Carlo sampling (for scattering) can be computationally *expensive* using direct calculations, which can prohibit meaningful Bayesian UQ.

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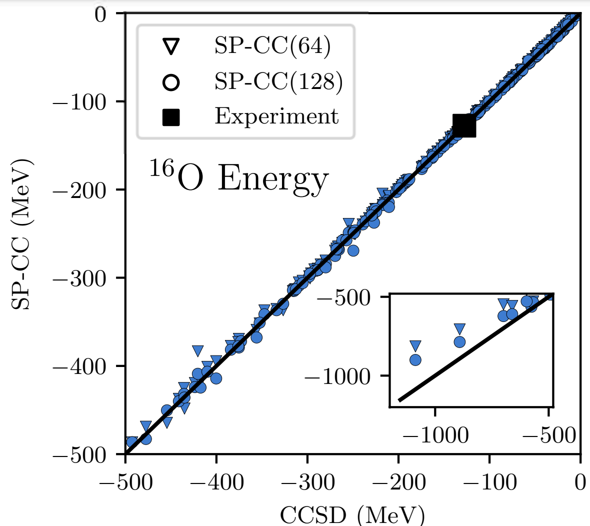
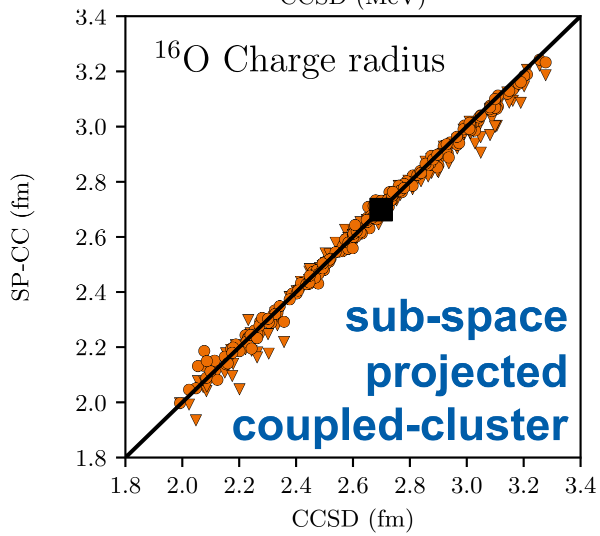
Rigorous UQ and global sensitivity analysis



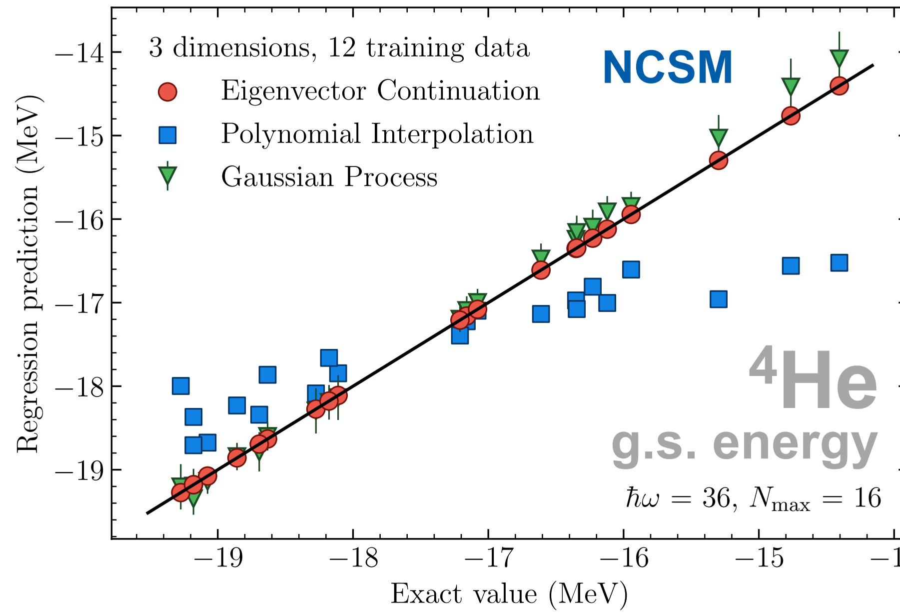


Ekström & Hagen, PRL **123**, 252501

Eigenvector Continuation

Frame *et al.*, PRL **121**, 032501

accurate & fast emulators
efficient resummation tool



König, Ekström *et al.*, PLB **810**, 135814
Demol, Duguet *et al.*, PRC **101**, 041302
Wesolowski, Svensson *et al.*, arXiv:2104.04441

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Rigorous UQ and global sensitivity analysis

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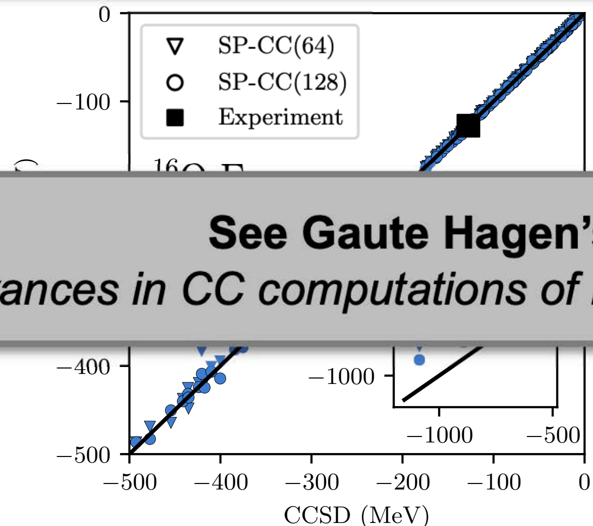
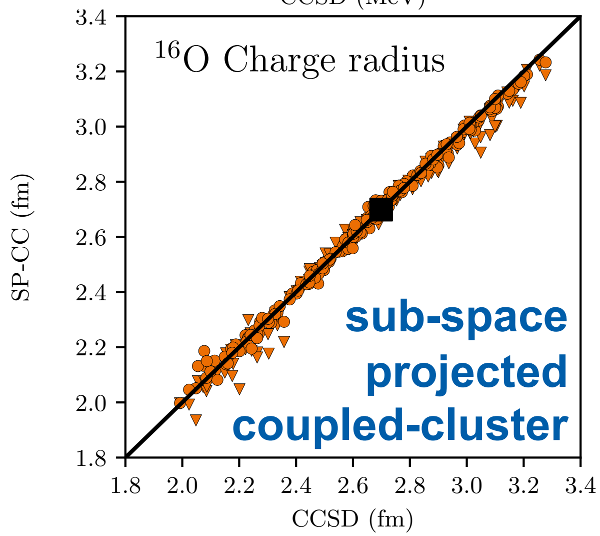


See Gaute Hagen's talk
Advances in CC computations of nuclei



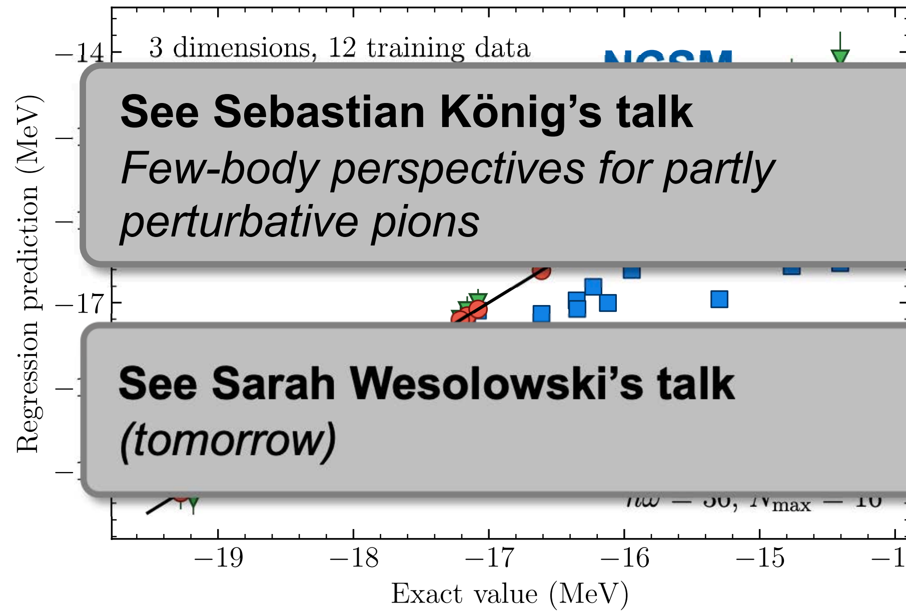
sub-space projected coupled-cluster

Ekström & Hagen, PRL **123**, 252501

Eigenvector Continuation

Frame *et al.*, PRL **121**, 032501

accurate & fast emulators
efficient resummation tool



See Sebastian König's talk
Few-body perspectives for partly perturbative pions

See Sarah Wesolowski's talk
(tomorrow)

König, Ekström *et al.*, PLB **810**, 135814
Demol, Duguet *et al.*, PRC **101**, 041302
Wesolowski, Svensson *et al.*, arXiv:2104.04441

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Kohn Variational Principle

Furnstahl, Garcia, Millican, and Zhang, PLB **809**, 10135719

$$\beta\left[|\psi_{\text{trial}}\rangle\right] = \frac{K_\ell}{p} - 2\mu\,\langle\psi_{\text{trial}}\,|\,H(\boldsymbol{\theta}) - E\,|\,\psi_{\text{trial}}\rangle \qquad p = \sqrt{2\mu E}$$

stationary **approximation to exact K_l matrix [accurate up to $O(\delta u^2)$]**

$$u_{\ell,E}^{\text{trial}}(r) \sim \frac{1}{p}\sin(\eta_\ell) + \frac{K_\ell}{p}\cos(\eta_\ell) \qquad \eta_\ell = kr - \frac{\pi}{2}\ell \qquad H(\boldsymbol{\theta}) = T + V(\boldsymbol{\theta})$$

for EC in *R* matrix theory,
see also Bai & Ren, PRC **103**, 014612

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Kohn Variational Principle 1

Furnstahl, Garcia, Millican, and Zhang, PLB **809**, 10135719

$$\beta\,[|\psi_{\rm trial}\rangle] = \frac{K_\ell}{p} - 2\mu\,\langle\psi_{\rm trial}\,|\,H(\boldsymbol{\theta}) - E\,|\,\psi_{\rm trial}\rangle \qquad p = \sqrt{2\mu E}$$

2 ***stationary*** **approximation to exact K_l matrix [accurate up to $O(\delta u^2)$]**

$$u^{\rm trial}_{\ell,E}(r) \sim \frac{1}{p}\sin(\eta_\ell) + \frac{K_\ell}{p}\cos(\eta_\ell) \qquad \eta_\ell = kr - \frac{\pi}{2}\ell \qquad H(\boldsymbol{\theta}) = T + V(\boldsymbol{\theta})$$

3

4

Training: solve RSE *exactly* for a set $\{\boldsymbol{\theta}_i\}_{i=1}^{N_b}$ and construct the trial wave function:

$$|\psi_{\rm trial}\rangle = \sum_{i=1}^{N_b} c_i\,|\psi_E(\boldsymbol{\theta}_i)\rangle$$

Given $H(\boldsymbol{\theta})$, the *stationary point* is obtained by simple linear algebra:

$$\delta\beta[\psi_{\rm trial}] = 0 \quad \text{s.t.} \quad \textstyle\sum_{i=1}^{N_b} c_i = 1$$

$$c_i = \sum_j (\Delta\widetilde{U})^{-1}_{ij}\left(\frac{K^{(j)}_\ell(E)}{p} - \lambda\right) \qquad \lambda = \frac{-1 + \sum_{ij}(\Delta\widetilde{U})^{-1}_{ij}\frac{K^{(j)}_\ell(E)}{p}}{\sum_{ij}(\Delta\widetilde{U})^{-1}_{ij}}$$

with matrix $\Delta\widetilde{U}_{ij} = 2\mu\,\langle\psi_E(\boldsymbol{\theta}_i)\,|\,2V(\boldsymbol{\theta}) - V(\boldsymbol{\theta}_i) - V(\boldsymbol{\theta}_j)\,|\,\psi_E(\boldsymbol{\theta}_j)\rangle$

5

Approximate $K_l = \tan\delta_l$: $[K_\ell(E)]_{\rm exact} \approx \sum_i c_i K^{(i)}_\ell(E) - \frac{p}{2}\sum_{ij} c_i \Delta\widetilde{U}_{ij} c_j$

emulate

validate

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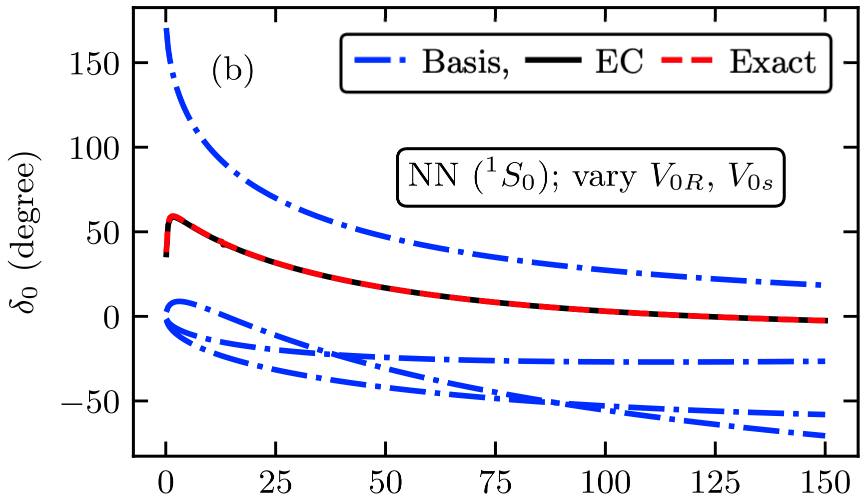
Furnstahl, Garcia, Millican, and Zhang, PLB **809**, 10135719

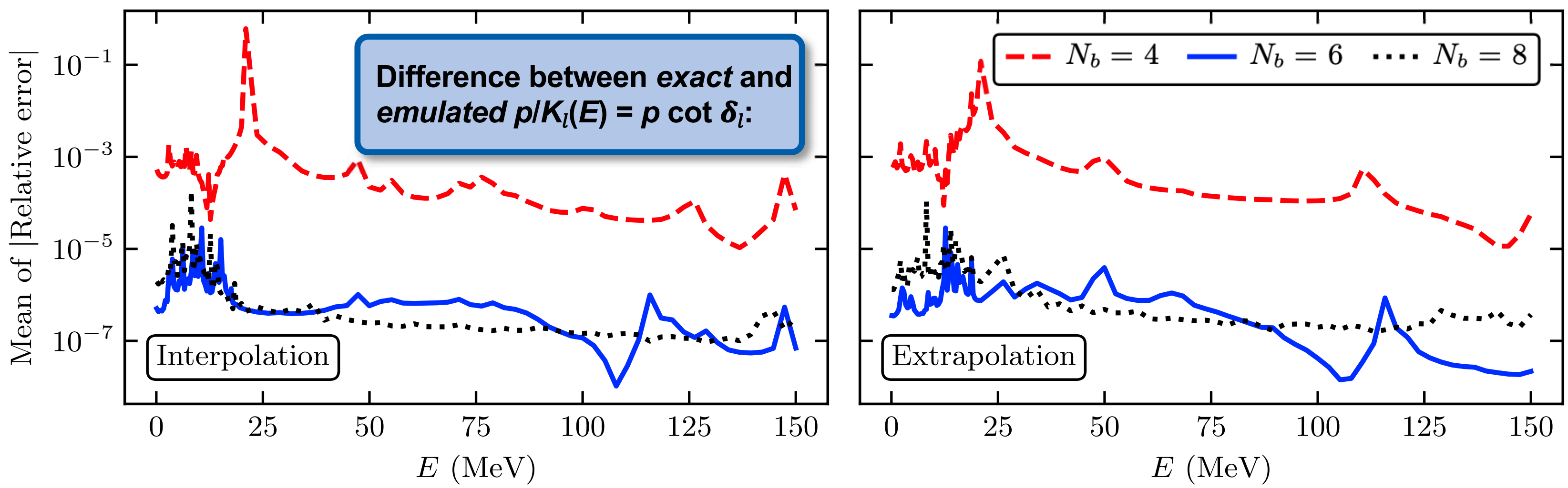


EC for scattering is effective for inter- and extrapolation

- local & nonlocal potentials
- incl. optical potentials
- high partial waves

Minnesota interaction:

$$V_{^1S_0}(r) \equiv V_{0R} e^{-\kappa_R r^2} + V_{0s} e^{-\kappa_s r^2}$$



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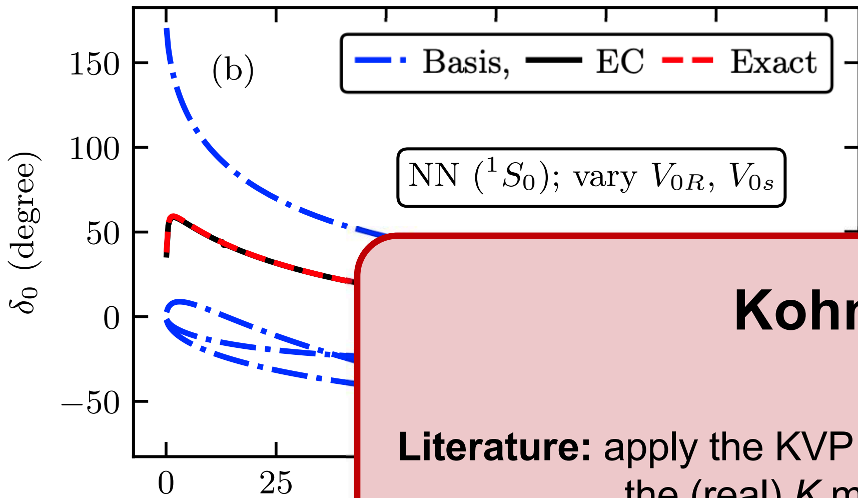
Furnstahl, Garcia, Millican, and Zhang, PLB **809**, 10135719



EC for scattering is effective for inter- and extrapolation

- local & nonlocal potentials
- incl. optical potentials

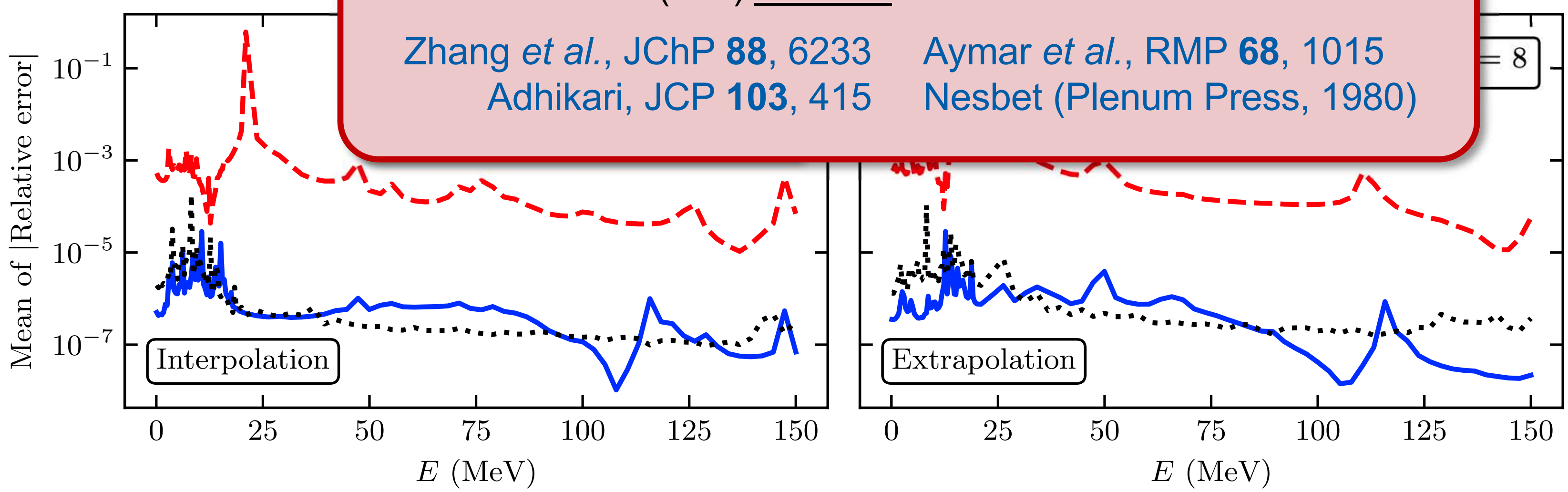
Kohn anomalies

Schwartz, PR **124**, 1468 (1961)

Literature: apply the KVP to the (complex) *S matrix* rather than the (real) *K* matrix to avoid anomalies

Zhang *et al.*, JChP **88**, 6233
Adhikari, JCP **103**, 415

Aymar *et al.*, RMP **68**, 1015
Nesbet (Plenum Press, 1980)



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Generalized Kohn Variational Principle

Lucchese, PRA **40**, 112

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stationary **approximation to exact L_l matrix [accurate up to $O(\delta u^2)$]**

$$u_{\ell,E}^{\text{trial}}(r) \sim \phi_0(r) + L\,\phi_1(r) \qquad \begin{aligned}\phi_0(r) &\sim u_{00}\sin(\eta_\ell) + u_{01}\cos(\eta_\ell)\\ \phi_1(r) &\sim u_{10}\sin(\eta_\ell) + u_{11}\cos(\eta_\ell)\end{aligned} \qquad \eta_\ell = kr - \frac{\pi}{2}\ell$$

$$L = K \quad \text{for} \quad u = \begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}$$

$$L = S \quad \text{for} \quad u = \begin{bmatrix}i & -1\\ i & 1\end{bmatrix}$$

$$L = T \quad \text{for} \quad u = \begin{bmatrix}1 & 0\\ i & 1\end{bmatrix}$$

… any nonsingular matrix

$$K = \frac{u_{01} + u_{11}L}{u_{00} + u_{10}L}$$

for applications to N-d and p-d scattering, see
Viviani, Kievsky, and Rosati, FBS **30**, 3
Kievsky, NPA **624**, 125
Kievsky, Viviani, and Rosati, NPA **577**, 511

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with matrix $$\Delta\tilde{U}_{ij} = \frac{2\mu}{\det u}\langle\psi_E(\boldsymbol{\theta}_i)\,|\,2V(\boldsymbol{\theta}) - V(\boldsymbol{\theta}_i) - V(\boldsymbol{\theta}_j)\,|\,\psi_E(\boldsymbol{\theta}_j)\rangle$$

Approximate L_l: $$[L_\ell(E)]_{\text{exact}} \approx \sum_i c_i L^{(i)}_\ell(E) - \frac{1}{2}\sum_{ij} c_i \Delta\tilde{U}_{ij} c_j$$

emulate

validate

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Generalized KVP in practice

CD, Giuliani, Quinonez *et al.*, in prep.

$$[L_\ell(E)]_{\text{exact}} \approx \sum_i c_i L_\ell^{(i)}(E) - \frac{1}{2}\sum_{ij} c_i \Delta\widetilde{U}_{ij} c_j$$

Considered a wide range of KVPs:

- *S*, *T*, *K*, their inverses, and random complex parametrizations *u*
- uncoupled channels
- local coordinate-space potentials

Potentials $V(r;\boldsymbol{\theta})$ implemented:

- Minnesota (real, nonlinear in $\boldsymbol{\theta}$)
- Woods-Saxon (real, nonlinear in $\boldsymbol{\theta}$)
- Optical (complex, nonlinear in $\boldsymbol{\theta}$)
- **Local chiral GT+ (real, linear in $\boldsymbol{\theta}$)**

We sample $H(\boldsymbol{\theta})$ randomly for different channels, energies, and basis sizes, and **investigate deviations** of **emulated from exact phase shifts.**

To measure the efficacy of EC, we fit the c_i's to the exact wave function.

$$|\psi_{\text{trial}}\rangle = \sum_{i=1}^{N_b} c_i\, |\psi_E(\boldsymbol{\theta}_i)\rangle$$

The EC basis usually is still effective in energy regions where the KVP is affected by Kohn anomalies.

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Complex vs real KVP

CD, Giuliani, Quinonez *et al.*, in prep.

Why is the complex KVP less prone to *Kohn anomalies*?

$$\lambda = \frac{-1 + \sum_{ij} (\Delta \widetilde{U})^{-1}_{ij} L^{(j)}_{\ell}(E)}{\sum_{ij} (\Delta \widetilde{U})^{-1}_{ij}}$$

There are several sources of Kohn anomalies. For instance, no *stationary* point of the functional can be found if

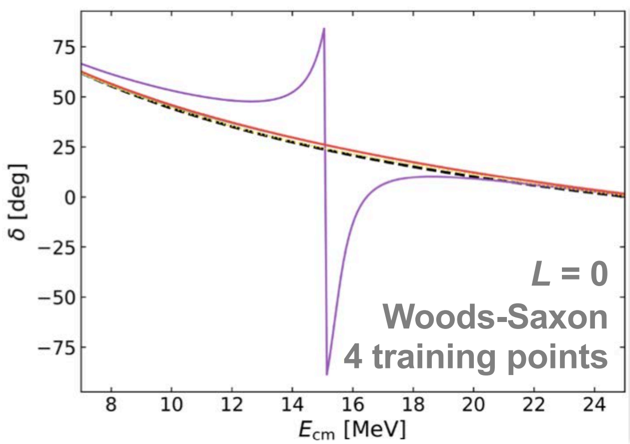
$$\sum_{ij} (\Delta \widetilde{U})^{-1}_{ij} = 0$$

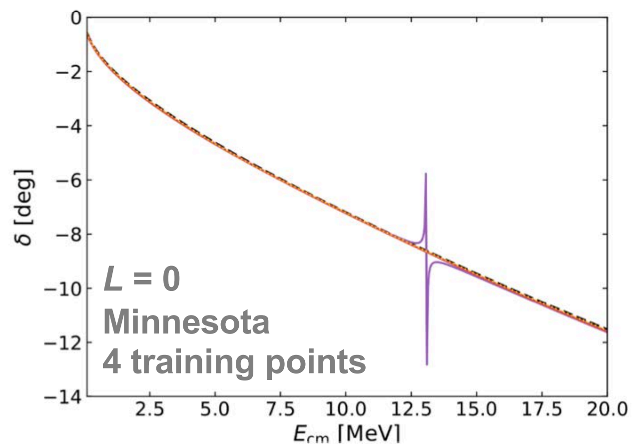
(can be used to pinpoint anomalies)

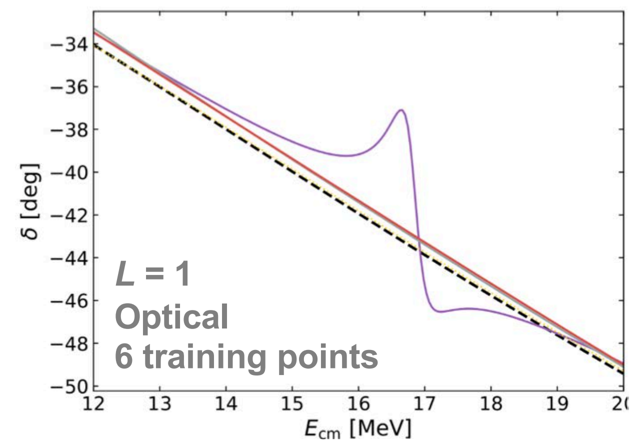
Advantage: the denominator is complex for the complex KVP and/or optical potentials, hence improving issues with zero crossings

No guarantee: we found Kohn anomalies in the *K* matrix for all but chiral potentials.

Other sources: bound states, resonances…







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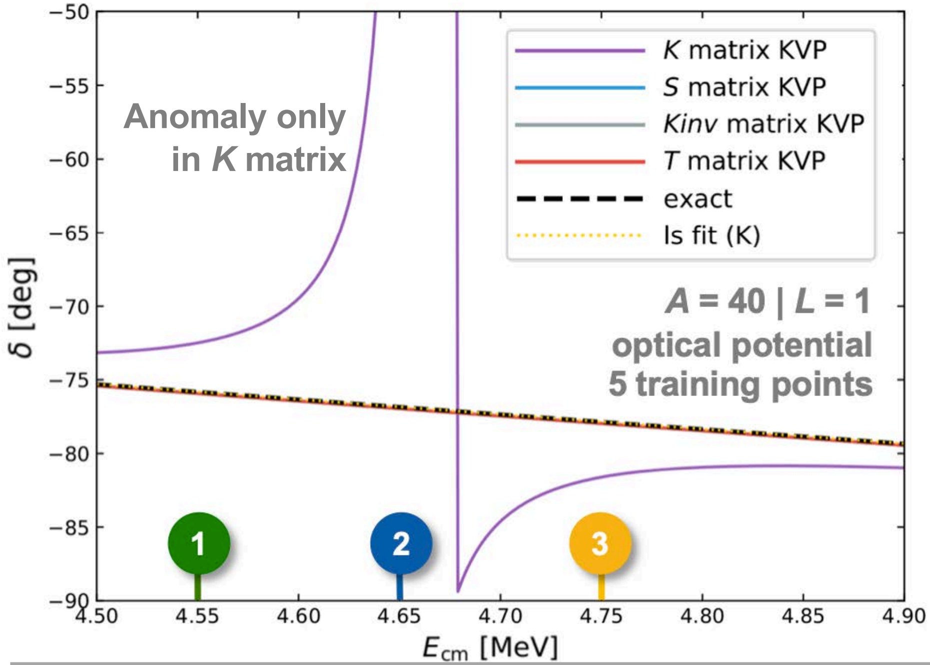
Phase shifts and (differential) cross sections

CD, Giuliani, Quinonez *et al.*, in prep.

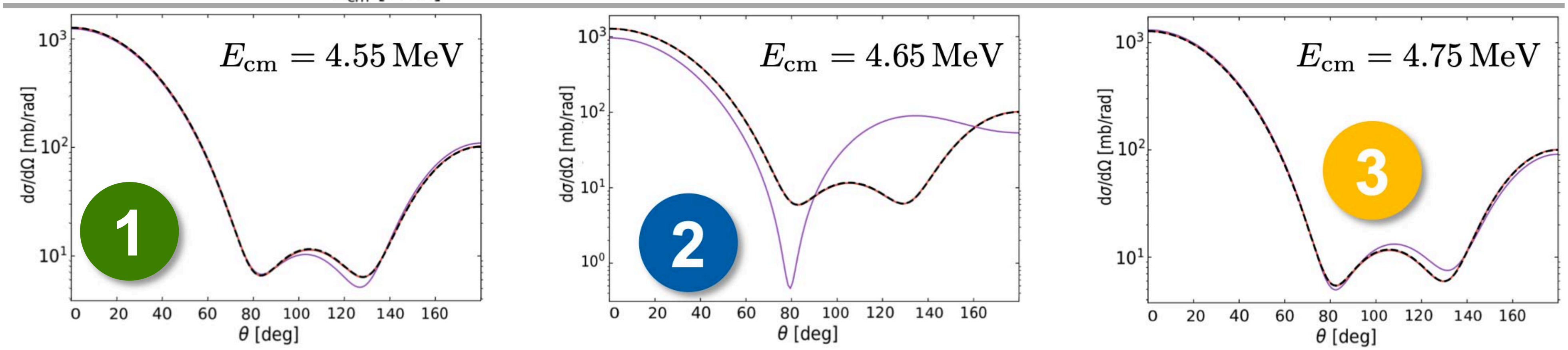


$$\frac{d\sigma}{d\Omega} = \left| \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) P_l(\cos\theta)(S_l - 1) \right|^2$$

Overall, the complex KVP reproduces well phase shifts and cross sections in contrast to the real KVP.

In absence of anomalies, the real KVP may be slightly more accurate for some *E*

differential cross sections



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Diagnostic tools

see also: Lucchese, PRA **40**, 112

Does that imply that the complex KVP is free of *Kohn anomalies*?

$$[L_\ell(E)]_{\text{exact}} \approx \sum_i c_i L_\ell^{(i)}(E) - \frac{1}{2}\sum_{ij} c_i \Delta\widetilde{U}_{ij} c_j$$

Diagnostic tools for anomalies:

- Use **multiple KVPs in parallel**
- Check KVPs for consistency

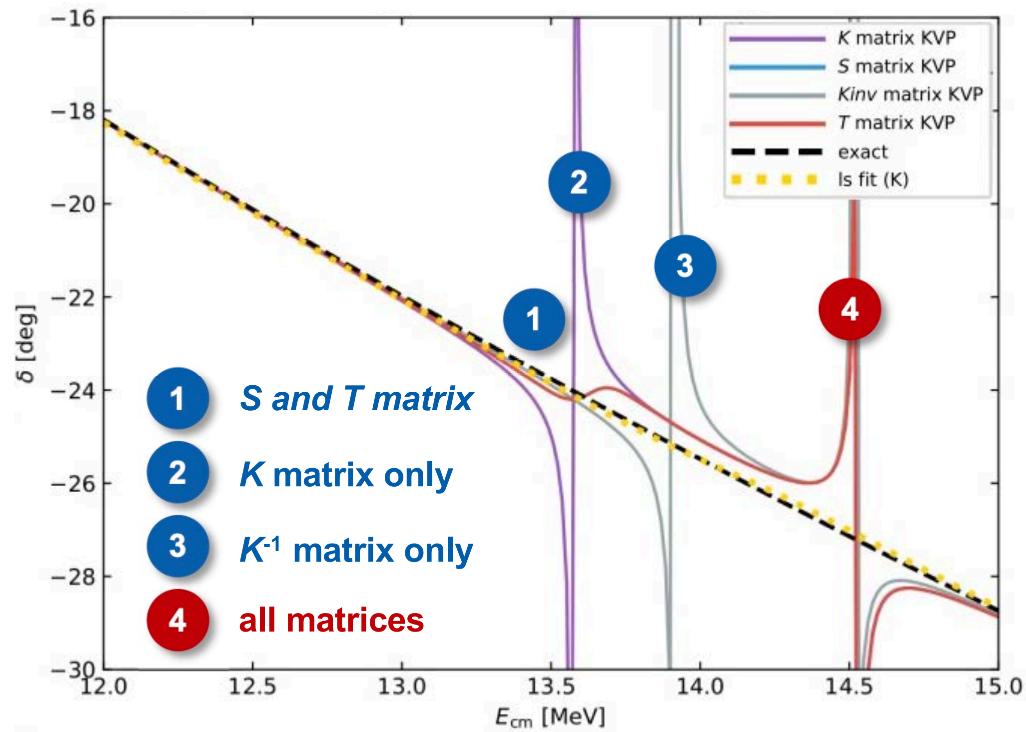
$$S = 1 + 2iT \qquad L^{-1}L = 1$$

$$|S| = 1 \text{ (for real } V\text{)} \qquad (\ldots)$$

- Track and find zero crossings of

$$\Gamma(E) = \sum_{ij} (\Delta\widetilde{U})^{-1}_{ij}$$

- **Change the size of the training basis** (double, add/remove, etc.)



see also: Lucchese, PRA **40**, 112
Viviani, Kievsky, and Rosati, FBS **30**, 3

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Numerical noise

CD, Giuliani, Quinonez *et al.*, in prep.

$$c_i = \sum_j (\Delta\widetilde{U})^{-1}_{ij} \left(L_\ell^{(j)}(E) - \lambda \right)$$

$$\lambda = \frac{-1 + \sum_{ij} (\Delta\widetilde{U})^{-1}_{ij} L_\ell^{(j)}(E)}{\sum_{ij} (\Delta\widetilde{U})^{-1}_{ij}}$$

The condition number increases with increasing number of training points.

Methods to control the noise in matrix inversions are *not* efficient (fine-tuned)

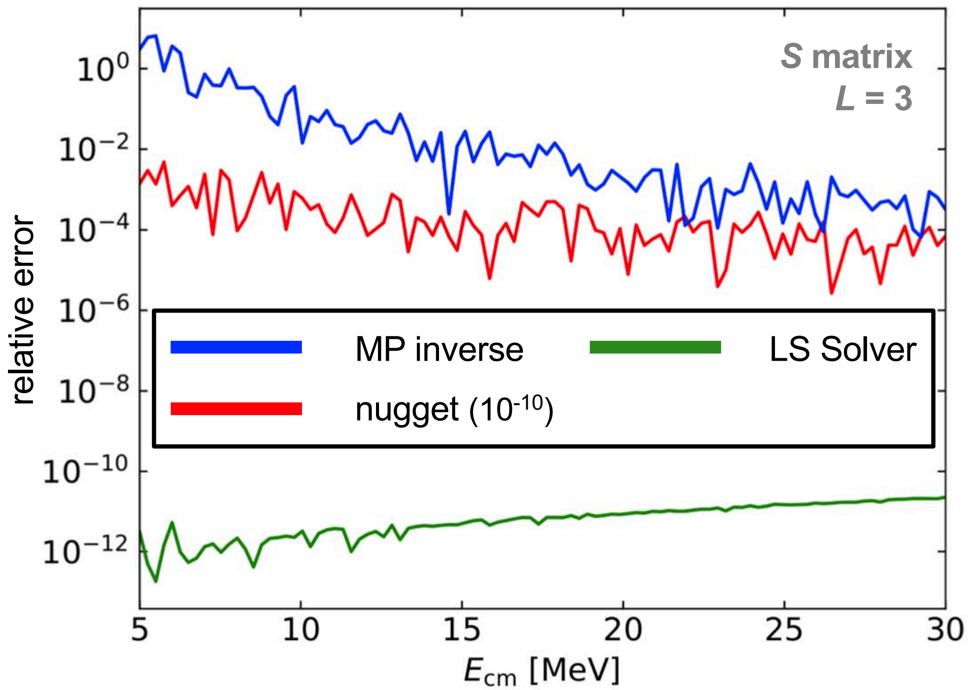
- nugget regularization
- Moore-Penrose inverse

***S* matrix especially prone to noise, whereas the *T* matrix is more stable**

Simple yet robust: find *stationary point* numerically (*e.g.*, using an LS solver)

$$\begin{pmatrix} \Delta\tilde{U} & 1 \\ \mathbf{1}^T & 0 \end{pmatrix} \begin{pmatrix} \boldsymbol{c} \\ \lambda \end{pmatrix} = \begin{pmatrix} \boldsymbol{L} \\ 1 \end{pmatrix}$$

inverse-free, if possible



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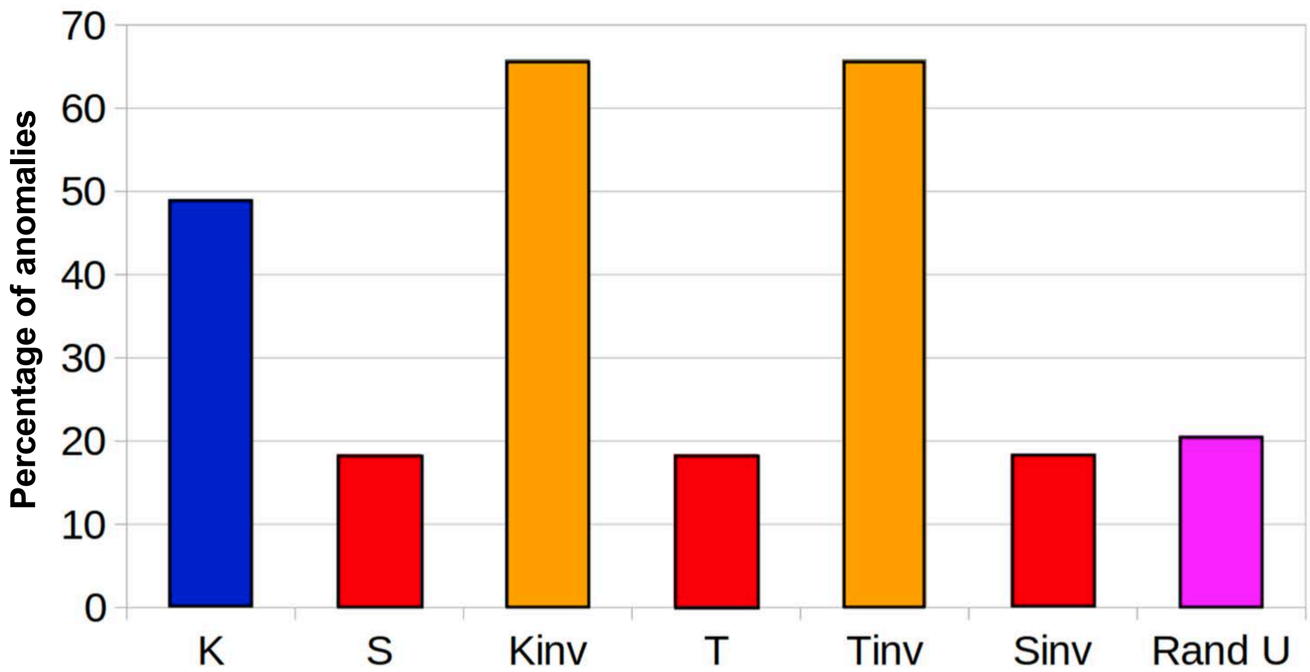
Abundance of Kohn anomalies

Which KVP performs best in terms of reducing *Kohn anomalies*?

But be careful: this depends on the interaction, channel, …



15 random matrices with a wide range in |det(u)|

L = 0 | A = 40 | E = 5-20 MeV
Woods-Saxon potential
5 training points

sample size: 500

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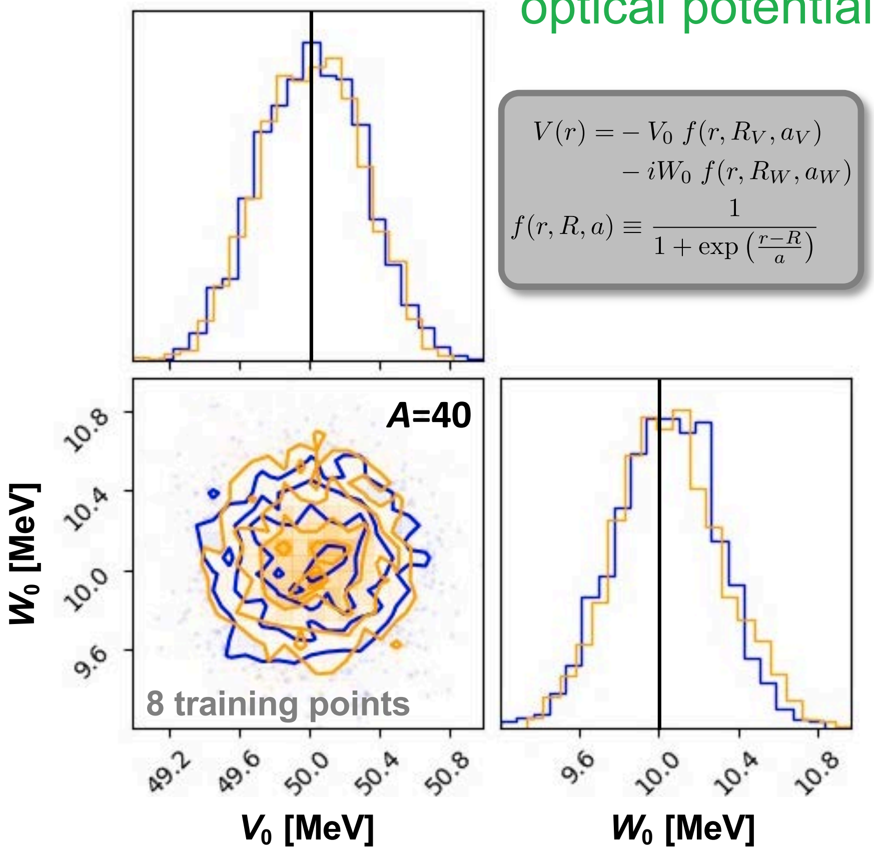
Proof of principle: MCMC sampling

CD, Giuliani, Quinonez *et al.*, in prep.

Possible application:
Bayesian model comparison for optical potentials

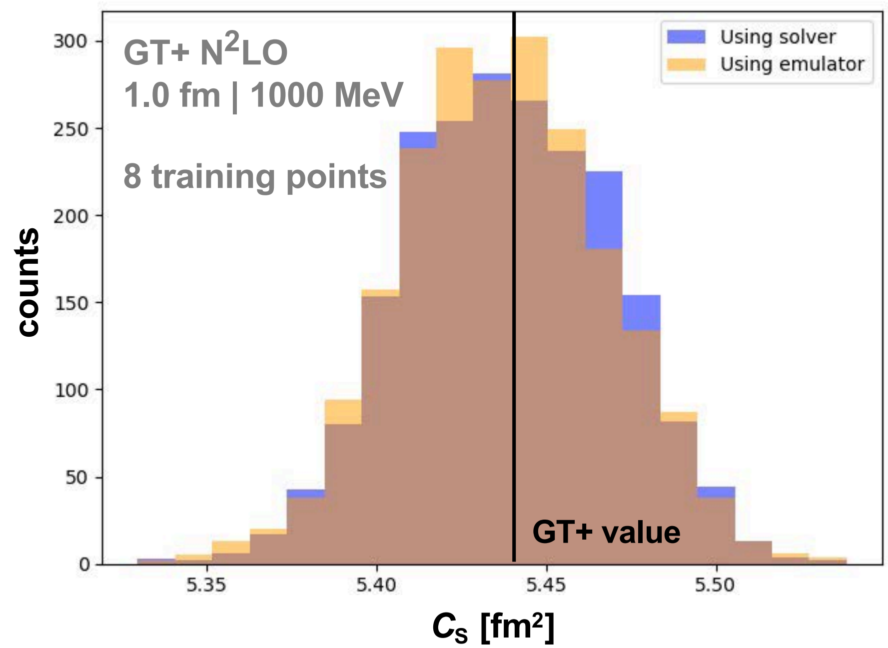
$$V(r) = -V_0\, f(r, R_V, a_V) - iW_0\, f(r, R_W, a_W)$$

$$f(r, R, a) \equiv \frac{1}{1+\exp\left(\frac{r-R}{a}\right)}$$



Optical potential

Local chiral potential



Gezerlis, Tews *et al.*, PRC **90**, 054323

Possible application:
parameter estimation for constructing next-generation (local) chiral interactions

Buchner (“UltraNest”), arXiv:2101.09604
needs coupled channels; Kamimura, PTPS **62**, 236

Eigenvector Continuation for scattering with local chiral NN and optical potentials

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Christian Drischler

April 26, 2021 | INT 21-1b: Nuclear Forces for Precision Nuclear Physics

This week's topic:
Improving nuclear forces with *novel fitting strategies* and higher orders in chiral EFT

1. using EC as an efficient emulator for scattering with local chiral interactions and optical potentials

2. statistical quantification and propagation of EFT truncation errors in nuclear matter calculations

Keywords:

+ ChEFT + scattering
+ Variational principles
+ Eigenvector Continuation
+ Bayesian UQ
+ infinite nuclear matter
+ N^3LO NN + 3N forces
+ …

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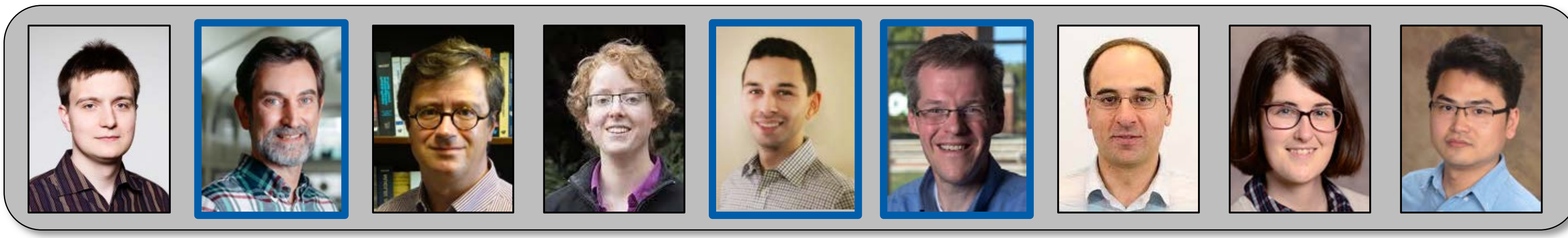
New framework for UQ of the infinite-matter EOS

buqeye.github.io

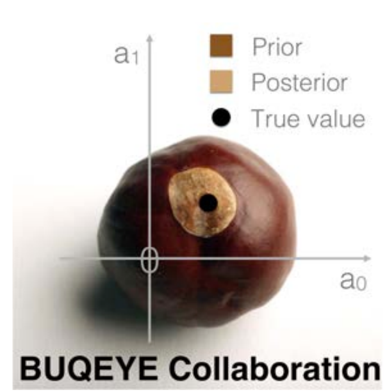


CD, Furnstahl, Melendez, and Phillips

How well do we know the neutron-matter equation of state at the densities inside neutron stars? A Bayesian approach with correlated uncertainties, PRL **125**, 202702

CD, Melendez, Furnstahl, and Phillips

Effective Field Theory Convergence Pattern of Infinite Nuclear Matter, PRC **102**, 054315



Bayesian
Uncertainty
Quantification:
Errors for
Your
EFT

UQ framework available at https://buqeye.github.io

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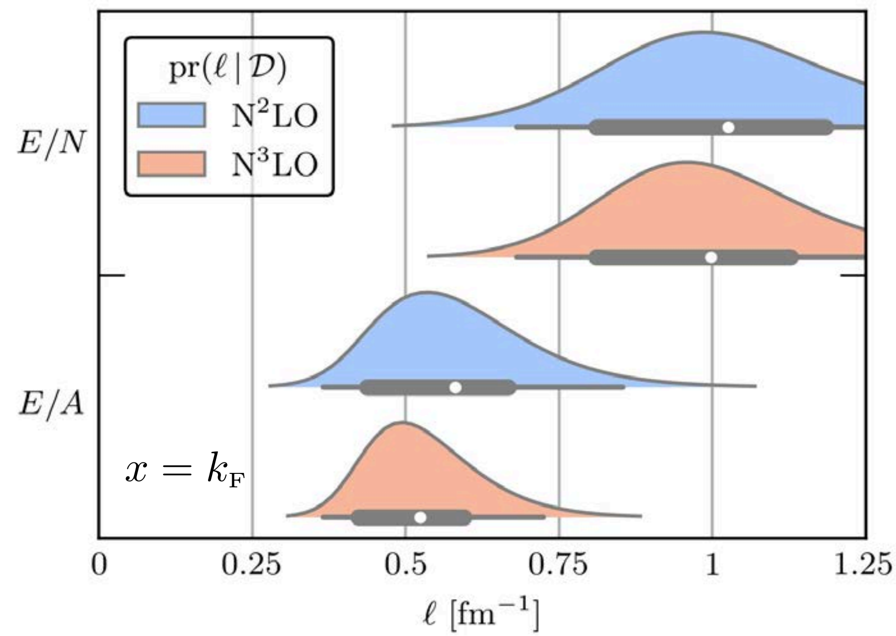
Propagating type-x uncertainties

CD, Melendez *et al.*, PRC **102**, 054315

How correlated is nuclear matter ?

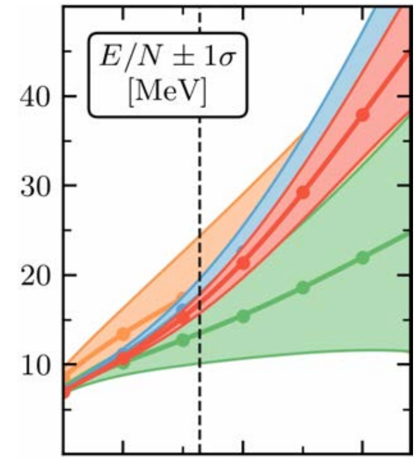
$\mathrm{pr}\,(\ell\,|\,\mathcal{D})$
correlation length



to be compared with

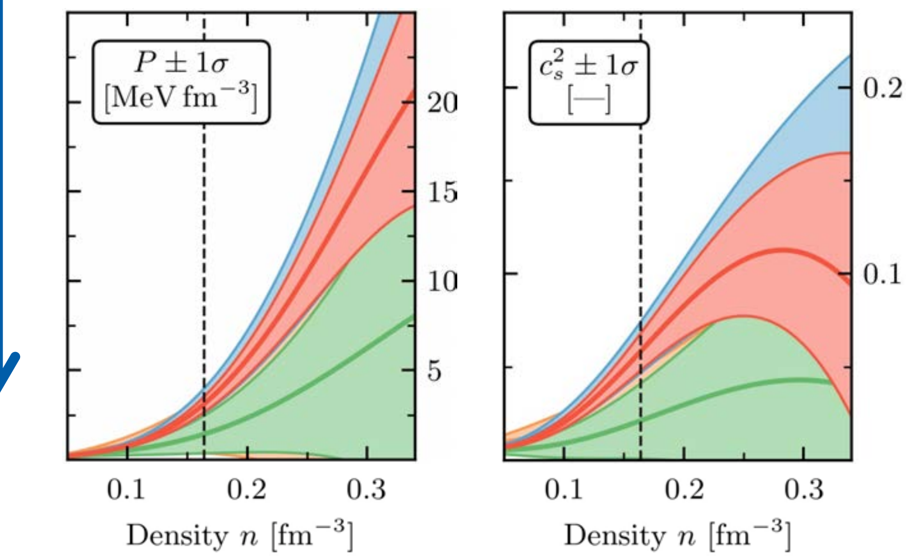
$$k_{\mathrm{F}}^{\mathrm{max}} = \begin{cases} 2.2\,\mathrm{fm}^{-1} & \mathrm{PNM} \\ 1.7\,\mathrm{fm}^{-1} & \mathrm{SNM} \end{cases}$$

derivative(s)



regression

consistent **propagation** of theoretical uncertainties to **derived quantities**



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Bayesian inference

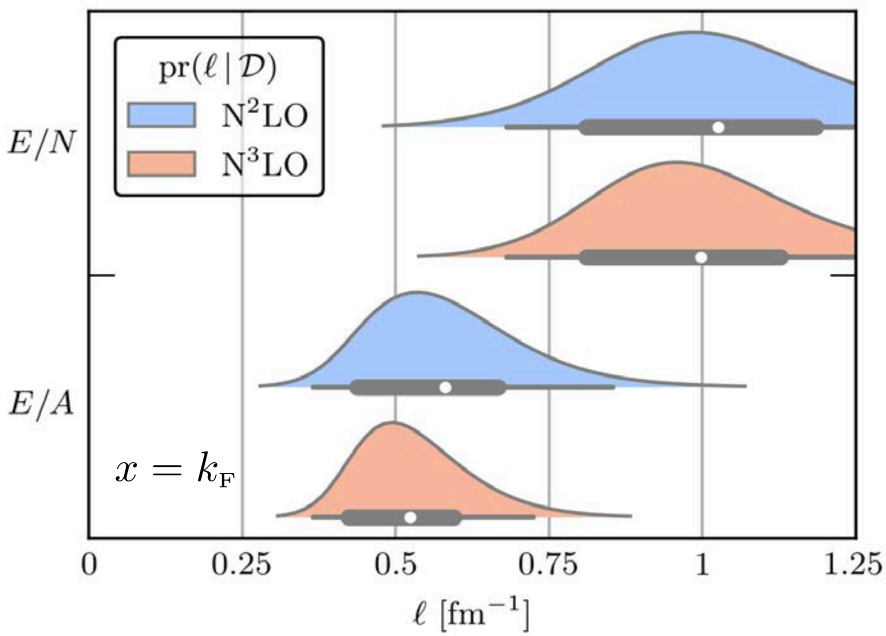
CD, Melendez *et al.*, PRC **102**, 054315

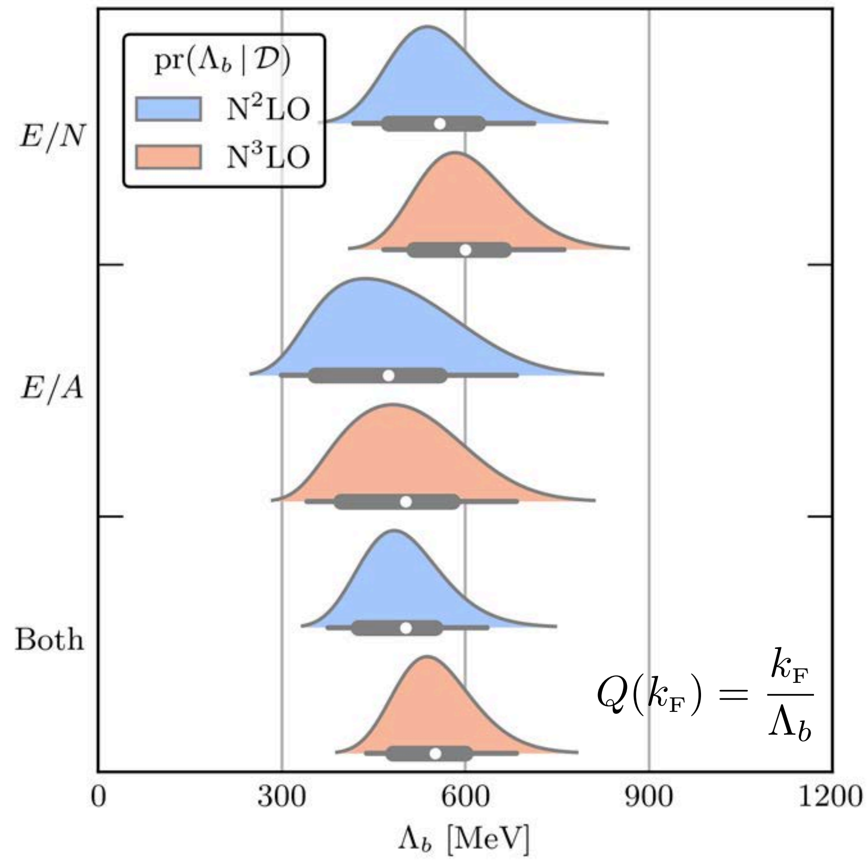
How correlated is nuclear matter ?

$\mathrm{pr}\,(\ell \,|\, \mathcal{D})$
correlation length

Where does the EFT break down ?

$\mathrm{pr}\,(\Lambda_b \,|\, \mathcal{D})$
breakdown scale





to be compared with

$$k_{\mathrm{F}}^{\max} = \begin{cases} 2.2\,\mathrm{fm}^{-1} & \text{PNM} \\ 1.7\,\mathrm{fm}^{-1} & \text{SNM} \end{cases}$$

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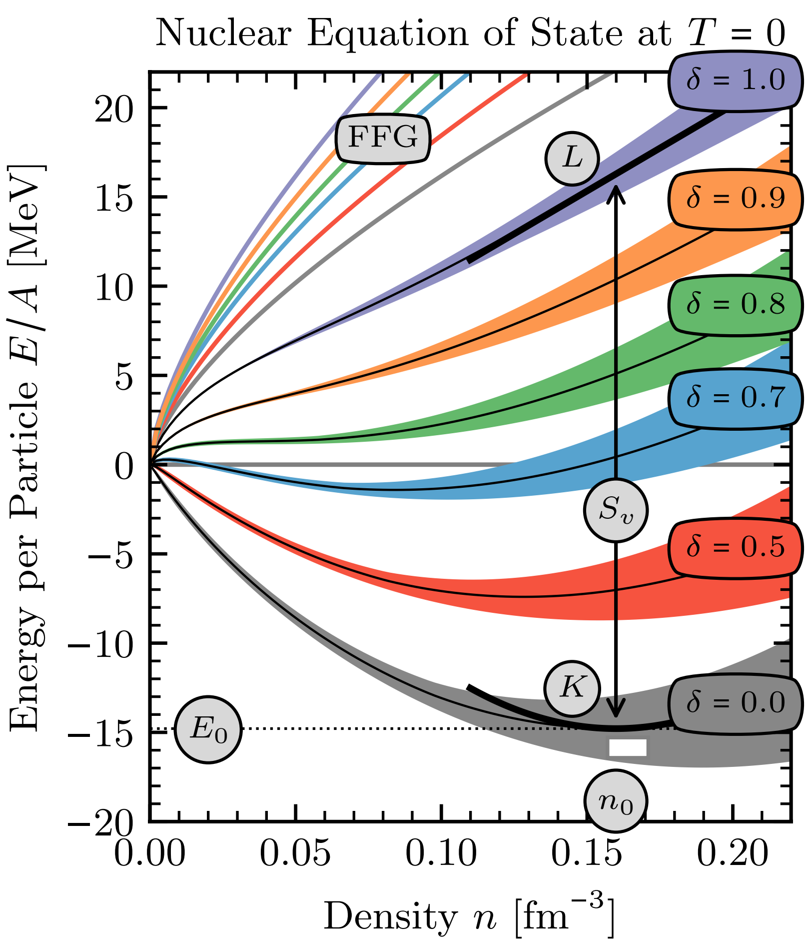
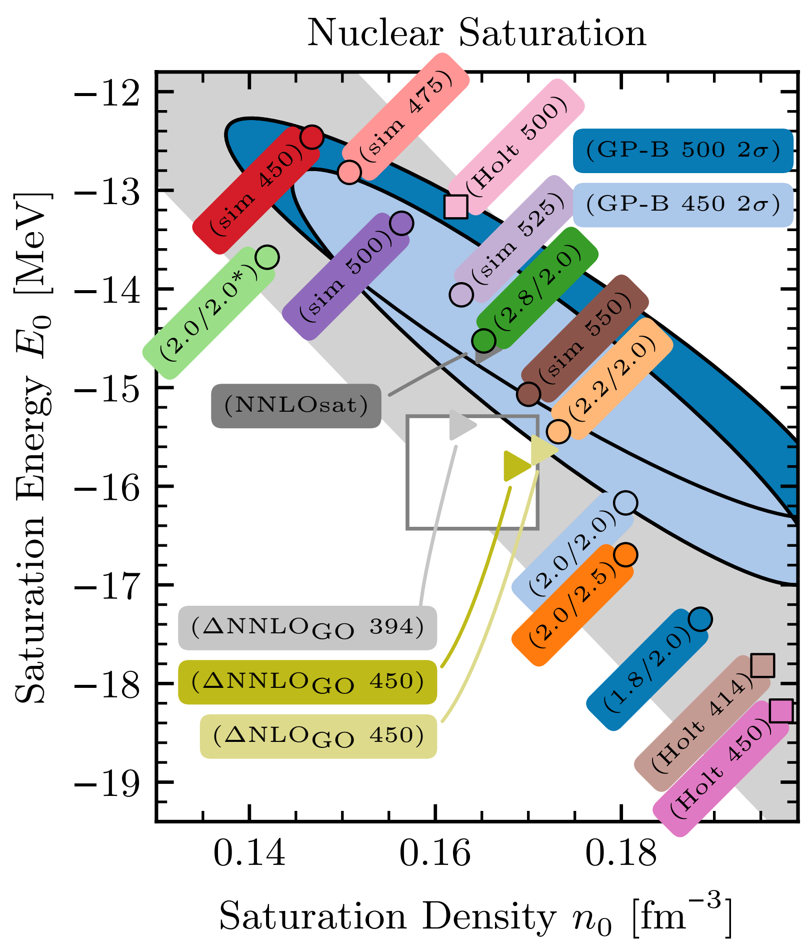
Parameters of the low-density EOS

CD, Holt, and Wellenhofer, arXiv:2101.01709





FFG: free Fermi gas; $\boldsymbol{\delta} = (n_n - n_p)/n$: isospin asymmetry

Annotations: **(λ / Λ$_{3N}$)** in fm^{-1} or **(Λ)** in MeV

for nuclear saturation, see also Atkinson *et al.*, PRC **102**, 044333; Dewulf *et al*, PRL **90**, 152501

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Summary

buqeye.github.io

1 Presented an efficient emulator using EC and complex KVP

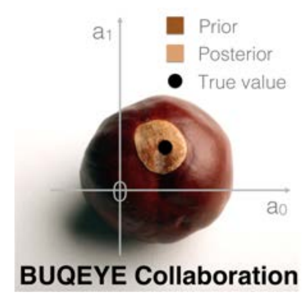
- with local chiral nucleon-nucleon interactions and optical potentials
- KVPs for the *T* matrix and *S* matrix can reproduce well phase shifts and cross sections
- EC is efficient in providing trial wave functions for interpolation and extrapolation

2 Studied diagnostic tools for Kohn anomalies

- Kohn anomalies can be encountered in variational calculations
- Consistency checks and variable basis sizes are key to Bayesian UQ
- An improved method for finding stationary points reduces numerical noise substantially

3 Set a new standard for UQ in infinite-matter calculations

- Need for *statistically* robust comparisons between theory, observation, and experiment
- Correlations within *and* between observables are crucial for reliable UQ
- Efficiently quantify and propagate EOS uncertainties to derived quantities



Thanks to my collaborators:

P. Giuliani **A. Lovell** F. Nunes **M. Quinonez**
R. Furnstahl **J. Melendez** **K. McElvain** D. Phillips

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Some topics for the discussion session

Convergence of Eigenvector Continuation

Avik Sarkar & Dean Lee, PRL **126**, 032501 | Can scattering provide general insights?

Extension to three-body scattering with EC

See Xilin Zhang's talk on Wednesday

Improved variational principles: insights from pre-EC era?

e.g., Viviani, Kievsky, and Rosati, FBS **30**, 3 and Zhang *et al.*, JChP **88**, 6233

Improving nuclear forces with novel fitting strategies

How would the workflow look like in practice?