Emulators for Uncertainty Propagation: From Nuclear Forces to Many-Body Physics

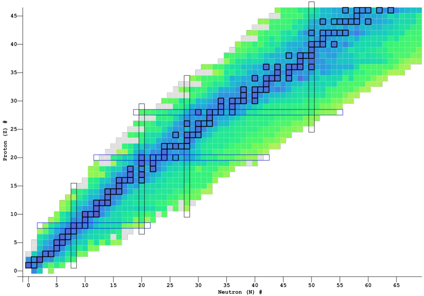
Ryan Curry

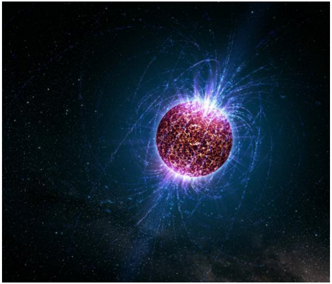
University of Guelph

2026-02-25

2026 Workshop on Progress in Ab Initio Nuclear Theory

From nuclear structure to neutron stars





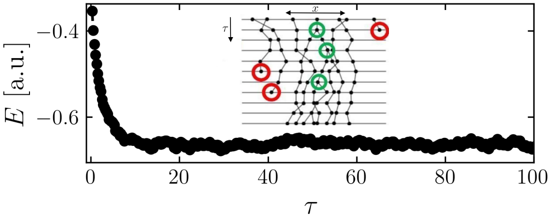
We want to describe diverse nuclear systems from first principles

Diffusion Monte Carlo

Solve Schrödinger equation in imaginary time $$-\frac{\partial}{\partial\tau}\Psi = \left(-\frac{\hbar}{2m}\nabla^2 + V\right)$$

$$\psi(\tau) = e^{-(H-E_T)\tau}\psi_T$$

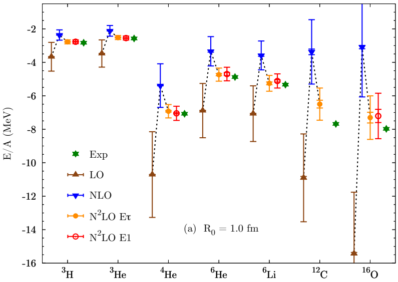
- Projects out the ground-state energy

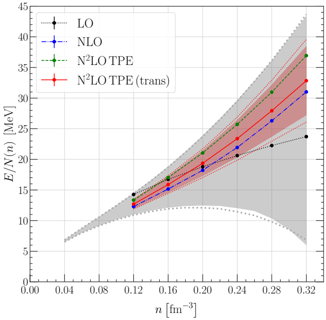


- Can straightforwardly handle high-cutoff / hard-core interactions
- Works well for central interactions $e^{-\sum_{i<j} v(\boldsymbol{r}_{ij})\tau}$
- Care needed for spin/isospin dependent interactions (chiral EFT)

Auxiliary Field Diffusion Monte Carlo

- Instead of summing over possible spin-isospin states (GFMC), we sample them with Hubbard-Stratonovich transformations
- Trade off in precision due to sampling auxiliary fields
- Extend calculations to $A \leq 18$ as well as dense matter





D. Lonardoni, S. Gandolfi, J.E. Lynn, *et. al*, Phys. Rev. C. **97**, 044318 (2018)

I. Tews, R. Somasundaram, *et. al*, Phys. Rev. Res. **7**, 033024 (2025)

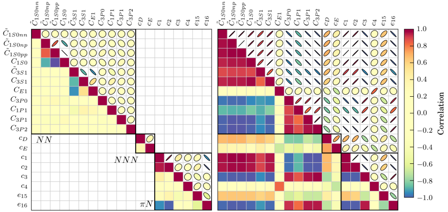
Uncertainty Quantification

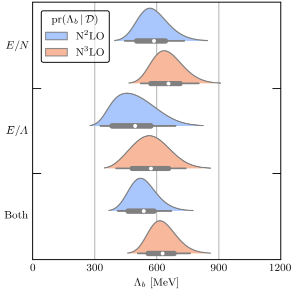
There are fundamental uncertainties that should be accounted for in a many-body calculation.

- Nuclear Interaction (Experimental / Theoretical)
  - Interactions are fit to experimental measurement (which come with some associated error)
  - Chiral EFT Hamiltonian must be truncated at a finite order

- Many-Body Methods (Computational / Theoretical)
  - Model space truncation (NCSM)
  - Fixed-node / constrained-path approximation (QMC methods)
  - Retaining only two-body operators (IMSRG(2), CCSD)

Lots of exciting work being done on UQ!





- Ongoing UQ programs from BUQEYE, BAND, Chalmers, and many more
- Chiral EFT interactions, nuclei across the nuclear chart, infinite matter, hypernuclei, and more
- Many talks and posters this week!

B.D. Carlsson, A. Ekstrom, C. Forssen, *et. al*, Phys. Rev. X. **1**, 011019 (2016)
C. Drischler, J.A. Melendez, R.J. Furnstahl, and D.R. Phillips, Phys. Rev. C. **102**, 5, 054315 (2020)

Uncertainty Propagated Quantum Monte Carlo

- Train emulators on exact few-body calculations
- Bayesian inference fit of all 2N and 3N LECs at N^2LO
- Propagate relevant uncertainties to many-body predictions

Quantum Monte Carlo Calculations of Light Nuclei with Fully Propagated Theoretical Uncertainties

Ryan Curry,[1,2] Kai Hebeler,[3,4,5] Stefano Gandolfi,[2] Alexandros Gezerlis,[1]
Achim Schwenk,[3,4,5] Rahul Somasundaram,[2] and Ingo Tews[2]

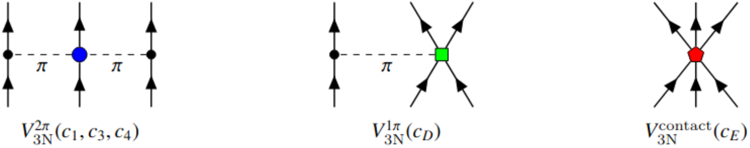
[1] *Department of Physics, University of Guelph, Guelph, Ontario N1G 2W1, Canada*
[2] *Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*
[3] *Technische Universität Darmstadt, Department of Physics, 64289 Darmstadt, Germany*
[4] *ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung GmbH, 64291 Darmstadt, Germany*
[5] *Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany*

We report on the first quantum Monte Carlo calculations of helium isotopes with fully propagated theoretical uncertainties from the interaction to the many-body observables. To achieve this, we build emulators for solutions to the Faddeev equations for the binding energy and Gamow-Teller matrix element of ^{3}H, as well as for auxiliary-field diffusion Monte Carlo calculations of the ^{4}He charge radius, employing local two- and three-body interactions up to next-to-next-to-leading order in chiral effective field theory. We use these emulators to determine the posterior distributions for all low-energy couplings that appear in the interaction up to this order using Bayesian inference while accounting for theoretical uncertainties. We then build emulators for auxiliary-field diffusion Monte Carlo for helium isotopes and propagate the full posterior distributions to these systems. Our approach serves as a framework for *ab initio* studies of atomic nuclei with consistently treated and correlated theoretical uncertainties.

arxiv:2510.015860

Fitting chiral EFT interactions

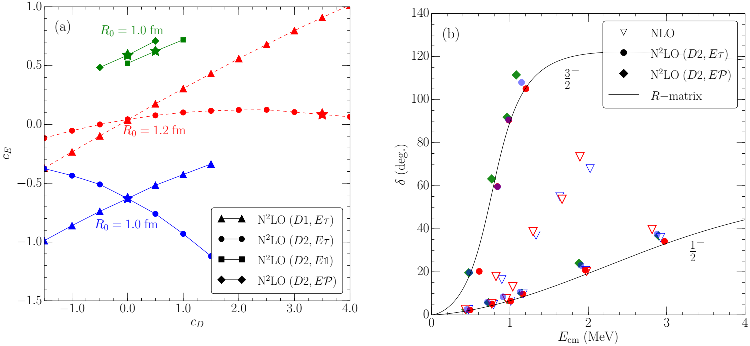
- 9 two-body LECS (C_S, C_T, C_{1-7}) up to N^{2}LO fit against experimental phase shift data
- Long-range 3N couplings c_1, c_3, and c_4 are constrained by πN scattering data.
- Short-range 3N couplings c_D and c_E need to be constrained by few-body observables.



K. Hebeler, Phys. Rep. **890**, 1-116 (2021)

Previously

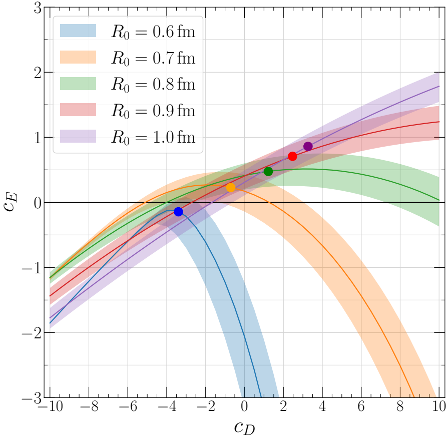
- c_D and c_E fit to GFMC binding energy of ^{4}He and n-α p-wave phase shifts
- Using a least-squares minimization approach



J.E. Lynn, I. Tews, A. Gezerlis, K.E. Schmidt, A. Schwenk, Phys. Rev. Lett. **116** 062501 (2016)

More recently...

- Fit against Faddeev calculations
- ^{3}H binding energy and β-decay (similar to Gazit *et. al* 2009)
- These calculations don't mix well with Bayesian inference.
- A single Faddeev calculation takes $\sim$ 1 hour
- Bayesian inference requires 10^5-10^6 evaluations



I. Tews, R. Somasundaram, *et. al*, Phys. Rev. Res. **7**, 033024 (2025)

A Tale of Two Emulators

Algorithm that mimics the behavior of a high-fidelity calculation for a fraction of the computational cost.

- In our case:
  - High fidelity means *ab initio* few-body calculation
  - Computational cost $\sim 10^3$s (Faddeev) or 10^6s (AFDMC)

- The goal:
  - Eigenvector Continuation (EC)
  - Parametric Matrix Model (PMM)
  - Dramatic reduction in computational cost

D. Frame, R. He, I. Ipsen, D. Lee, D. Lee, and E. Rrapaj Phys. Rev. Lett. **121**, 032501 (2018)

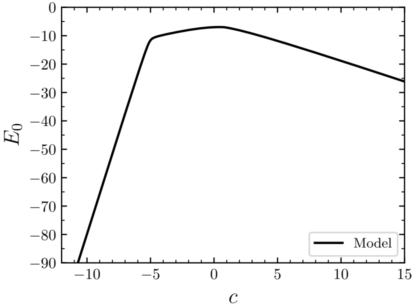
P. Cook, D. Jammooa, M. Hjorth-Jensen, D. Lee, and D. Lee, Nat. Commun. **16**, 5929 (2025)

An example...

Consider a "high-fidelity model" with a single control parameter c

$$H = H^0 + cH^1 \tag{1}$$

We can solve for the lowest eigenvalue of H for any value of c
(but let's pretend it's very expensive)

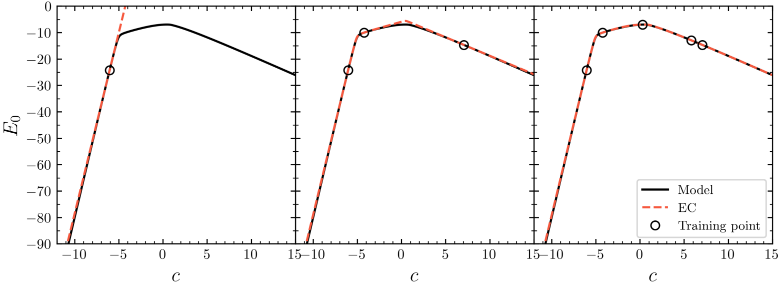


Eigenvector Continuation

- Projects the Hamiltonian to a subspace where its ground state can be rapidly evaluated
- For two training points c_1 and c_2, with eigenvectors $|\psi_1\rangle$ and $|\psi_2\rangle$

$$M = \begin{bmatrix} \langle\psi_1|H^0|\psi_1\rangle & \langle\psi_1|H^0|\psi_2\rangle \\ \langle\psi_2|H^0|\psi_1\rangle & \langle\psi_2|H^0|\psi_2\rangle \end{bmatrix} + c \begin{bmatrix} \langle\psi_1|H^1|\psi_1\rangle & \langle\psi_1|H^1|\psi_2\rangle \\ \langle\psi_2|H^1|\psi_1\rangle & \langle\psi_2|H^1|\psi_2\rangle \end{bmatrix}$$

- Solve for smallest eigenvalue in the projected subspace for all values of the control parameter



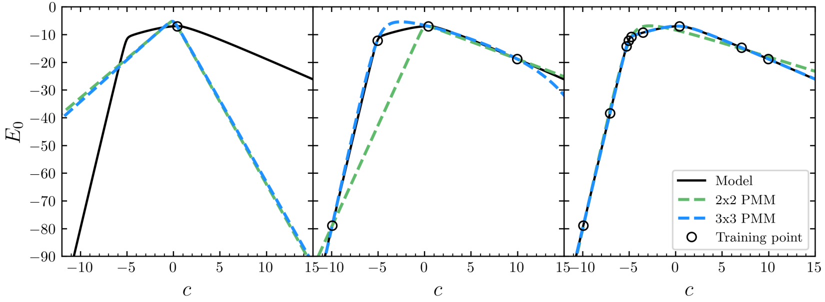
- Exact eigenstate requirement very tricky for AFDMC

Parametric Matrix Model

- Instead of explicit overlaps, fit matrix elements by minimizing cost function
- Dimensionality of PMM matrices is a free hyperparameter
- Can train against any number of training points

$$\tilde{H} = \begin{bmatrix} x_1 & 0 \\ 0 & x_2 \end{bmatrix} + c \begin{bmatrix} x_3 & x_4 \\ x_4 & x_5 \end{bmatrix}$$

- Does not require any knowledge about exact eigenstates of the high-fidelity model (i.e. can be straightforwardly used for QMC)

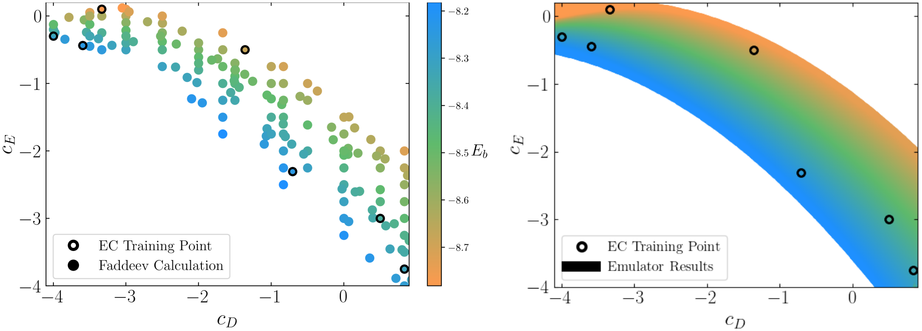


Emulating Solutions to the Faddeev Equations

$$H = T + V_{NN} + V_{3N}^{TPE} + V_{3N}^{D} + V_{3N}^{E}$$

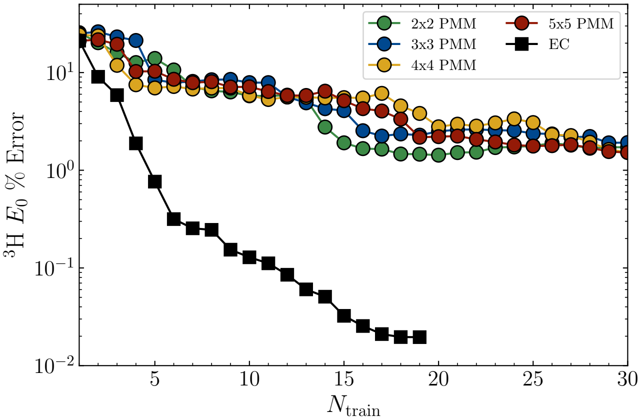
$$\tilde{H} = H^0 + C_S H^S + C_T H^T + \sum_{i=1}^{7} C_i H^i + c_D H^D + c_E H^E$$

- High-cutoff interaction $R_0 = 0.6$ fm or $\Lambda_c \approx 660$ MeV
- Faddeev equations give exact solution for three-body wavefunction
- Solve for E_0 of ^{3}H for ~ 100 LEC sets (c_D/c_E shown for example)



Parametric Matrix Model vs Eigenvector Continuation

- Study how % error decreases with number of training points
- Additional computational overhead for eigenvector continuation (*seemingly* worth the effort)



R. Curry, K. Hebeler, S. Gandolfi, A. Gezerlis, A. Schwenk, R. Somasundaram, and I. Tews arXiv:2510.15860

Bayesian Inference

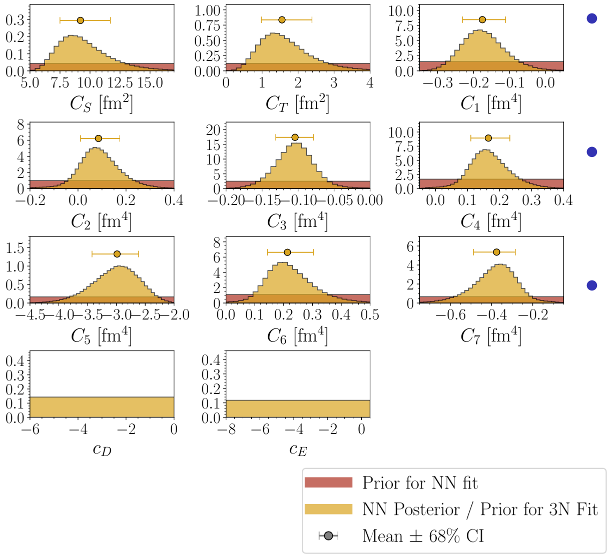
$$\mathcal{L} \propto \prod_i \exp\left[-\frac{1}{2}\left(\frac{X_i^{\text{exp.}} - X_i^{\text{theo.}}}{\sigma_i}\right)^2\right]$$

- X_i includes ^{3}H binding energy, GT matrix element (Faddeev) and ^{4}He charge radius (AFDMC)
- $\sigma_i^2 = \sigma_{i,\text{exp}}^2 + \sigma_{i,\text{theo}}^2$
- Theoretical uncertainty $\sigma_{i,\text{theo}} = \Delta X_i$, estimated by performing calculations at lower chiral orders

$$\Delta X_{\text{N}^2\text{LO}}^{\text{EKM}} = \max\left[Q^4|X_{\text{LO}}|, \quad Q^2|X_{\text{LO}} - X_{\text{NLO}}|, \quad Q|X_{\text{NLO}} - X_{\text{N}^2\text{LO}}|\right]$$

R. Curry, K. Hebeler, S. Gandolfi, A. Gezerlis, A. Schwenk, R. Somasundaram, and I. Tews
arXiv:2510.15860

Determining full N^2LO LEC Posteriors

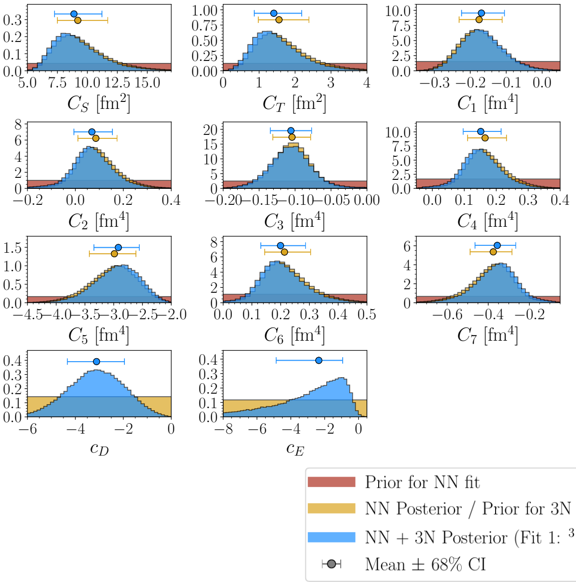


- Somasundaram *et. al* performed NN Bayesian fit at N^2LO
- We take their posteriors as our priors for the NN LECs
- Include additional uniform priors on c_D and c_E

R. Somasundaram, J.E. Lynn, L. Huth, A. Schwenk, and I. Tews, Phys. Rev. C. **109**, 034005 (2024)

R. Curry, K. Hebeler, S. Gandolfi, A. Gezerlis, A. Schwenk, R. Somasundaram, and I. Tews arXiv:2510.15860

Bayesian Fit Against ^{3}H



- N^2LO posteriors when fit only against triton observables
- Likelihood factorizes, making this a global fit
- Very slight changes in NN LECs (strong dependence on prior)
- Long tail on c_E distribution

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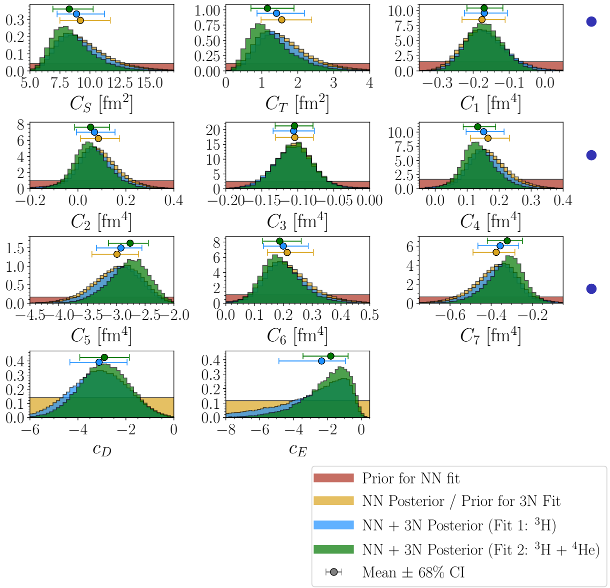
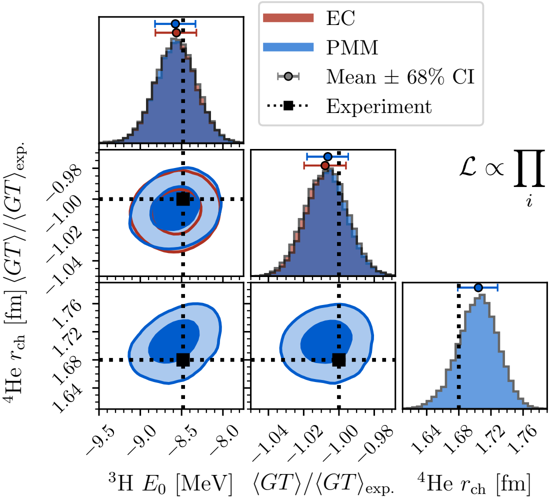
Additional ^{4}He Constraint



- AFDMC ^{4}He charge radius added to reduce long tail in c_E
- All NN LECs are also narrower due to its inclusion
- With LEC posteriors in hand, we can use them for many-body calculations

R. Curry, K. Hebeler, S. Gandolfi, A. Gezerlis, A. Schwenk, R. Somasundaram, and I. Tews
arXiv:2510.15860

Posterior Predictions: PMM vs EC



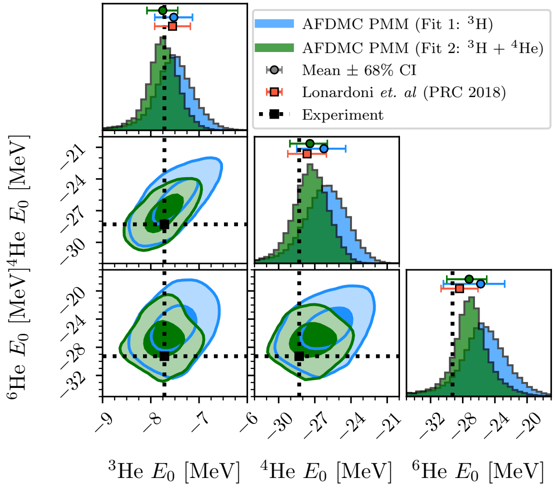
$$\mathcal{L} \propto \prod_i \exp\left[-\frac{1}{2}\left(\frac{X_i^{\rm exp.} - X_i^{\rm theo.}}{\sigma_i}\right)^2\right]$$

- PMM ≡ minimizing cost function
- EC ≡ explicit overlap calculations

- PMM/EC give essentially identical results when used in likelihood

R. Curry, K. Hebeler, S. Gandolfi, A. Gezerlis, A. Schwenk, R. Somasundaram, and I. Tews arXiv:2510.15860

AFDMC calculations of helium isotopes



- Evaluate AFDMC emulators over 2.5×10^5 LEC samples
- Full posterior predictions for helium isotope binding energies
- Uncertainties propagated to many-body predictions
- Able to study correlations between different nuclei with QMC

R. Curry, K. Hebeler, S. Gandolfi, A. Gezerlis, A. Schwenk, R. Somasundaram, and I. Tews, arXiv:2510.15860

Summary & Future Directions

- First Bayesian fit of local high-cutoff chiral EFT interactions containing all two- and three-nucleon operators at N^2LO
- Emulators employed at every step of the calculation (fitting the interaction $\rightarrow$ final many-body predictions)
- Opportunity to explore other fitting observables
- Framework for future Quantum Monte Carlo studies of more light- and medium-mass nuclei with fully propagated theoretical uncertainties

Thank you for listening!

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INNOVATION Canada Foundation for Innovation Fondation canadienne pour l'innovation

Collaborators:

- **Alex Gezerlis** (Guelph)
- **Ingo Tews** (LANL)
- **Stefano Gandolfi** (LANL)
- **Rahul Somasundaram** (LANL)
- **Achim Schwenk** (TUD)
- **Kai Hebeler** (TUD)