QMC and Chiral EFT: Uncertainty Quantification and Perturbation Theory

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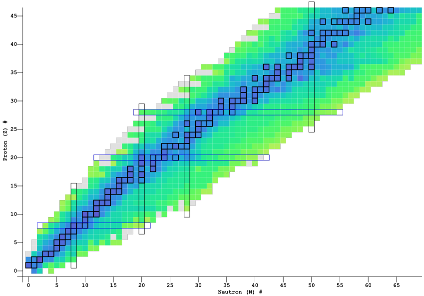
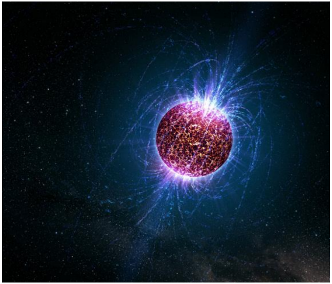
2026-05-18

Nuclear Hamiltonians for Advancing Nuclear Physics and Beyond
INT, Seattle, WA

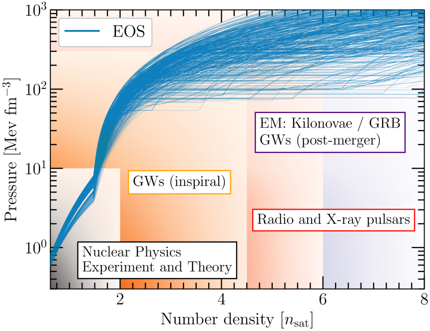
From nuclear structure to neutron stars





We want to describe diverse nuclear systems from first principles

The Multi-Messenger Era



P.T.H. Pang, *et. al*
Nature Communications **14**, 8352 (2023)

- Terrestrial experiments
  - Neutron skin thickness
  - Heavy ion collisions
- Astrophysical measurements
  - Gravitational Waves
  - NICER
  - Heavy pulsars
- Nuclear Theory Calculations

- Studies analyzing these events require input from nuclear theory
- We should do everything we can to quantify and reduce our theoretical uncertainties

Solving the Nuclear Many-Body Problem

Accurate description of the nuclear interaction + **Powerful computational approaches**

- Effective range expansion
- Fit to experimental data
  - Argonne V18 & similar
- EFT related to underlying theory (QCD)
  - Pionless
  - Chiral (Δ-less or -full)
  - Halo

- Hartree Fock (& extensions)
- BCS Theory
- Nuclear Shell Model
- Energy Density Functionals

- No-Core Shell Model
- Quantum Monte Carlo
- Many-Body Perturbation Theory
- Coupled Cluster
- In-Medium Similarity Renormalization Group
- Self-Consistent Green's Functions

What's the plan?

QMC requires local interactions, but at N^3LO this is impossible.

Can we include nonlocal operators perturbatively in our many-body calculations?

R. Curry, J.E. Lynn, K.E. Schmidt and A. Gezerlis, Phys. Rev. Res., **5**, (2023)

R. Curry, R. Somasundaram, S. Gandolfi, A. Gezerlis, and I. Tews, Phys. Rev. C, **111**, 015801 (2025)

There are fundamental uncertainties in our description of the nuclear interaction.

What is the best way to properly account for these in our many-body calculations?

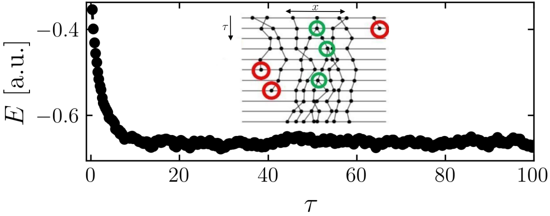
R. Curry, K. Hebeler, S. Gandolfi, A. Gezerlis, A. Schwenk, R. Somasundaram, and I. Tews, arXiv:2510.15860

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)

Green's Function Monte Carlo

How do we handle a propagator with spin/isospin degrees of freedom?

$$e^{-\sum_{i<j}[v_1(\boldsymbol{r}_{ij})\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2+v_2(\boldsymbol{r}_{ij})\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2+\ldots]\tau}$$

- Explicitly sum over all spin/isospin states

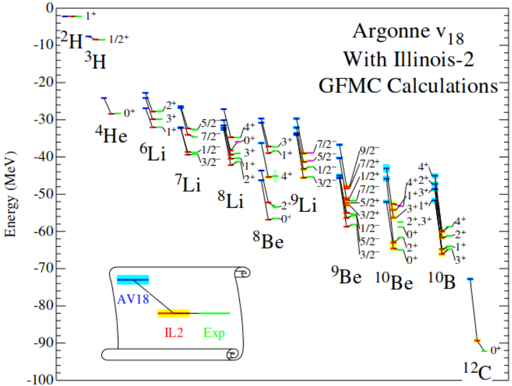
$$|\Phi\rangle = \begin{pmatrix} a_{\uparrow\uparrow\uparrow} \\ a_{\uparrow\uparrow\downarrow} \\ a_{\uparrow\downarrow\uparrow} \\ a_{\uparrow\downarrow\downarrow} \\ a_{\downarrow\uparrow\uparrow} \\ a_{\downarrow\uparrow\downarrow} \\ a_{\downarrow\downarrow\uparrow} \\ a_{\downarrow\downarrow\downarrow} \end{pmatrix} \qquad \boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\,|\Phi\rangle = \begin{pmatrix} a_{\uparrow\uparrow\uparrow} \\ a_{\uparrow\uparrow\downarrow} \\ 2a_{\downarrow\uparrow\uparrow} - a_{\uparrow\downarrow\uparrow} \\ 2a_{\downarrow\uparrow\downarrow} - a_{\uparrow\downarrow\downarrow} \\ 2a_{\uparrow\downarrow\uparrow} - a_{\downarrow\uparrow\uparrow} \\ 2a_{\uparrow\downarrow\downarrow} - a_{\downarrow\uparrow\downarrow} \\ a_{\downarrow\downarrow\uparrow} \\ a_{\downarrow\downarrow\downarrow} \end{pmatrix}$$

- Each of the $2^A \frac{A!}{Z!(A-Z)!}$ spin-isospin states must be propagated
- Limiting GFMC to $A \leq 12$

J. Carlson, Phys. Rev. C **36**, 2026, (1987)

Green's Function Monte Carlo

- GFMC is an exact calculation, limited to $A \leq 12$



S. Pieper, R.B. Wiringa,
Annu. Rev. Nucl. Part. Sci. **51** (2001)

- Used to study electroweak sector,
  G.B. King and S. Pastore, Annu. Rev. Nucl. Part. Sci. **74** (2024)
- Few-body nuclear reactions
  J.E. Lynn, I. Tews, J. Carlson, *et. al*, Phys. Rev. Lett., **116** (2016)
- Precision tests of standard model
  G.B. King, J. Carlson, A.R. Flores, *et. al*, arXiv:2509.07310

Auxiliary Field Diffusion Monte Carlo

- Instead of summing over all spin-isospin states, we can sample them
- Particles can be described by single-nucleon spinors

$$|S_i\rangle = a_i\,|p\uparrow\rangle + b_i\,|p\downarrow\rangle + c_i\,|n\uparrow\rangle + d_i\,|n\downarrow\rangle$$

- Linearize quadratic spin/isospin ($\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2, etc$) dependence through Hubbard-Stratonovich transformation

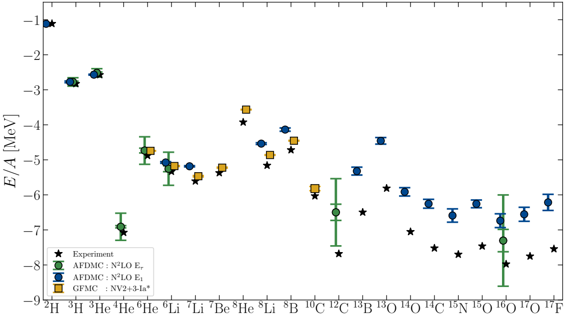
$$e^{-\frac{1}{2}\lambda O^2} = \frac{1}{\sqrt{2\pi}} \int dx\, e^{-\frac{x^2}{2}+\sqrt{-\lambda}xO}$$

- We have traded two body $\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$ type interactions for single particles interacting with external auxiliary fields x

K.E. Schmidt and S. Fantoni, Phys. Lett. B **446** (1999)

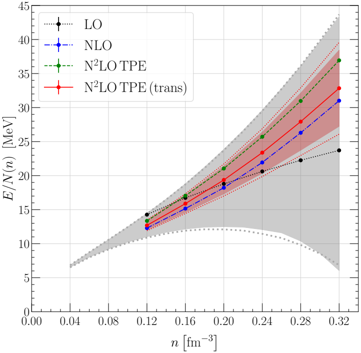
Auxiliary Field Diffusion Monte Carlo

- Trade off in precision due to sampling auxiliary fields
- Extend calculations to $A \leq 17$ as well as dense matter



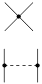
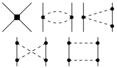
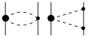
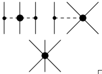
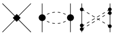
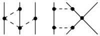
R. Curry, S. Gandolfi, A. Gezerlis, and I. Tews
PNPP, *in preparation.*

Results from D. Lonardoni, G.B. King, J. Martin



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

Chiral Effective Field Theory

	2N	3N	4N
LO $\nu = 0$	 2	—	—
NLO $\nu = 2$	 7	—	—
N^2LO $\nu = 3$	 $+ \cdots$ 0	 2	—
N^3LO $\nu = 4$	 $+ \cdots$ 12	 $+ \cdots$ 0	 $+ \cdots$ 0

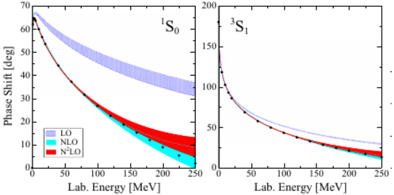
- Expansion in powers of Q/Λ_b
- Separation of scales quarks vs nucleons and pions
- Power counting
- Many-body forces emerge naturally
- Reduce uncertainty by going to higher chiral order

S. Weinberg, Phys. Lett. B, **251**, 288 (1990)

U. van Kolck, Phys. Rev. C, **49**, 2932 (1994)

E. Epelbaum, H.-W. Hammer, Ulf-G. Meissner, Rev. Mod. Phys. **81**, 1773 (2009)

- Use only half of the operators in calculation
- Recover the rest through anti-symmetrization



- $q \to r$ local
- $k \to \nabla$ nonlocal

$$V^{(0)} = \alpha_1 + \alpha_2 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + \alpha_3 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 + \alpha_4 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$$

$$\begin{aligned} V^{(2)}_{\text{cont}} = & \gamma_1 q^2 + \gamma_2 q^2 \boldsymbol{\sigma_1} \cdot \boldsymbol{\sigma_2} + \gamma_3 q^2 \boldsymbol{\tau_1} \cdot \boldsymbol{\tau_2} \\ & + \gamma_4 q^2 \boldsymbol{\sigma_1} \cdot \boldsymbol{\sigma_2} \boldsymbol{\tau_1} \cdot \boldsymbol{\tau_2} \\ & + \gamma_5 k^2 + \gamma_6 k^2 \boldsymbol{\sigma_1} \cdot \boldsymbol{\sigma_2} + \gamma_7 k^2 \boldsymbol{\tau_1} \cdot \boldsymbol{\tau_2} \\ & + \gamma_8 k^2 \boldsymbol{\sigma_1} \cdot \boldsymbol{\sigma_2} \boldsymbol{\tau_1} \cdot \boldsymbol{\tau_2} \\ & + \gamma_9 (\boldsymbol{\sigma_1} + \boldsymbol{\sigma_2})(\boldsymbol{q} \times \boldsymbol{k}) \\ & + \gamma_{10} (\boldsymbol{\sigma_1} + \boldsymbol{\sigma_2})(\boldsymbol{q} \times \boldsymbol{k}) \boldsymbol{\tau_1} \cdot \boldsymbol{\tau_2} \\ & + \gamma_{11} (\boldsymbol{\sigma_1} \cdot \boldsymbol{q})(\boldsymbol{\sigma_2} \cdot \boldsymbol{q}) \\ & + \gamma_{12} (\boldsymbol{\sigma_1} \cdot \boldsymbol{q})(\boldsymbol{\sigma_2} \cdot \boldsymbol{q}) \boldsymbol{\tau_1} \cdot \boldsymbol{\tau_2} \\ & + \gamma_{13} (\boldsymbol{\sigma_1} \cdot \boldsymbol{k})(\boldsymbol{\sigma_2} \cdot \boldsymbol{k}) \\ & + \gamma 14 (\boldsymbol{\sigma_1} \cdot \boldsymbol{k})(\boldsymbol{\sigma_2} \cdot \boldsymbol{k}) \boldsymbol{\tau_1} \cdot \boldsymbol{\tau_2} \end{aligned}$$

A. Gezerlis, I. Tews, E. Epelbaum, S. Gandolfi, K. Hebeler, A. Nogga, and A. Schwenk, Phys. Rev. Lett. **111** (2013)

Trouble on the horizon ...

- 30 new contact operators at N^{3}LO (reduce to 12: Fierz, UT)
- Nonlocal operators cannot be totally avoided

$$
\begin{aligned}
V^{(4)}_{\rm cont} = {} & \alpha_1\, \boldsymbol{q}^4 + \alpha_2\, \boldsymbol{q}^4 \boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 + \alpha_3\, \boldsymbol{q}^4 \boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 + \alpha_4\, \boldsymbol{q}^4 \boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 \boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 \\
& + \alpha_5\, \boldsymbol{k}^4 + \alpha_6\, \boldsymbol{k}^4 \boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 + \alpha_7\, \boldsymbol{k}^4 \boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 + \alpha_8\, \boldsymbol{k}^4 \boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 \boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 \\
& + \alpha_9\, \boldsymbol{q}^2\boldsymbol{k}^2 + \alpha_{10}\, \boldsymbol{q}^2\boldsymbol{k}^2 \boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 + \alpha_{11}\, \boldsymbol{q}^2\boldsymbol{k}^2 \boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 + \alpha_{12}\, \boldsymbol{q}^2\boldsymbol{k}^2 \boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 \boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 \\
& + \alpha_{13}\, (\boldsymbol{q}\times\boldsymbol{k})^2 + \alpha_{14}\, (\boldsymbol{q}\times\boldsymbol{k})^2 \boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 + \alpha_{15}\, (\boldsymbol{q}\times\boldsymbol{k})^2 \boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 + \alpha_{16}\, (\boldsymbol{q}\times\boldsymbol{k})^2 \boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 \boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 \\
& + \frac{i}{2}\alpha_{17}\, \boldsymbol{q}^2 (\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\cdot(\boldsymbol{q}\times\boldsymbol{k}) + \frac{i}{2}\alpha_{18}\, \boldsymbol{q}^2 (\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\cdot(\boldsymbol{q}\times\boldsymbol{k}) \boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 \\
& + \frac{i}{2}\alpha_{19}\, \boldsymbol{k}^2 (\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\cdot(\boldsymbol{q}\times\boldsymbol{k}) + \frac{i}{2}\alpha_{20}\, \boldsymbol{k}^2 (\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\cdot(\boldsymbol{q}\times\boldsymbol{k}) \boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 \\
& + \alpha_{21}\, \boldsymbol{q}^2\, \boldsymbol{\sigma}_1\cdot\boldsymbol{q}\, \boldsymbol{\sigma}_2\cdot\boldsymbol{q} + \alpha_{22}\, \boldsymbol{q}^2\, \boldsymbol{\sigma}_1\cdot\boldsymbol{q}\, \boldsymbol{\sigma}_2\cdot\boldsymbol{q}\, \boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 + \alpha_{23}\, \boldsymbol{k}^2\, \boldsymbol{\sigma}_1\cdot\boldsymbol{q}\, \boldsymbol{\sigma}_2\cdot\boldsymbol{q} \\
& + \alpha_{24}\, \boldsymbol{k}^2\, \boldsymbol{\sigma}_1\cdot\boldsymbol{q}\, \boldsymbol{\sigma}_2\cdot\boldsymbol{q}\, \boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 + \alpha_{25}\, \boldsymbol{q}^2\, \boldsymbol{\sigma}_1\cdot\boldsymbol{k}\, \boldsymbol{\sigma}_2\cdot\boldsymbol{k} + \alpha_{26}\, \boldsymbol{q}^2\, \boldsymbol{\sigma}_1\cdot\boldsymbol{k}\, \boldsymbol{\sigma}_2\cdot\boldsymbol{k}\, \boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 \\
& + +\alpha_{27}\, \boldsymbol{k}^2\, \boldsymbol{\sigma}_1\cdot\boldsymbol{k}\, \boldsymbol{\sigma}_2\cdot\boldsymbol{k} + \alpha_{28}\, \boldsymbol{k}^2\, \boldsymbol{\sigma}_1\cdot\boldsymbol{k}\, \boldsymbol{\sigma}_2\cdot\boldsymbol{k}\, \boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 \\
& + \alpha_{29}\, \boldsymbol{\sigma}_1\cdot(\boldsymbol{q}\times\boldsymbol{k})\, \boldsymbol{\sigma}_2\cdot(\boldsymbol{q}\times\boldsymbol{k}) + \alpha_{30}\, \boldsymbol{\sigma}_1\cdot(\boldsymbol{q}\times\boldsymbol{k})\, \boldsymbol{\sigma}_2\cdot(\boldsymbol{q}\times\boldsymbol{k}) \boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 \,.
\end{aligned}
$$

- Need to develop a way to consistently treat nonlocal operators perturbatively in Quantum Monte Carlo

R. Somasundaram, J.E. Lynn, L. Huth, A. Schwenk, and I. Tews, Phys. Rev. C. **111** (2013)

Tricky beyond first order

First- and Second-order Corrections

$$E_0^{(1)} = \langle \psi_0 | V' | \psi_0 \rangle$$

$$E_0^{(2)} = -\sum_{k \neq 0}^{\infty} \frac{|\langle \psi_0 | V' | \psi_k \rangle|^2}{E_k - E_0}$$

The problem?

$$\lim_{\tau \to \infty} \psi(\tau) = \lim_{\tau \to \infty} e^{-(H - E_T)\tau} \psi_T \propto \psi_0 \longrightarrow E_0$$

R. Curry, J.E. Lynn, K.E. Schmidt and A. Gezerlis, Phys. Rev. Res., **5**, L042021, (2023)
R. Curry, R. Somasundaram, S. Gandolfi, A. Gezerlis, and I. Tews, Phys. Rev. C, **111**, 015801, (2025)

A solution - In very brief

$$I(\mathcal{T}) = \int_0^{\mathcal{T}} d\tau \left\langle\psi_0\right| V' e^{-[H_0 - E_0]\tau} V' \left|\psi_0\right\rangle$$

$$I(\mathcal{T}) = (E_0^{(1)})^2 \mathcal{T} - \sum_{k \neq 0}^{\infty} \frac{|\langle\psi_k|V'|\psi_0\rangle|^2}{E_k - E_0} [e^{-[E_k - E_0]\mathcal{T}} - 1]$$

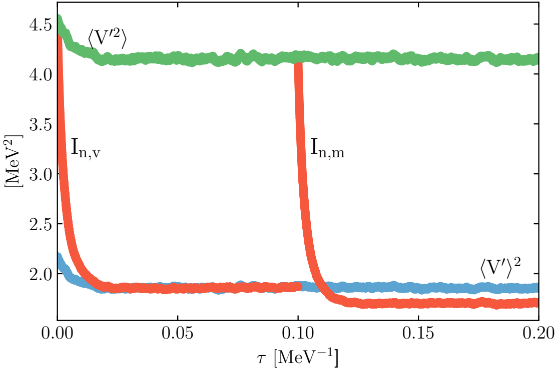
$$I(\mathcal{T} \to \infty) = (E_0^{(1)})^2 \mathcal{T} - E_0^{(2)}$$

R. Curry, J.E. Lynn, K.E. Schmidt and A. Gezerlis, Phys. Rev. Res., **5**, L042021, (2023)

R. Curry, R. Somasundaram, S. Gandolfi, A. Gezerlis, and I. Tews, Phys. Rev. C, **111**, 015801, (2025)

Practically speaking

$$I(\mathcal{T}) = \int_0^{\mathcal{T}} d\tau \, \langle\psi_0| \, V' e^{-[H_0 - E_0]\tau} V' \, |\psi_0\rangle \longrightarrow I \approx \frac{\sum_i^{\mathcal{N}} w_i V'(\boldsymbol{R}_i) V'(\boldsymbol{R}_i')}{\sum_i^{\mathcal{N}} w_i}$$



R. Curry, J.E. Lynn, K.E. Schmidt and A. Gezerlis, Phys. Rev. Res., **5**, L042021, (2023)

R. Curry, R. Somasundaram, S. Gandolfi, A. Gezerlis, and I. Tews, Phys. Rev. C, **111**, 015801, (2025)

Non-Local Operators

- Non-local operators cannot be avoided at higher chiral orders.
- Non-local operators cannot easily be included in imaginary time propagator
- Let's replace a local operator at NLO with a nonlocal equivalent and treat perturbatively

$$V^{(0)} = \alpha_1 + \alpha_2 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + \alpha_3 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 + \alpha_4 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$$

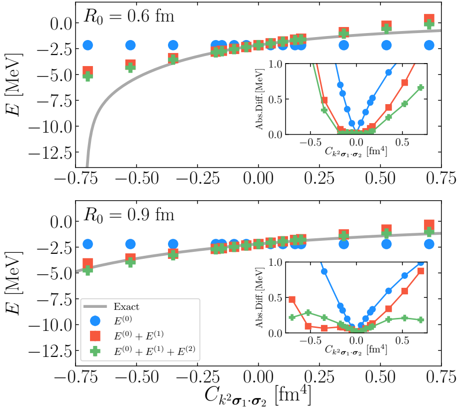
$$\begin{aligned} V^{(2)}_{\text{cont}} = & \gamma_1 q^2 + \gamma_2 q^2 \boldsymbol{\sigma_1} \cdot \boldsymbol{\sigma_2} + \gamma_3 q^2 \boldsymbol{\tau_1} \cdot \boldsymbol{\tau_2} \\ & + \gamma_4 q^2 \boldsymbol{\sigma_1} \cdot \boldsymbol{\sigma_2} \boldsymbol{\tau_1} \cdot \boldsymbol{\tau_2} \\ & + \gamma_5 k^2 + \gamma_6 k^2 \boldsymbol{\sigma_1} \cdot \boldsymbol{\sigma_2} + \gamma_7 k^2 \boldsymbol{\tau_1} \cdot \boldsymbol{\tau_2} \\ & + \gamma_8 k^2 \boldsymbol{\sigma_1} \cdot \boldsymbol{\sigma_2} \boldsymbol{\tau_1} \cdot \boldsymbol{\tau_2} \\ & + \gamma_9 (\boldsymbol{\sigma_1} + \boldsymbol{\sigma_2})(\boldsymbol{q} \times \boldsymbol{k}) \\ & + \gamma_{10} (\boldsymbol{\sigma_1} + \boldsymbol{\sigma_2})(\boldsymbol{q} \times \boldsymbol{k}) \boldsymbol{\tau_1} \cdot \boldsymbol{\tau_2} \\ & + \gamma_{11} (\boldsymbol{\sigma_1} \cdot \boldsymbol{q})(\boldsymbol{\sigma_2} \cdot \boldsymbol{q}) \\ & + \gamma_{12} (\boldsymbol{\sigma_1} \cdot \boldsymbol{q})(\boldsymbol{\sigma_2} \cdot \boldsymbol{q}) \boldsymbol{\tau_1} \cdot \boldsymbol{\tau_2} \\ & + \gamma_{13} (\boldsymbol{\sigma_1} \cdot \boldsymbol{k})(\boldsymbol{\sigma_2} \cdot \boldsymbol{k}) \\ & + \gamma 14 (\boldsymbol{\sigma_1} \cdot \boldsymbol{k})(\boldsymbol{\sigma_2} \cdot \boldsymbol{k}) \boldsymbol{\tau_1} \cdot \boldsymbol{\tau_2} \end{aligned}$$

- $q \rightarrow r$ local
- $k \rightarrow \nabla$ nonlocal

R. Curry, R. Somasundaram, S. Gandolfi, A. Gezerlis, and I. Tews, Phys. Rev. C, **111**, 015801, (2025)

Deuteron with nonlocal operator

$$k^2 \longrightarrow \left[-\frac{1}{4}(\nabla^2\delta_{R_0}\psi(\boldsymbol{r}) - \frac{1}{r}\frac{\partial\delta_{R_0}}{\partial r}\left(\boldsymbol{r}\cdot\nabla\psi(\boldsymbol{r})\right) - \delta_{R_0}\nabla^2\psi(\boldsymbol{r})\right]$$

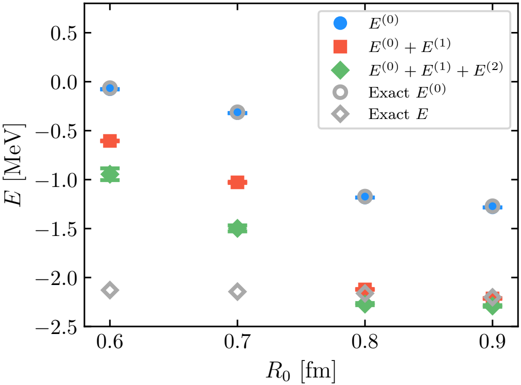


- Non-local operator <u>not included</u> in fit to phase shifts
- $k^2\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2$ included perturbatively for two cutoffs
- Compare against exact Lippmann-Schwinger solution

R. Curry, R. Somasundaram, S. Gandolfi, A. Gezerlis, and I. Tews, Phys. Rev. C, **111**, 015801, (2025)

A more realistic test case

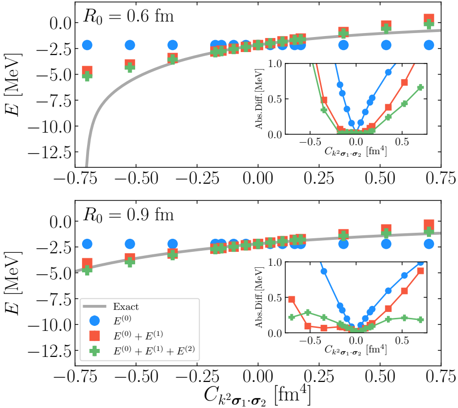
- Non-local operator included in fit to phase shifts

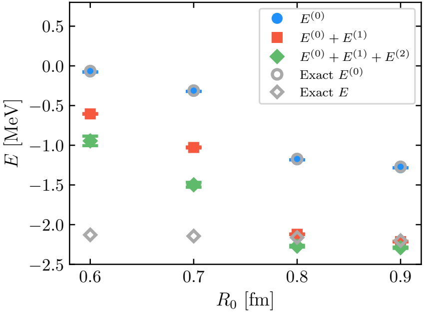


- Full range of coordinate space cutoffs
- Issues with perturbativeness at harder cutoffs

R. Curry, R. Somasundaram, S. Gandolfi, A. Gezerlis, and I. Tews, Phys. Rev. C, **111**, 015801, (2025)

Wait a minute...

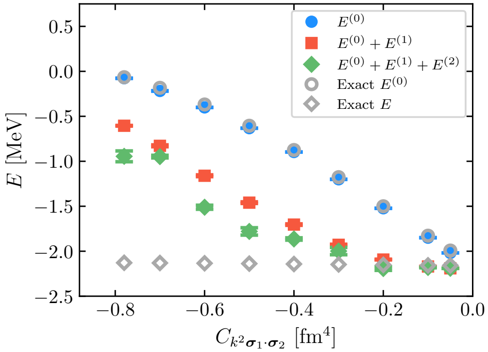




Can we take inspiration from the first case, and improve on the hard cutoff?

R. Curry, R. Somasundaram, S. Gandolfi, A. Gezerlis, and I. Tews, Phys. Rev. C, **111**, 015801, (2025)

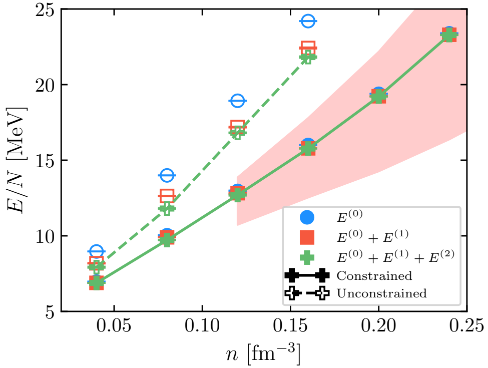
Constraining the nonlocal operator



- Hard-cutoff interaction $R_0 = 0.6$ fm ($\Lambda_c \approx 600$ MeV)
- Non-local operator included in fit to phase shifts
- Create a series of NLO interactions with a variable nonlocal LEC
- Clear region where perturbation theory is sufficient!

R. Curry, R. Somasundaram, S. Gandolfi, A. Gezerlis, and I. Tews, Phys. Rev. C, **111**, 015801, (2025)

Neutron Matter

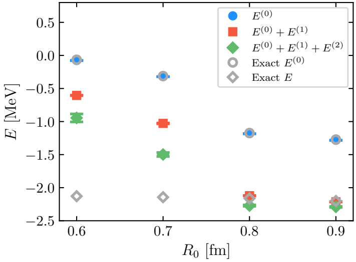


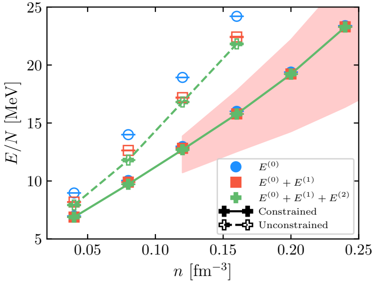
- Use constrained NLO interaction for calculation of neutron matter EOS
- Clear improvement from constraining the nonlocal operator
- Able to include nonlocal operators perturbatively even for hard cutoff interactions!

R. Curry, R. Somasundaram, S. Gandolfi, A. Gezerlis, and I. Tews, Phys. Rev. C, **111**, 015801, (2025)

Summary

- Novel method for calculating second-order perturbation theory in a QMC context
- Treat nonlocal operators perturbatively for diverse nuclear systems
- Constrained nonlocal operator to treat perturbatively for hard-cutoff interactions
- Paves the way for perturbative inclusion of N^3LO nonlocal contacts in AFDMC





Changing gears

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)

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]

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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.

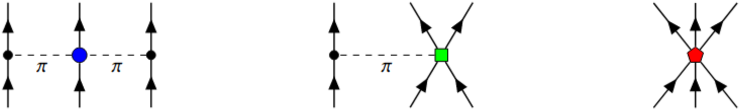
arxiv:2510.015860

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.

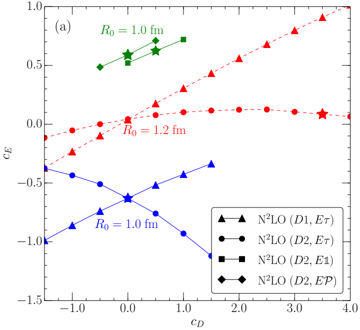


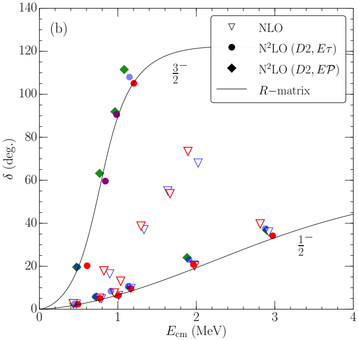
$V_{3N}^{2\pi}(c_1, c_3, c_4)$ $V_{3N}^{1\pi}(c_D)$ $V_{3N}^{\text{contact}}(c_E)$

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

Previously for local interactions

- 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

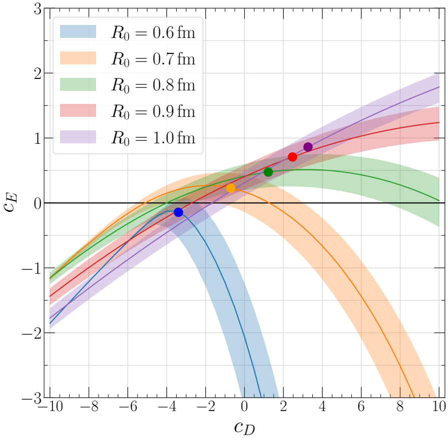




J.E. Lynn, I. Tews, A. Gezerlis, K.E. Schmidt, A. Schwenk, Phys. Rev. Lett. **116** 062501 (2016)

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

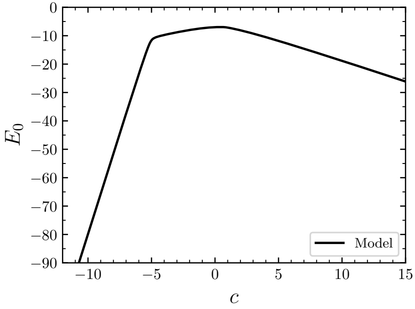
D. Frame, R. He, I. Ipsen, D. Lee, D. Lee, and E. Rrapaj Phys. Rev. Lett. **121**, 032501 (2018)
P. Cook, D. Jammooa, M. Hjorth-Jensen, D. Lee, and D. Lee, Nat. Commun. **16**, 5929 (2025)

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)

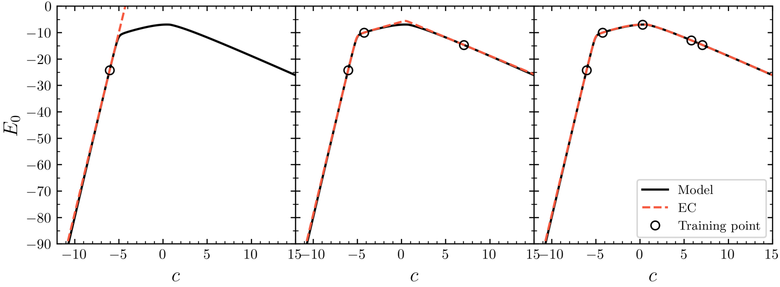


Eigenvector Continuation

- 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



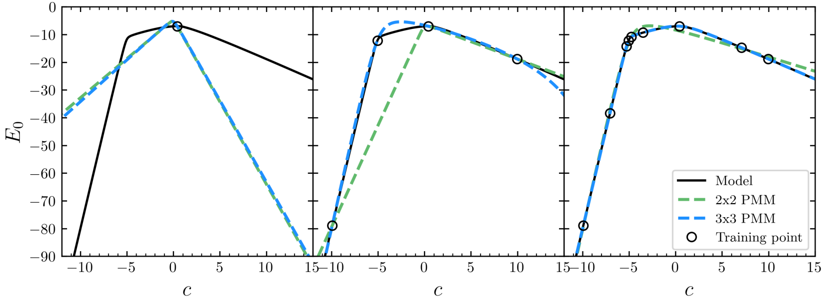
- Exact eigenstate requirement very tricky for AFDMC

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)

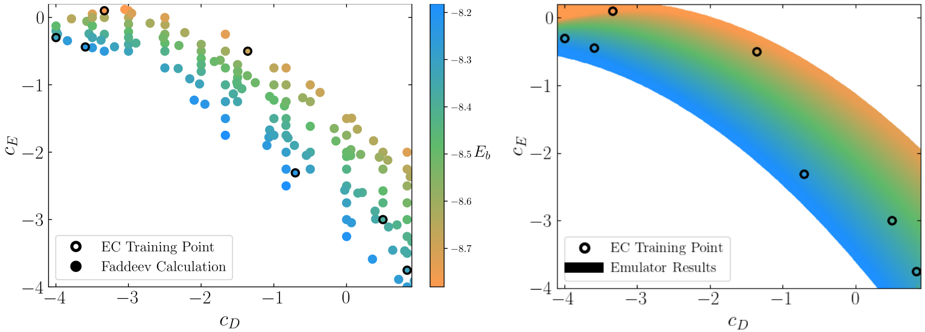


Emulating Solutions to the Faddeev Equations

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

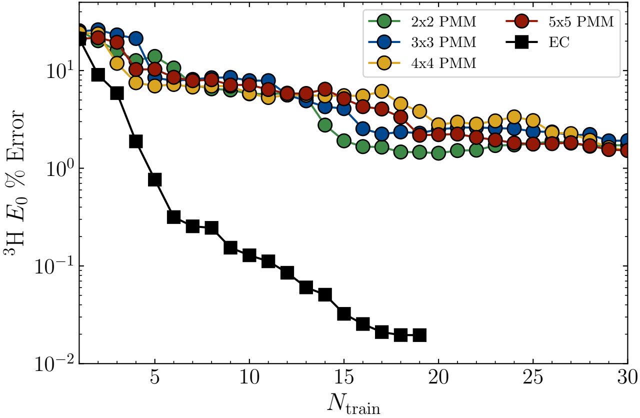
$$\tilde{H} = H_0 + C_S H_S + C_T H_T + \sum_{i=1}^{7} C_i H_i + c_D H_D + c_E H_E$$

- 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

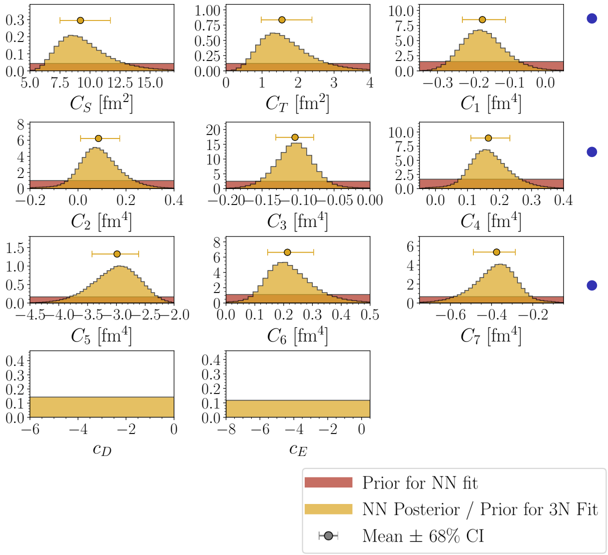
$$\mathcal{L} \propto \prod_i \exp\left[-\frac{1}{2}\left(\frac{X_i^{\text{exp.}} - X_i^{\text{theo.}}}{\sigma_i}\right)^2\right]$$

- 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

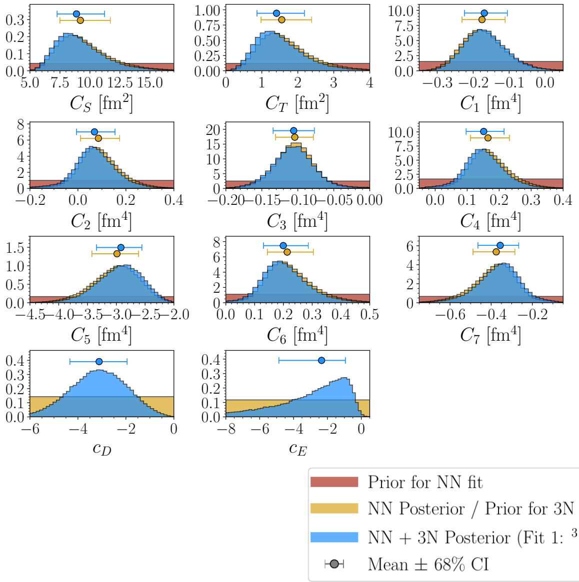


- Somasundaram *et. al* performed NN Bayesian fit at N^2LO
- We take their posteriors as our priors for the NN LECs
- Include additional uniform priors on c_D and c_E

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

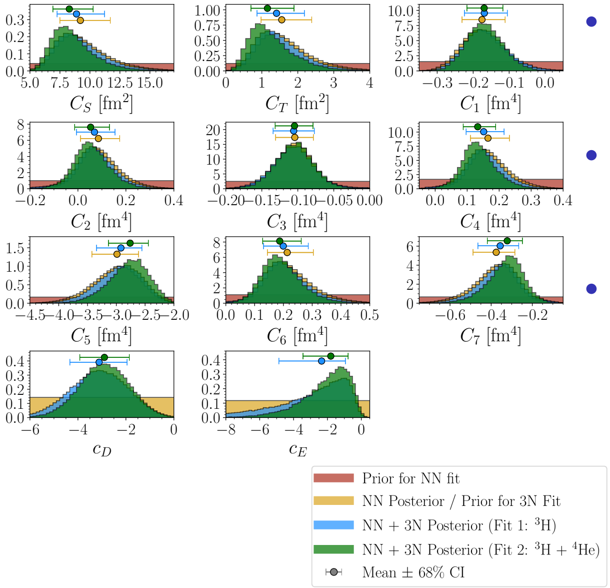
Bayesian Fit Against ^{3}H



- N^{2}LO 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

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

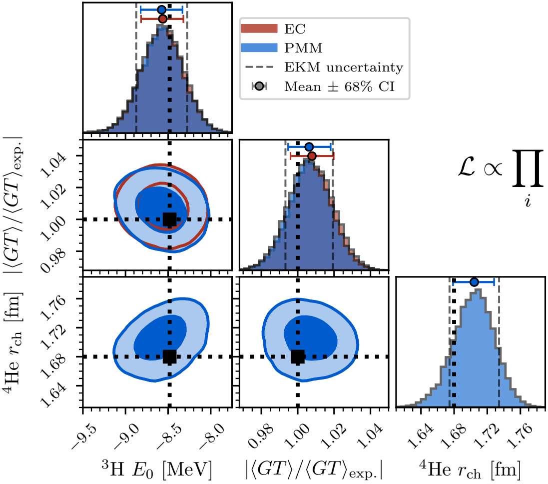
Additional ^{4}He Constraint



- 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



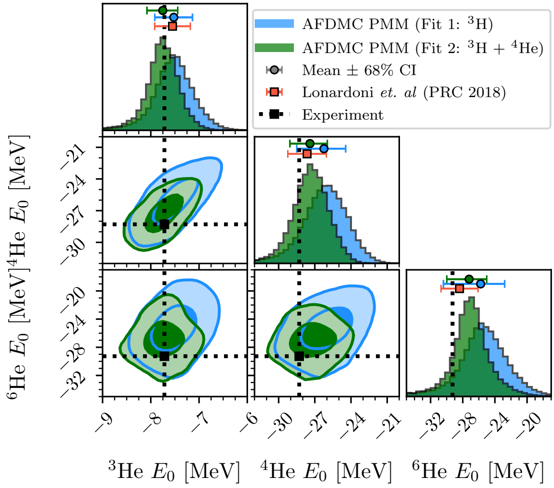
$$\mathcal{L} \propto \prod_i \exp\left[-\frac{1}{2}\left(\frac{X_i^{\rm exp.} - X_i^{\rm theo.}}{\sigma_i}\right)^2\right]$$

- 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

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

Thank you for your attention!

Collaborators:

- **Alex Gezerlis** (Guelph)
- **Ingo Tews** (LANL)
- **Stefano Gandolfi** (LANL)
- **Rahul Somasundaram** (LANL)
- **Achim Schwenk** (TUD)
- **Kai Hebeler** (TUD)
- **Joel Lynn** (TUD)
- **Kevin Schmidt** (ASU)

Funding / Computational Resources:

NSERC CRSNG

Los Alamos NATIONAL LABORATORY

Digital Research Alliance of Canada

INNOVATION Canada Foundation for Innovation Fondation canadienne pour l'innovation

Some questions

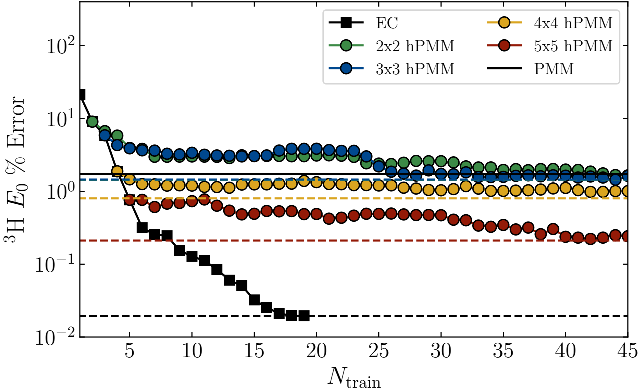
- How can we move towards treating chiral EFT consistently (perturbative vs non-perturbatve where appropriate)

- Additional few-body observables for fitting 3N interactions? Is it kosher to use medium mass nuclei, etc when fitting 3N force?

- What lessons can we learn from renormalizable theories that can be applied to chiral EFT?

Hybrid PMM-EC Emulator

- hPMM emulator starts from an EC starting matrix, and trains on additional data as a PMM
- All hPMM tests outperform previous best PMM (solid black line)
- 5×5 hPMM outperforms 8×8 EC



R. Curry, J. Kozar, C.L. Armstrong, K. Hebeler, S. Gandolfi, A. Gezerlis, A. Schwenk, R. Somasundaram, and I. Tews, *in preparation*