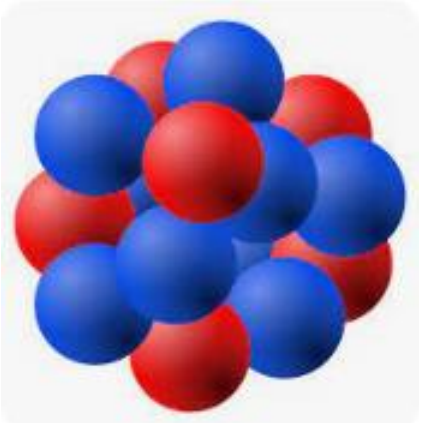
Progress of Perturbative Quantum Monte Carlo Calculations

Bing-Nan Lu
吕炳楠

Graduate School of China Academy of Engineering Physics

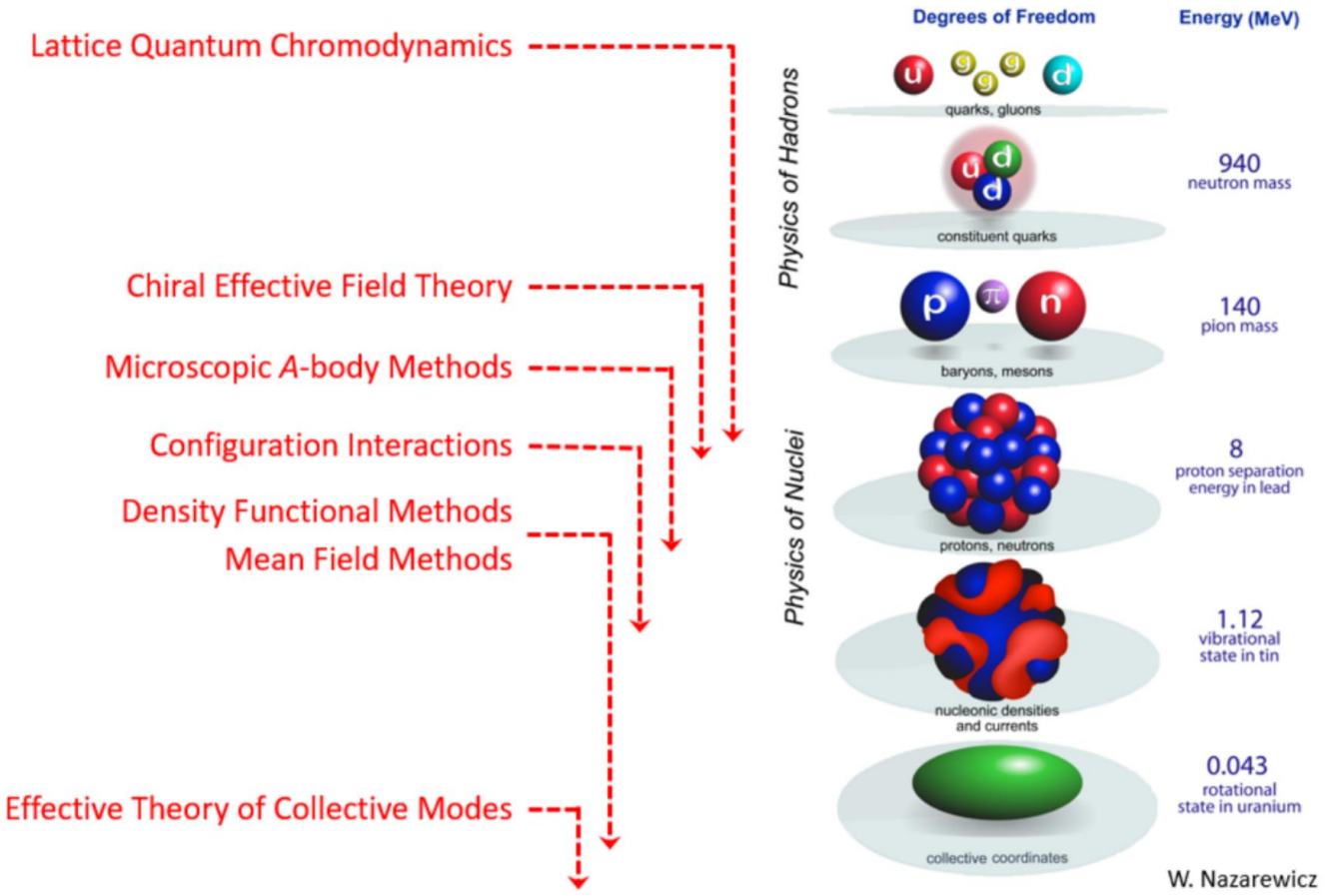


基于第一性原理的手征核力与核物理研究研讨会
2025-02-22, 北京航空航天大学

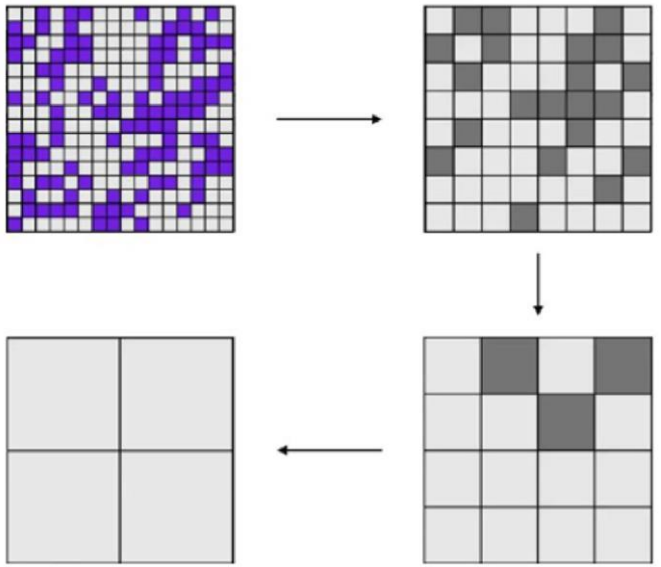
Contents

- Brief introduction to nuclear lattice EFT
- Nuclear force with Wigner-SU(4) symmetry
- Perturbative quantum Monte Carlo method
- Summary and perspective

What is a nuclear EFT?



- **Modern nuclear force constructions are based on the Effective Field Theory**
- **Theoretical foundation of EFT is the Wilsonian renormalization group**:
  - **High-momentum** details can be integrated out & hidden in LECs
  - **Low-momentum** physics kept invariant under ren. group transformations

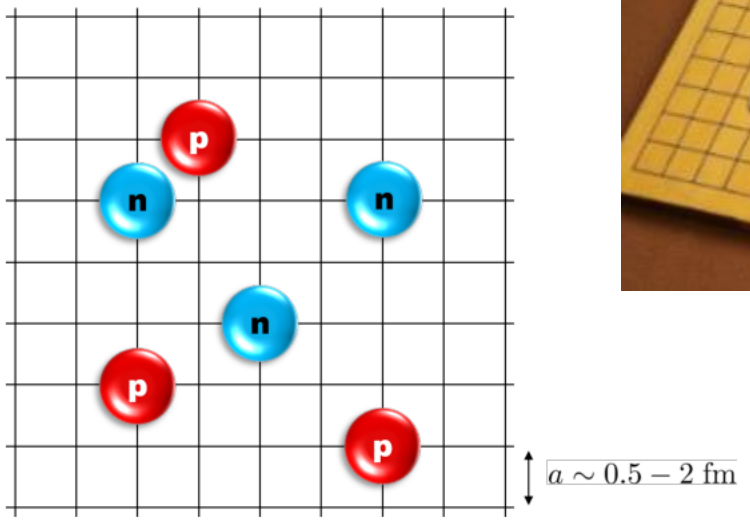


Lattice EFT: A many-body EFT solver

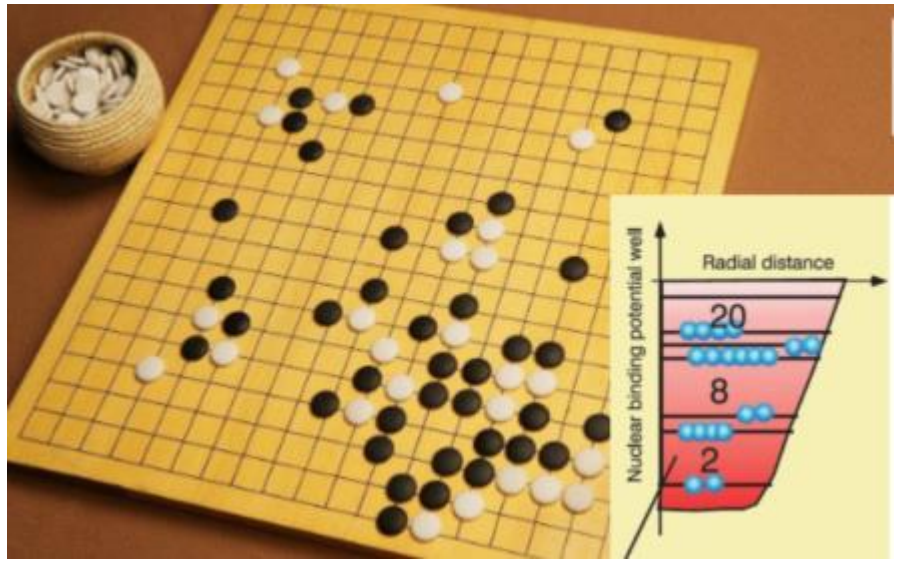
Lattice EFT = Chiral EFT + Lattice + Monte Carlo

Review: Dean Lee, Prog. Part. Nucl. Phys. 63, 117 (2009),
Lähde, Meißner, "Nuclear Lattice Effective Field Theory", Springer (2019)

- Discretized chiral nuclear force
- Lattice spacing $a \approx 1$ fm $= 620$ MeV (∼chiral symmetry breaking scale)
- Protons & neutrons interacting via **short-range, δ-like** and **long-range, pion-exchange** interactions
- Exact method, polynomial scaling ($\sim A^2$)



Lattice adapted for nucleus



- Solve the non-perturbative nuclear many-body problem by sampling all configurations

Lattice EFT: A many-body EFT solver

- Get *interacting g. s.* from imaginary time projection:

$$|\Psi_{g.s.}\rangle \propto \lim_{\tau\to\infty} \exp(-\tau H)|\Psi_A\rangle$$

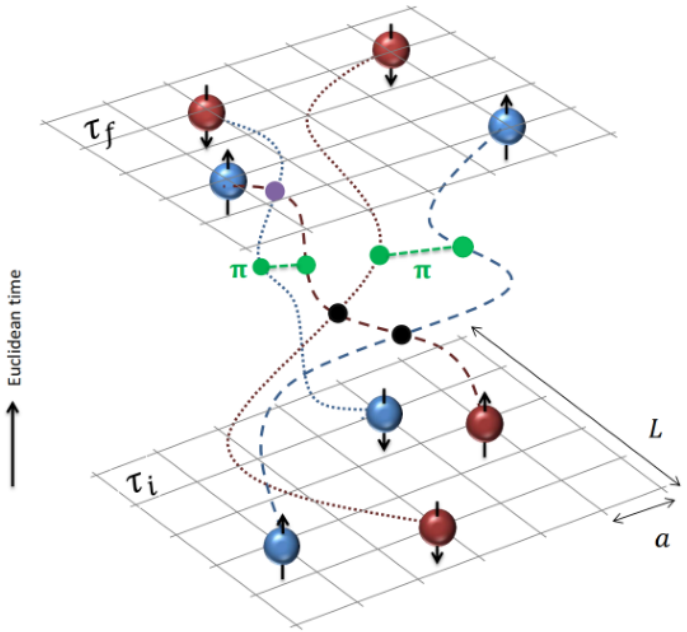
with $|\Psi_A\rangle$ representing A *free* nucleons.

- Expectation value of any operator $\mathscr{O}$:

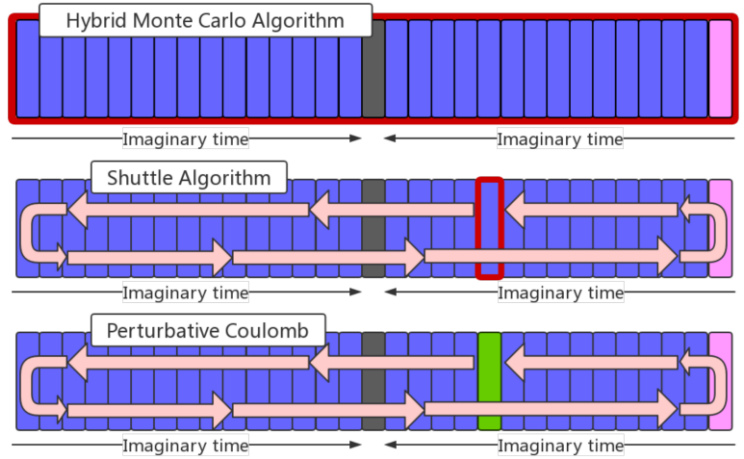
$$\langle O\rangle = \lim_{\tau\to\infty} \frac{\langle\Psi_A|\exp(-\tau H/2)\mathscr{O}\exp(-\tau H/2)|\Psi_A\rangle}{\langle\Psi_A|\exp(-\tau H)|\Psi_A\rangle}$$

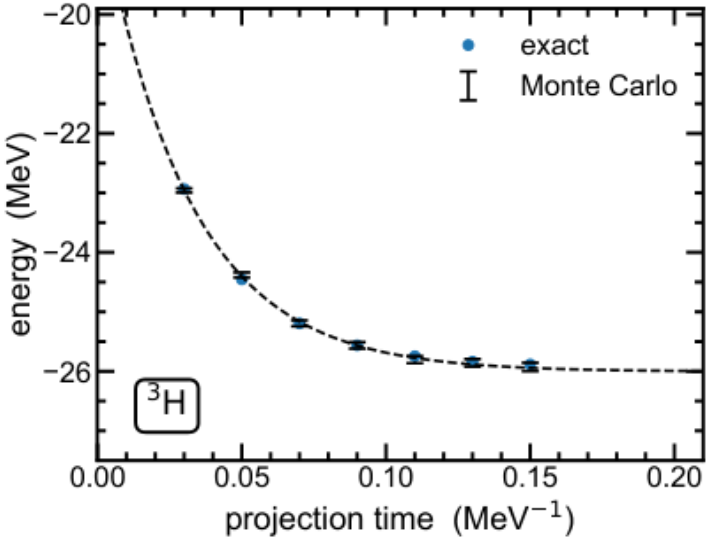
- τ is discretized into time slices:

$$\exp(-\tau H) \simeq \left[:\exp(-\frac{\tau}{L_t}H):\right]^{L_t}$$



All possible configurations in $\tau \in [\tau_i, \quad \tau_f]$ are sampled.
Complex structures like nucleon clustering emerges naturally.



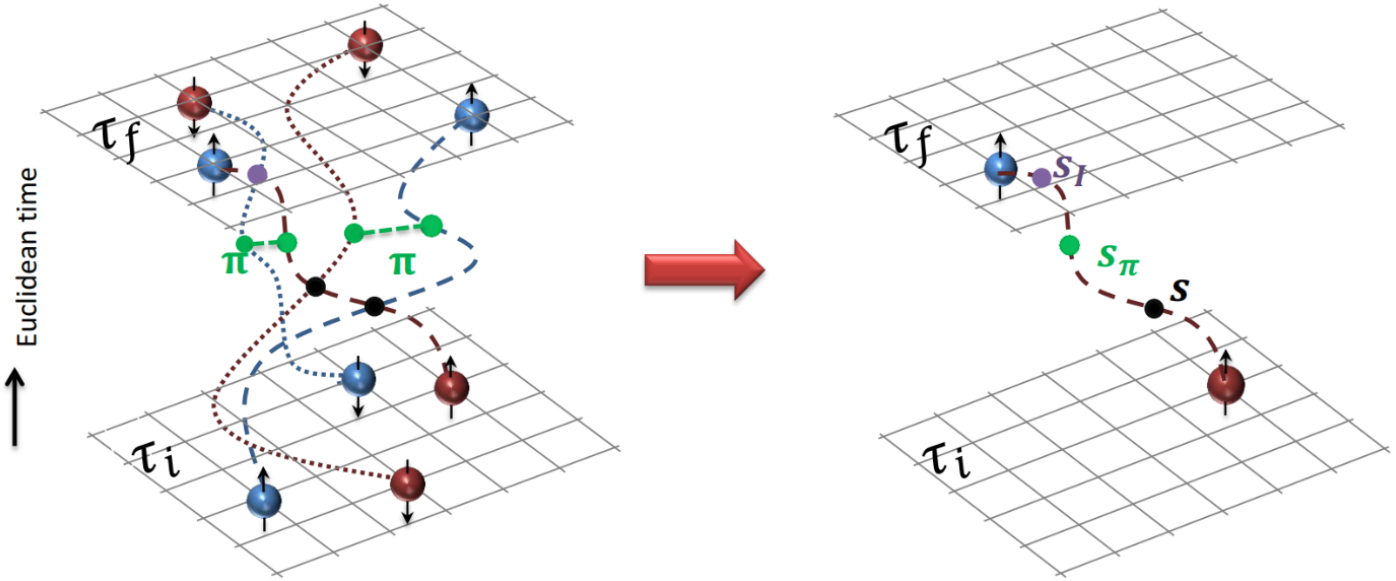


Lattice EFT: A many-body EFT solver

- Quantum correlations between nucleons are represented by fluctuations of the auxiliary fields.

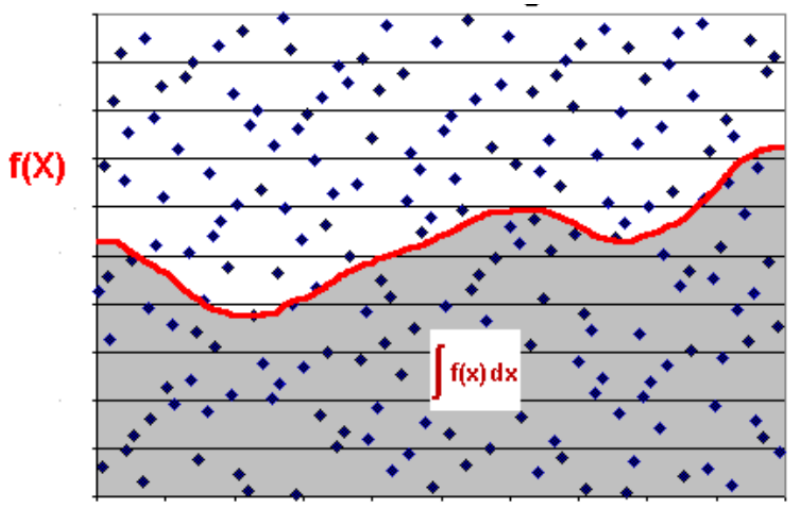
$$:\exp\left[-\frac{a_t C}{2}(\psi^\dagger\psi)^2\right]:=\frac{1}{\sqrt{2\pi}}\int ds:\exp\left[-\frac{s^2}{2}+\sqrt{-a_t C}s(\psi^\dagger\psi)\right]:$$

- Long-range interactions such as OPEP or more complex interactions can be represented similarly.
- For fixed aux. fields, product of s.p. states (e.g., Slater determinant) keep the form of product of s.p. states in propagations. ⟸**No *N*-*N* interaction**



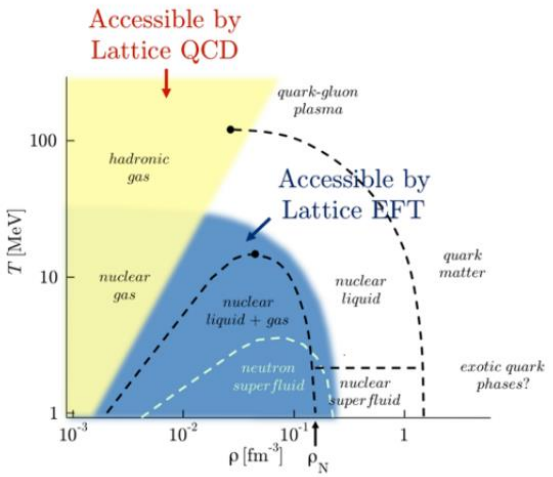
In lattice EFT, solving a general Hamiltonian consists of 5 steps:

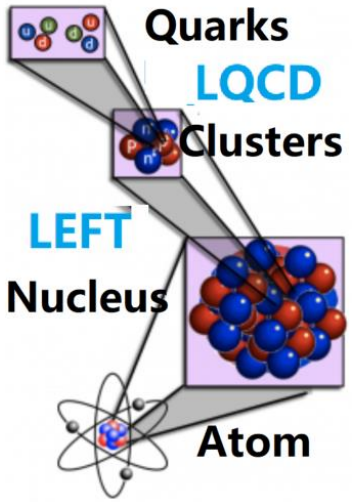
1. Rewrite expectation value as a path integral using auxiliary field transformation.
2. For each field configuration, calculate the amplitude.
3. Integrate over the field variables using Monte Carlo algorithms.
4. Take the limit $\tau \to \infty$ to find the true ground state.
5. Take the limit $L \to \infty$ to eliminate the finite volume effects.



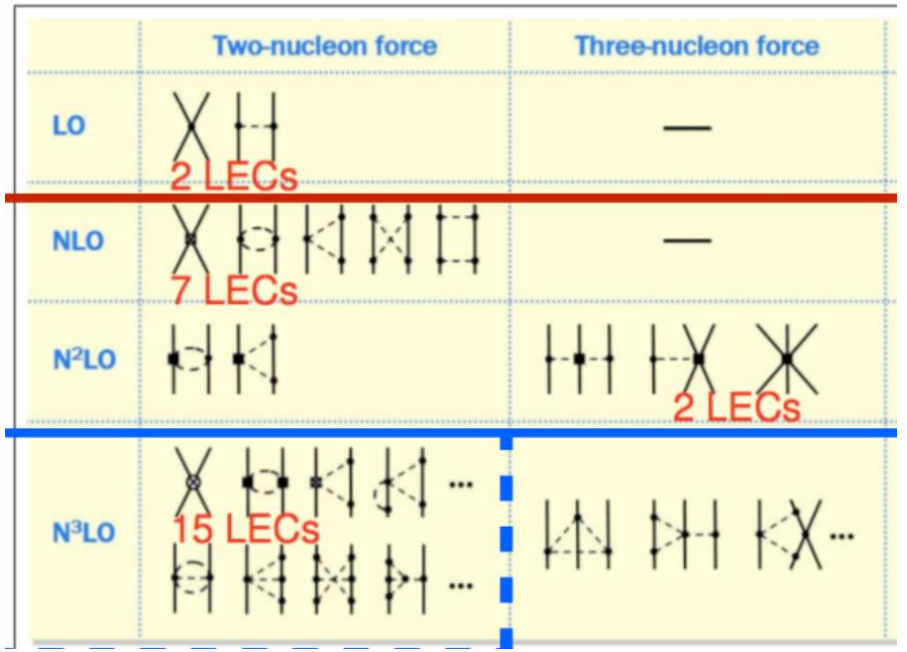
Compare Lattice EFT and Lattice QCD

	LQCD	LEFT
degree of freedom	quarks & gluons	nucleons and pions
lattice spacing	$\sim$0.1 fm	$\sim$1 fm
dispersion relation	relativistic	non-relativistic
renormalizability	renormalizable	effective field theory
continuum limit	yes	no
Coulomb	difficult	easy
accessibility	high T / low ρ	low T / $\rho_{\rm sat}$
sign problem	severe for $\mu > 0$	moderate





- Lattice EFT share a lot of common features with Lattice QCD. However,
  - Non-rel. → particle number conservation
  - Quadratic dispersion relation
    → no Fermion doubling problem
  - EFT contains non-renormalizable terms
    → no continuum limit

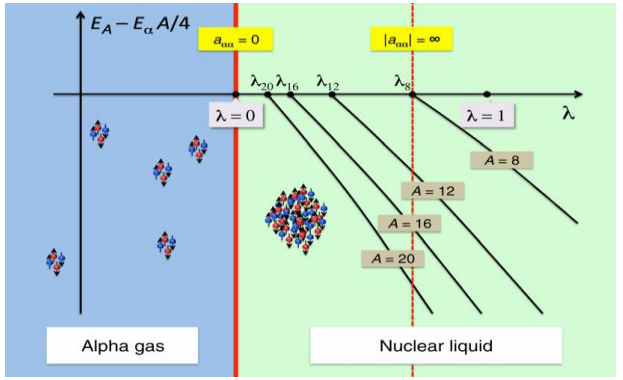


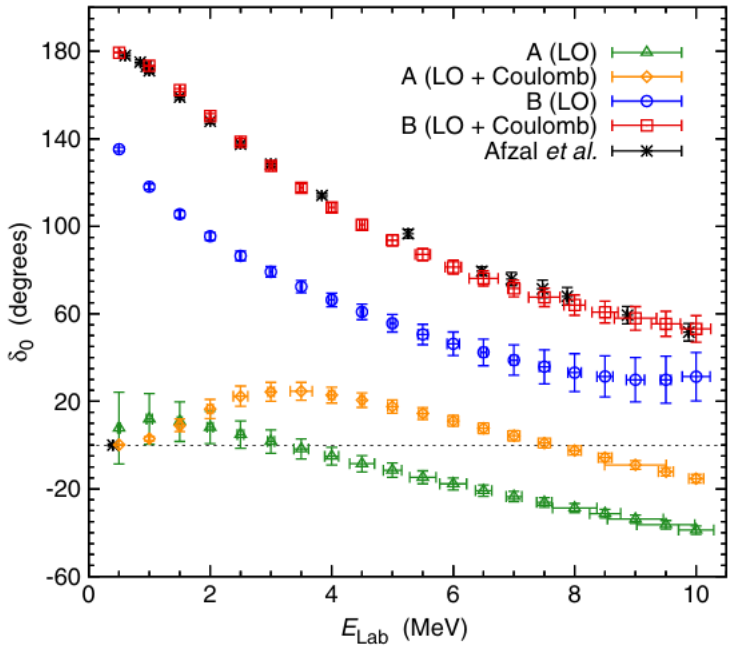
Nuclear binding near a quantum phase transition

PRL 117, 132501 (2016) Selected for a Viewpoint in *Physics* PHYSICAL REVIEW LETTERS week ending 23 SEPTEMBER 2016

Nuclear Binding Near a Quantum Phase Transition

Serdar Elhatisari,[1] Ning Li,[2] Alexander Rokash,[3] Jose Manuel Alarcón,[1] Dechuan Du,[2] Nico Klein,[1] Bing-nan Lu,[2] Ulf-G. Meißner,[1,2,4] Evgeny Epelbaum,[3] Hermann Krebs,[3] Timo A. Lähde,[2] Dean Lee,[5] and Gautam Rupak[6]





Nucleus	A (LO)	B (LO)	A (LO + Coulomb)	B (LO + Coulomb)	Experiment
^{3}H	−7.82(5)	−7.78(12)	−7.82(5)	−7.78(12)	−8.482
^{3}He	−7.82(5)	−7.78(12)	−7.08(5)	−7.09(12)	−7.718
^{4}He	−29.36(4)	−29.19(6)	−28.62(4)	−28.45(6)	−28.296
^{8}Be	−58.61(14)	−59.73(6)	−56.51(14)	−57.29(7)	−56.591
^{12}C	−88.2(3)	−95.0(5)	−84.0(3)	−89.9(5)	−92.162
^{16}O	−117.5(6)	−135.4(7)	−110.5(6)	−126.0(7)	−127.619
^{20}Ne	−148(1)	−178(1)	−137(1)	−164(1)	−160.645

- The nuclear force can be either local (position-dependent) or non-local (velocity-dependent).
- Locality is an essential element for nuclear binding.

Zeroth order Hamiltonian (perturbative order)

We use a zeroth order lattice Hamiltonian that respects the Wigner-SU(4) symmetry

$$H_0 = K + \frac{1}{2} C_{\mathrm{SU4}} \sum_{\boldsymbol{n}} : \tilde{\rho}^2(\boldsymbol{n}) :$$

The smeared density operator $\tilde{\rho}(\boldsymbol{n})$ is defined as

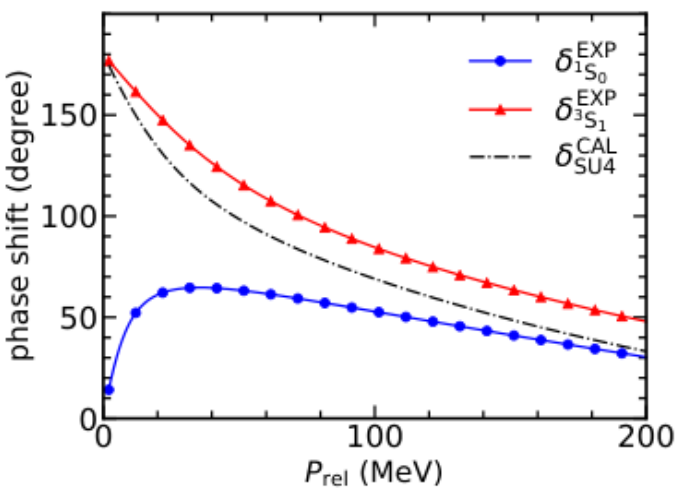
$$\tilde{\rho}(\boldsymbol{n}) = \sum_i \tilde{a}_i^\dagger(\boldsymbol{n}) \tilde{a}_i(\boldsymbol{n}) + s_L \sum_{|\boldsymbol{n}'-\boldsymbol{n}|=1} \sum_i \tilde{a}_i^\dagger(\boldsymbol{n}') \tilde{a}_i(\boldsymbol{n}'), \tag{1}$$

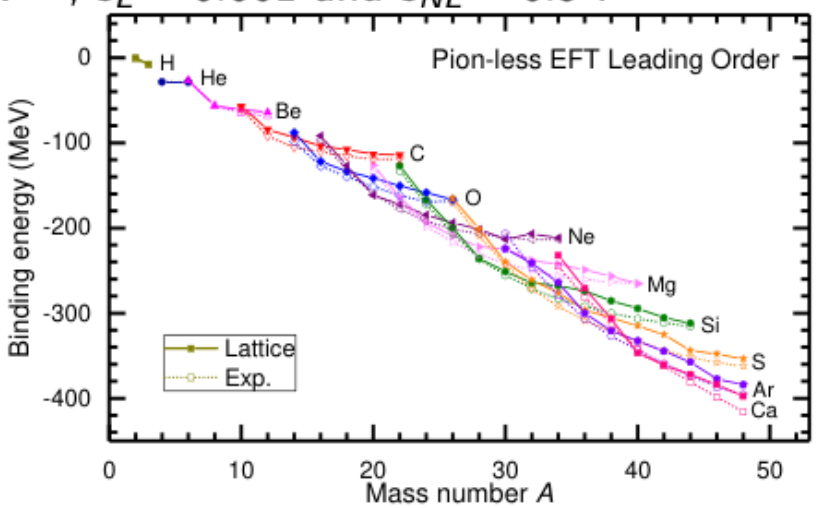
where i is the joint spin-isospin index

$$\tilde{a}_i(\boldsymbol{n}) = a_i(\boldsymbol{n}) + s_{NL} \sum_{|\boldsymbol{n}'-\boldsymbol{n}|=1} a_i(\boldsymbol{n}'). \tag{2}$$

In this work we use a lattice spacing $a = 1.32$ fm and the parameter set

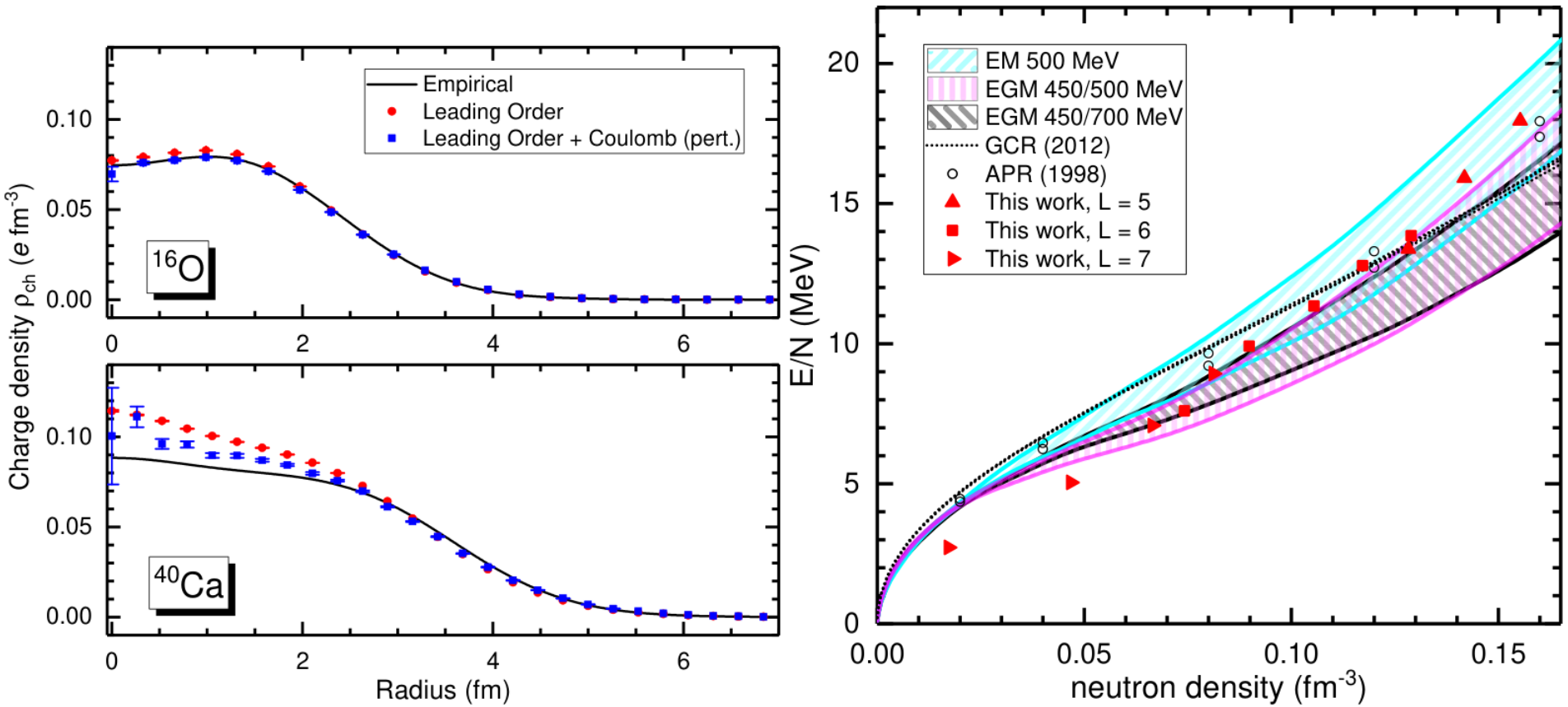
$C_{\mathrm{SU4}} = -3.41 \times 10^{-7}$ MeV^{-2}, $s_L = 0.061$ and $s_{NL} = 0.5$.





Essential elements for nuclear binding

Charge density and neutron matter equation of state
are impotant in element creation, neutron star merger, etc.



Lu, Li, Elhatisari, Lee, Epelbaum, Meissner, Phys. Lett. B 797 (2019) 134863

Nuclear mass Model

To better describe shell evolution, we introduce the **spin-orbit coupling interaction** without the problem.

$$H = H_{\text{free}} + \frac{1}{2!}C_2 \sum_{\vec{n}} \tilde{\rho}(\vec{n})^2 + \frac{1}{3!}C_3 \sum_{\vec{n}} \tilde{\rho}(\vec{n})^3 + \boxed{C_{sl} V_{\frac{i}{2}(\mathbf{q}\times S)\cdot\mathbf{k}}}$$

Nolocal density operator :

$$\tilde{\rho}(\vec{n}) = \sum_i \tilde{a}_i^\dagger(\vec{n})\tilde{a}_i(\vec{n}) + s_L \sum_{|n'-\vec{n}|=1} \sum_i \tilde{a}_i^\dagger(\vec{n}')\,\tilde{a}_i(\vec{n}')$$

$$\tilde{a}_i(\vec{n}) = a_i(\vec{n}) + s_{NL} \sum_{|\vec{n}'-\vec{n}|=1} a_i(\vec{n}')$$

With **small coupling constants** and appropriate auxiliary field transformations, the introduction of the spin-orbit coupling term does not lead to sign problems.

Nuclear mass Model

Experimental data is required to determine **five fitting parameters.**

$$H = H_{\text{free}} + \frac{1}{2!}C_2\sum_{\vec{n}}\tilde{\rho}(\vec{n})^2 + \frac{1}{3!}C_3\sum_{\vec{n}}\tilde{\rho}(\vec{n})^3 + \boxed{C_{sl}V_{\frac{i}{2}(\mathbf{q}\times S)\cdot\mathbf{k}}}$$

Loss function : $\chi^2 = \chi^2(s_L, s_{NL}, C_2, C_3, C_{sl}) = \sum_A \left(\frac{E(A) - E(A)_{\text{exp}}}{\epsilon}\right)^2$

Determine the parameters by **minimizing** the loss function.

Difficulties:

1.Each calculation **consumes a lot of computing resources**.

2.The **order of magnitude** of parameters varies greatly.

3.Monte Carlo calculations involve **statistical errors**.

Measure derivatives

$$\chi^2 = \sum_A \left(\frac{E(A) - E(A)_{exp}}{\varepsilon}\right)^2 \longrightarrow \frac{\partial \chi^2}{\partial \theta_i} = \sum_A \left[2\left(\frac{E(A) - E(A)_{exp}}{\varepsilon^2}\right)\frac{\partial E(A)}{\partial \theta_i}\right]$$

where θ_i is the **fitting parameters.**

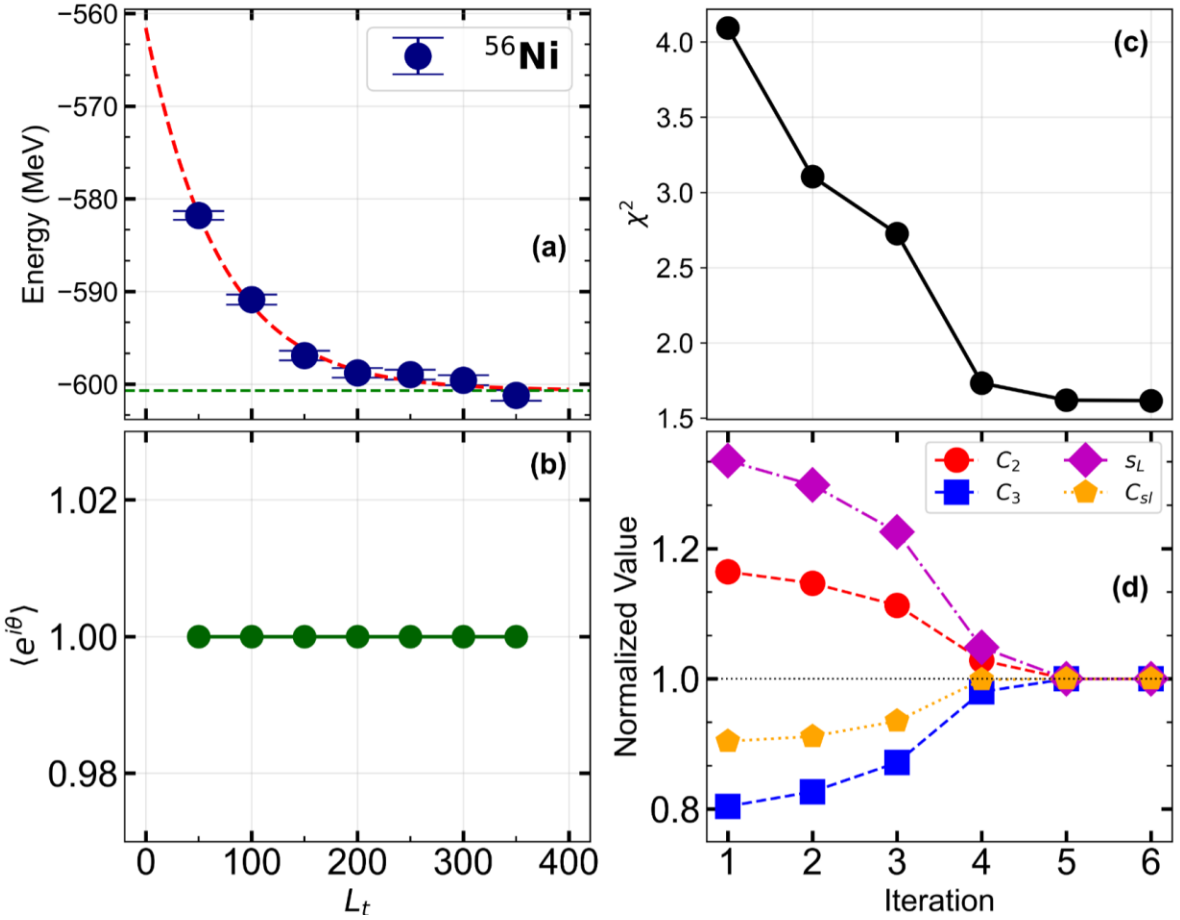
Therefore, we can directly **measure** $\frac{\partial E}{\partial \theta_i}$ as an operator in the Monte Carlo calculations, providing an exact derivative.

MC method → simultaneously measure → Operator $\frac{\partial \chi^2}{\partial \theta_i}$

we consider using **the gradient descent method**.

The Gredient Descending Method

Implementation: We implemented the Gradient Descending algorithm simply by introducing strategies such as **feature scaling** and **adaptive learning rates**.



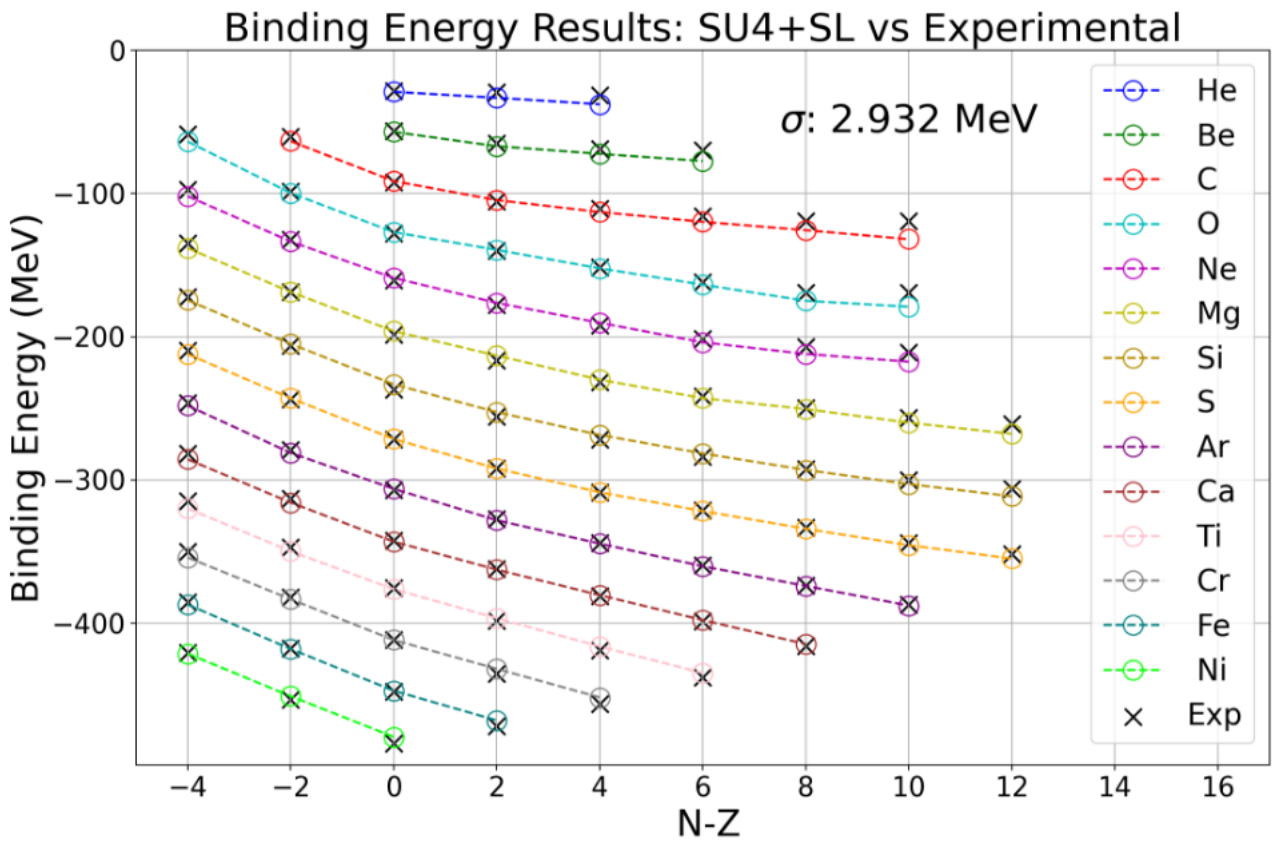
Target nucleus

^{4}He, ^{12}C, ^{16}O, ^{28}Si, ^{32}S, and ^{40}Ca

$$\chi^2 = \sum_A \left(\frac{E(A) - E(A)_{exp}}{\varepsilon}\right)^2$$

The plot shows a **significant decrease** in the loss function with successive iterations.

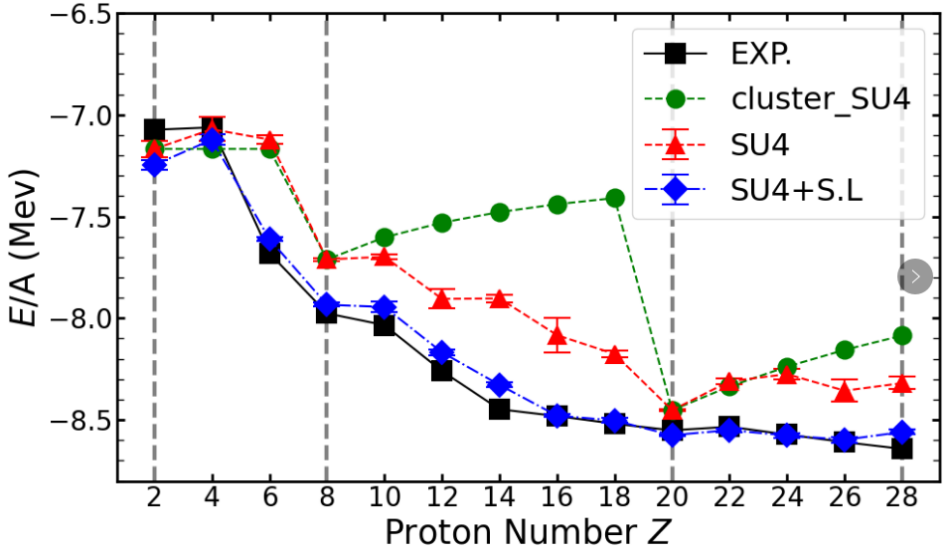
Nuclear binding energies with spin-orbit term (preliminary)



- **Spin-orbit term** is essential for **shell evolutions**. (proper SL term **do not induce sign problem**)
- SU(4) + SL Hamiltonian, **5 parameters** optimized with masses of ^{4}He, ^{16}O, ^{24}Mg, ^{28}Si, ^{40}Ca, etc.

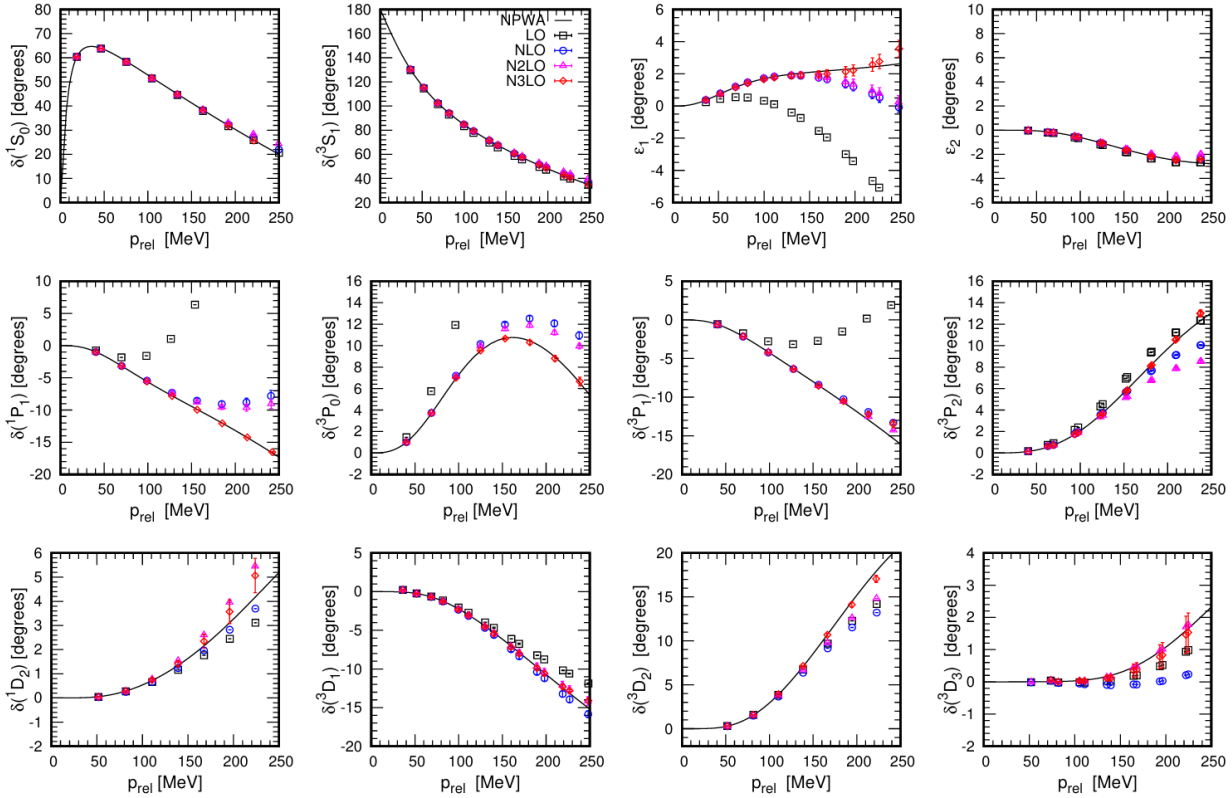
- Average error for **76** even-even nuclei: **2.932 MeV**
  Applicable to light/medium mass nuclei
  Zhong-Wang Niu, B.L., in preparation

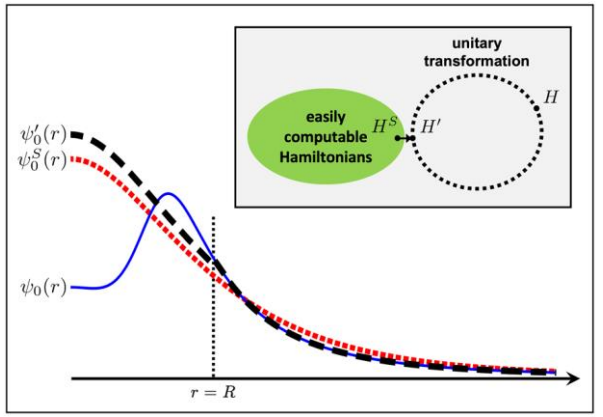
- Errors in other models
  - Relativistic mean field (PC-PK1): **2.258 MeV**
    Peng-Wei Zhao et al., PRC82, 054319 (2010)
  - Non-rel. mean field (UNDEF1): **3.380 MeV**
    Kortelainen et al., PRC 85, 024304 (2012).
  - Finite range droplet model: **1.142 MeV**
    P. Moller et al., **Atom. Data Nucl. Data Tables 109, 1 (2016)**

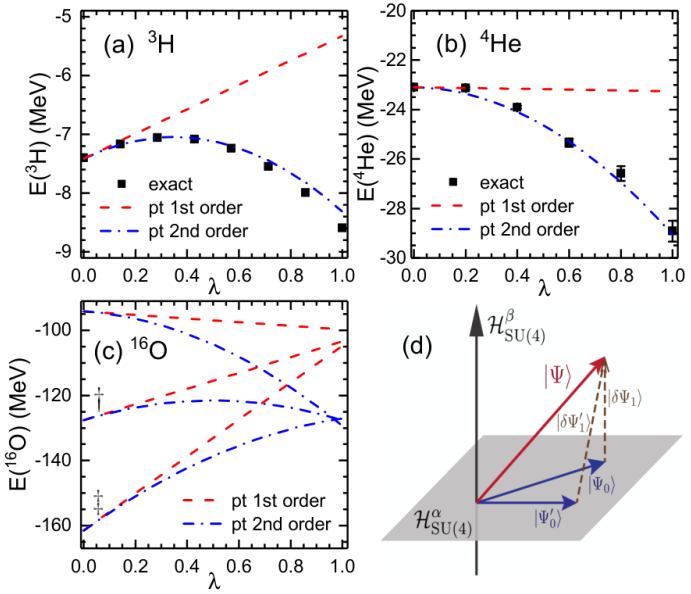


Precision lattice chiral nuclear forces

- High-precision fit to N-N scattering phase shifts at N^{3}LO
  Alarcon et al., EPJA 53, 83 (2017)
  Li et al., PRC 98, 044002 (2018)



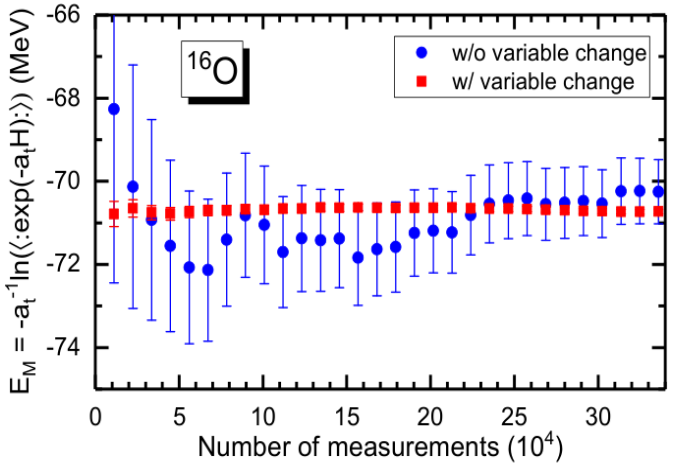


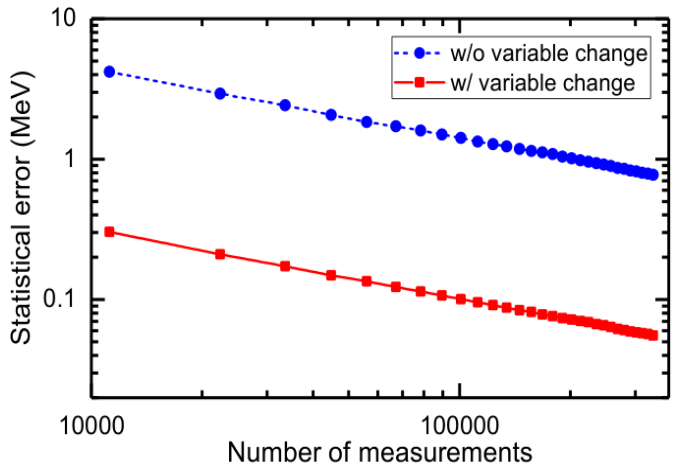


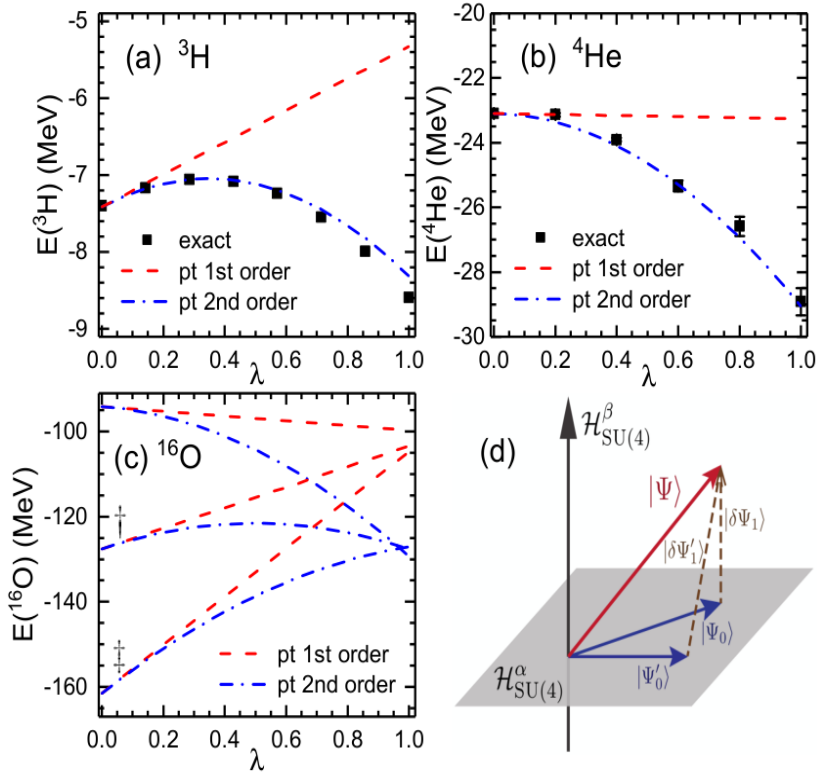
Implementation in lattice calculations:

- Wave function matching method
  Elhatisari et al.,
  Nature 630, 59 (2024)
- Perturbative quantum Monte Carlo method
  Lu et al.,
  PRL 128, 242501 (2022)
- Rank-one operator method
  Ma et al.,
  PRL 132, 232502 (2024)

Perturbative quantum Monte Carlo







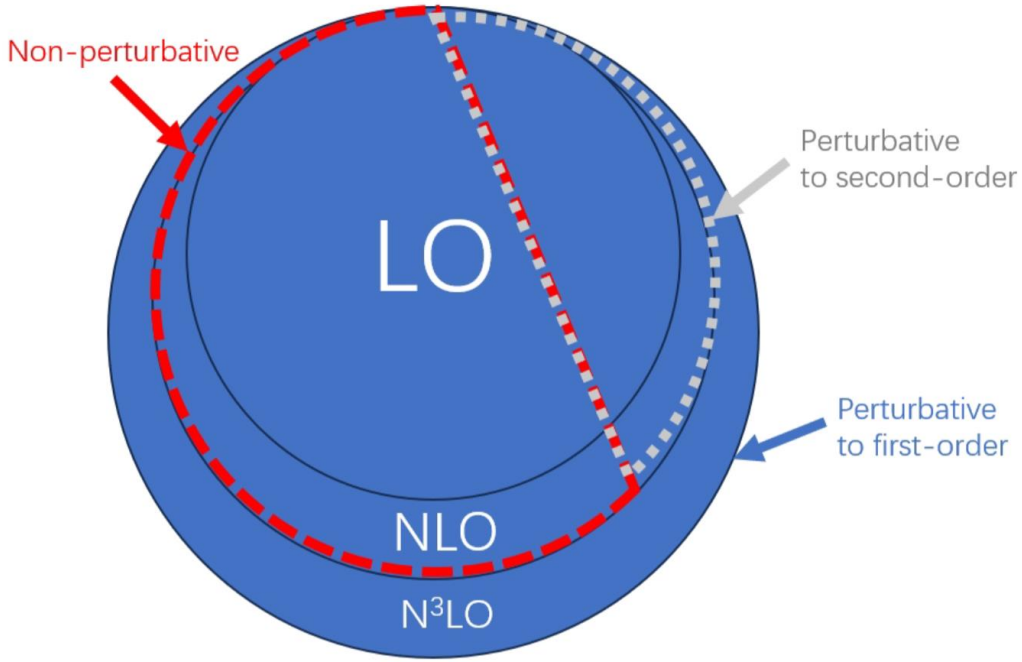
$$E_i = E_i^{(0)} + \lambda\langle\Psi_i^{(0)}|V_C|\Psi_i^{(0)}\rangle + \lambda^2\sum_{k\neq 0}\frac{\langle\Psi_k^{(0)}|V_C|\Psi_i^{(0)}\rangle}{E_k^{(0)} - E_i^{(0)}} + \mathcal{O}(\lambda^3)$$

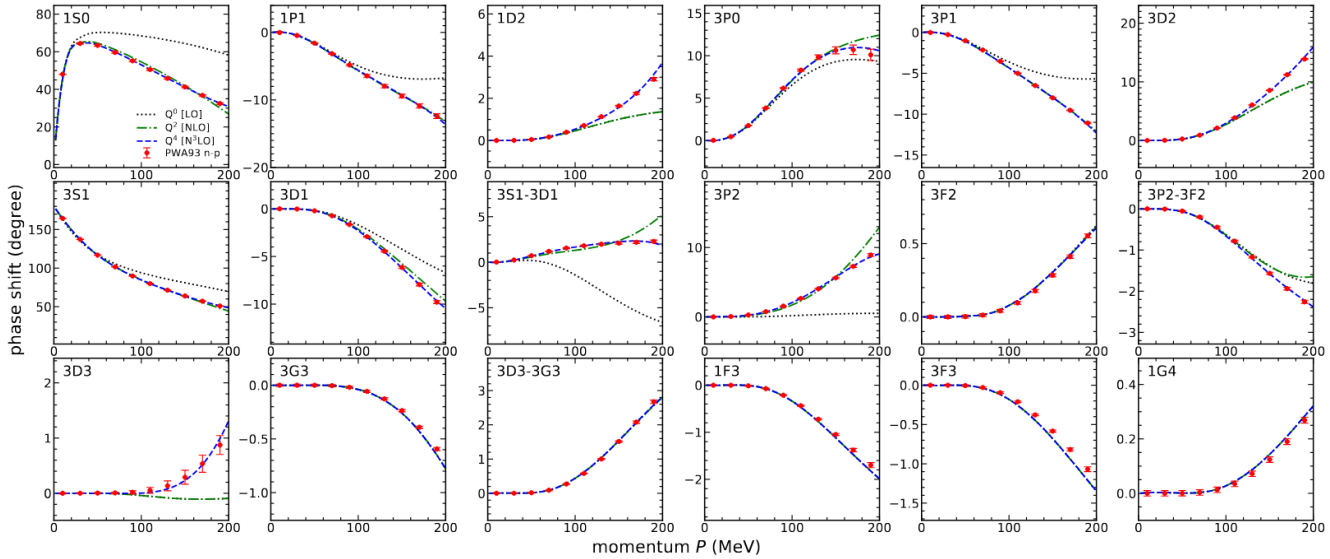
- Projection QMC targets the ground states, **excited states** are expensive
- Conventional Rayleigh-Schrodinger perturbation theory requires **excited states**

PRL 128, 242501 (2022) propose a novel perturbative QMC algorithm (ptQMC) that efficiently calculate the Second-order corrections.

In some cases, the second-order corrections are unexpectedly large!

Perturbative QMC for chiral forces





- We generate a chain of chiral Hamiltonian with progressively increasing precision
- The Hamiltonian converge and their difference are suppressed by powers of the momentum scale

J. Liu, T. Wang, B.L., arXiv:2502.13565 (2025)

$$
\begin{aligned}
H_{\mathrm{LO}} &= K + V_{\mathrm{2N}}^{(0)}, \\
H_{\mathrm{NLO}} &= K + V_{\mathrm{2N}}^{(0)} + V_{\mathrm{2N}}^{(2)} + V_{\mathrm{CSB}}^{\mathrm{nn}} + V_{\mathrm{CSB}}^{\mathrm{pp}} + V_{\mathrm{GIR}}, \\
H_{\mathrm{N3LO}} &= K + V_{\mathrm{2N}}^{(0)} + V_{\mathrm{2N}}^{(2)} + V_{\mathrm{2N}}^{(4)} + V_{\mathrm{CSB}}^{\mathrm{nn}} \\
&\quad + V_{\mathrm{CSB}}^{\mathrm{pp}} + V_{\mathrm{GIR}},
\end{aligned}
$$

Double expansion for N3LO chiral forces

$$H_{\mathrm{N3LO}} = H_{\mathrm{SU4}} + \lambda(H_{\mathrm{NLO}} - H_{\mathrm{SU4}}) + \mu(H_{\mathrm{N3LO}} - H_{\mathrm{NLO}})$$

$$E_{\mathrm{N3LO}}(\lambda,\mu) = \sum_{n,m=0}^{\infty} E_{\lambda^n\mu^m}\lambda^n\mu^m$$

The true wave function can be expanded into a series in correction term $V_C = H - H_0$

The partial amplitudes can be calculated efficiently with complexification of the field Variables.

$$|\Psi\rangle = \lim_{L_t\to\infty} M^{L_t/2}|\Psi_T\rangle = |\Psi_0\rangle + |\Psi_1\rangle + \mathcal{O}(V_C^2)$$

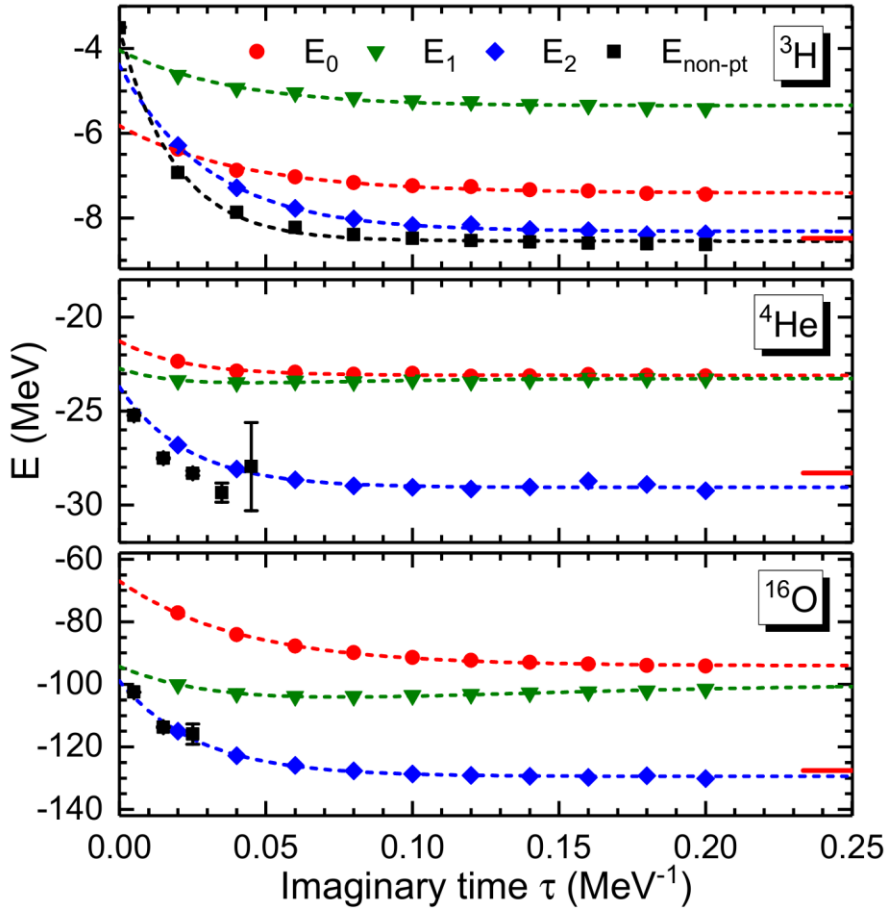
$$\langle O\rangle = \lim_{\tau\to\infty} \frac{\langle\Psi_T|\exp(-H\tau/2)O\exp(-H\tau/2)|\Psi_T\rangle}{\langle\Psi_T|\exp(-H\tau)|\Psi_T\rangle}$$

$$= O_0 + 2\mathrm{Re}\left(\frac{\langle\Psi_0|O|\Psi_1\rangle}{\langle\Psi_0|\Psi_0\rangle} - O_0\frac{\langle\Psi_0|\Psi_1\rangle}{\langle\Psi_0|\Psi_0\rangle}\right) + \mathcal{O}(V_C^2)$$

$$\mathcal{M}_k(O) = \int \mathcal{D}cP(c+\bar{c})\langle\cdots O\cdots M(s_k,c+\bar{c})\cdots\rangle_T$$

$$= \mathcal{M}(s)\exp\left(\frac{\bar{c}^2}{2}\right)\int \mathcal{D}c\exp\left(-\frac{c^2}{2}+\epsilon\right)$$

N2LO ptQMC calculation with 3NF



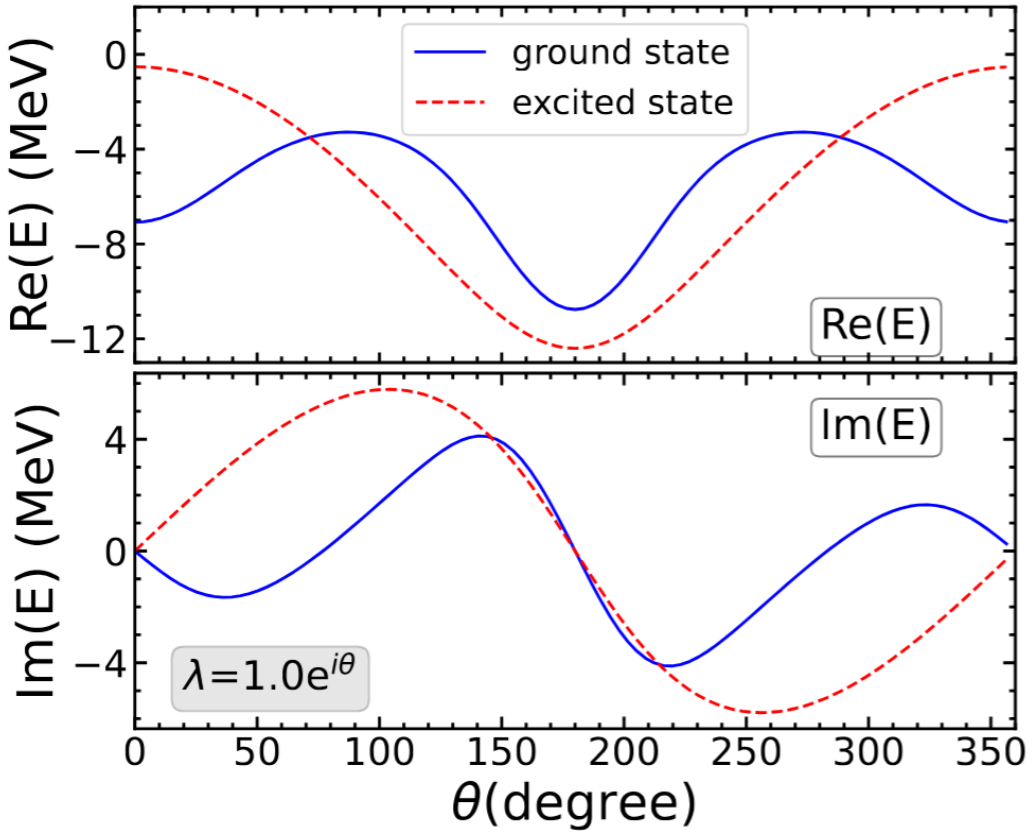
N2LO calculation with three-body interaction
Phys. Rev. Lett. 128, 242501 (2022)

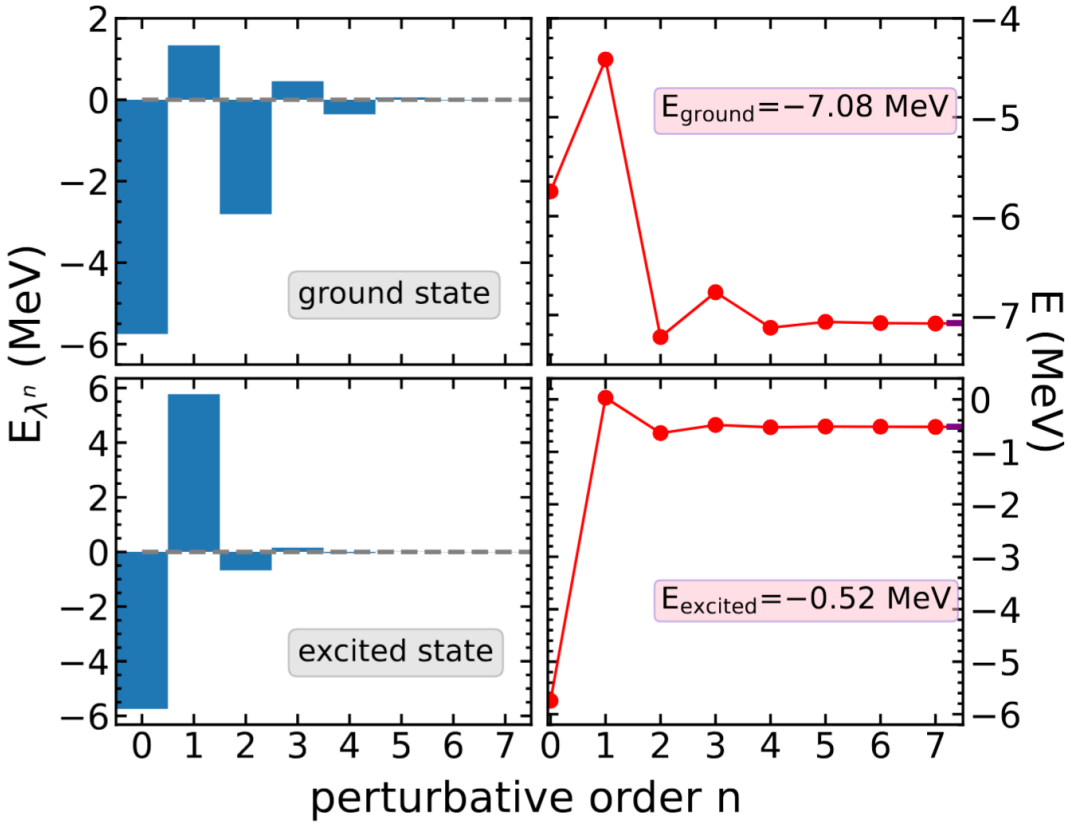
	E_0	δE_1	E_1	δE_2	E_2	$E_{\rm exp}$
^{3}H	$-7.41(3)$	$+2.08$	$-5.33(3)$	-2.99	$-8.32(3)$	-8.48
^{4}He	$-23.1(0)$	-0.2	$-23.3(0)$	-5.8	$-29.1(1)$	-28.3
^{8}Be	$-44.9(4)$	-1.7	$-46.6(4)$	-11.1	$-57.7(4)$	-56.5
^{12}C	$-68.3(4)$	-1.8	$-70.1(4)$	-18.8	$-88.9(3)$	-92.2
^{16}O	$-94.1(2)$	-5.6	$-99.7(2)$	-29.7	$-129.4(2)$	-127.6
^{16}O†	$-127.6(4)$	$+24.2$	$-103.4(4)$	-24.3	$-127.7(2)$	-127.6
^{16}O‡	$-161.5(1)$	$+56.8$	$-104.7(2)$	-22.3	$-127.0(2)$	-127.6

NLO ptQMC calculation for ^{2}H in a 7 fm box

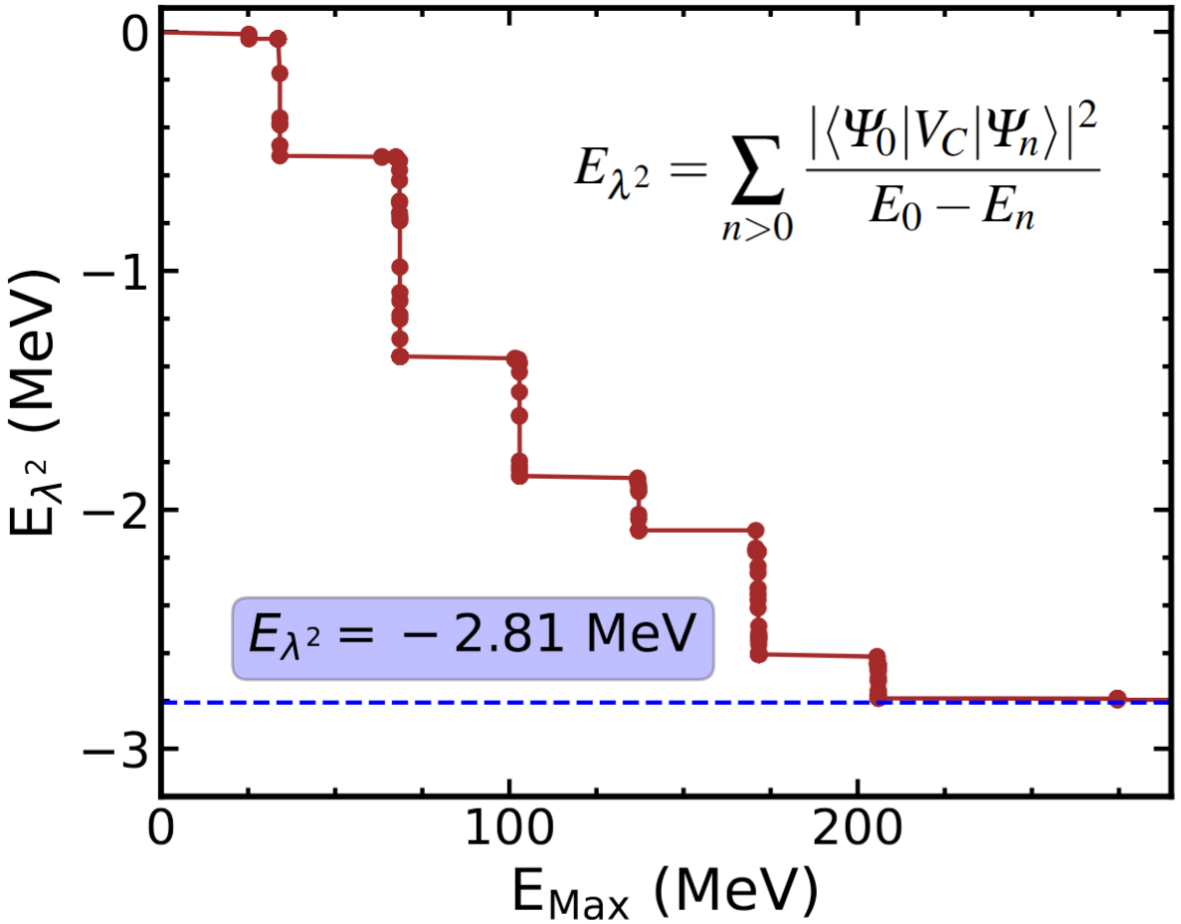
Deuteron energy can be expanded using Cauchy integral formula

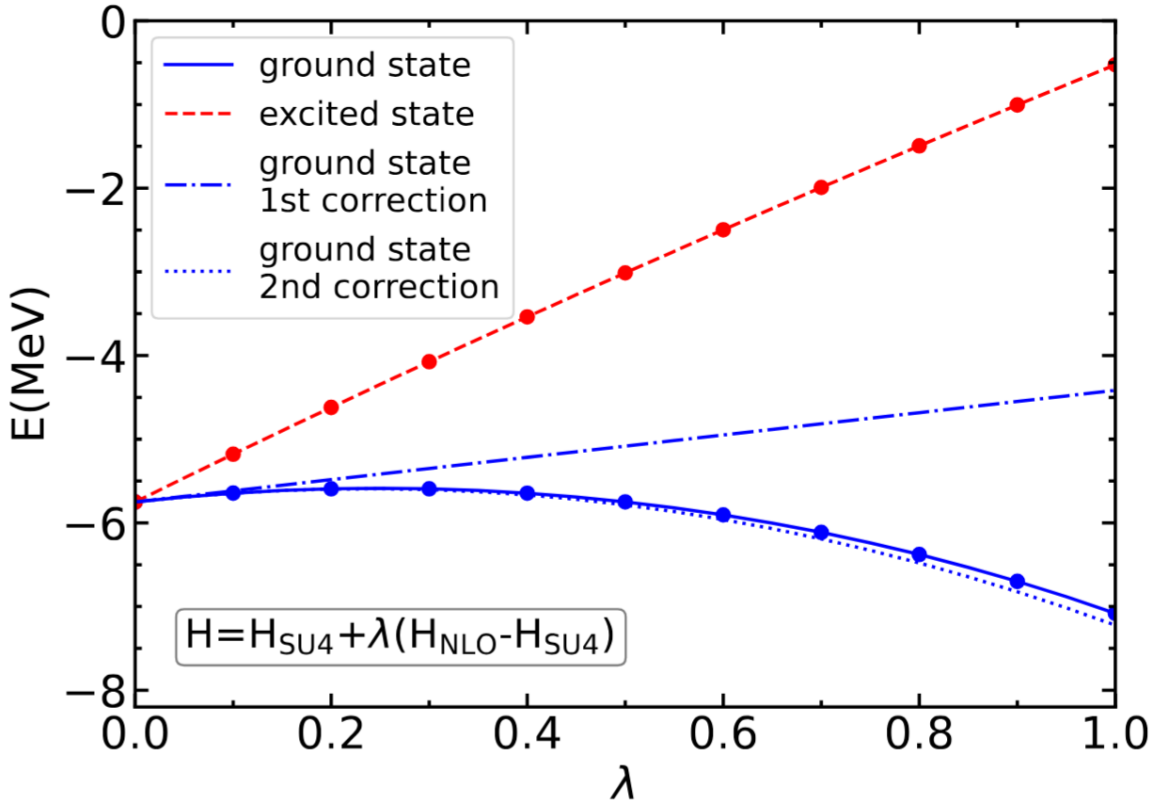
$$\left.\frac{\partial^n E}{\partial \lambda^n}\right|_{\lambda=0} = \frac{n!}{2\pi i}\oint_{|\lambda|=1}\frac{E(\lambda)}{\lambda^{n+1}}d\lambda$$



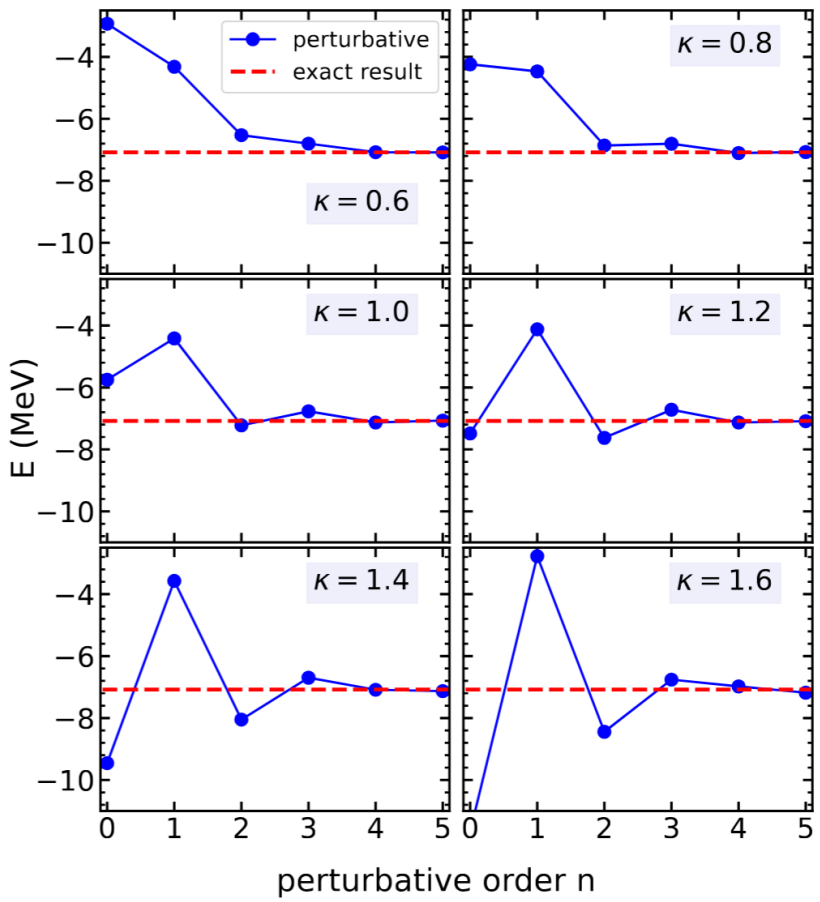


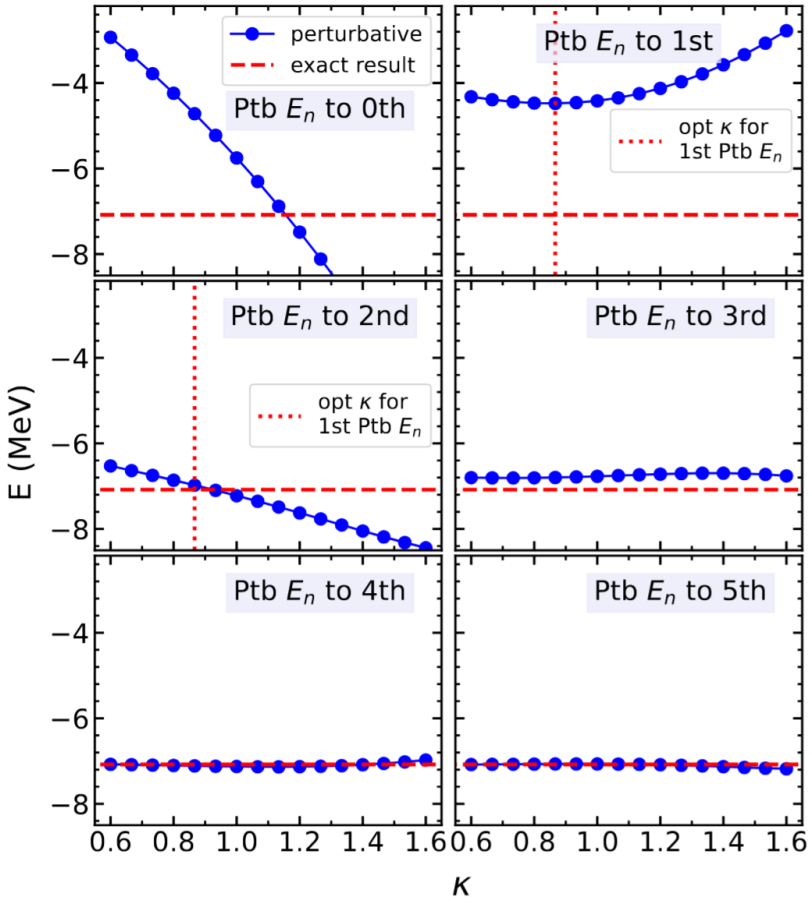
Comparison with Rayleigh-Schrodinger scheme





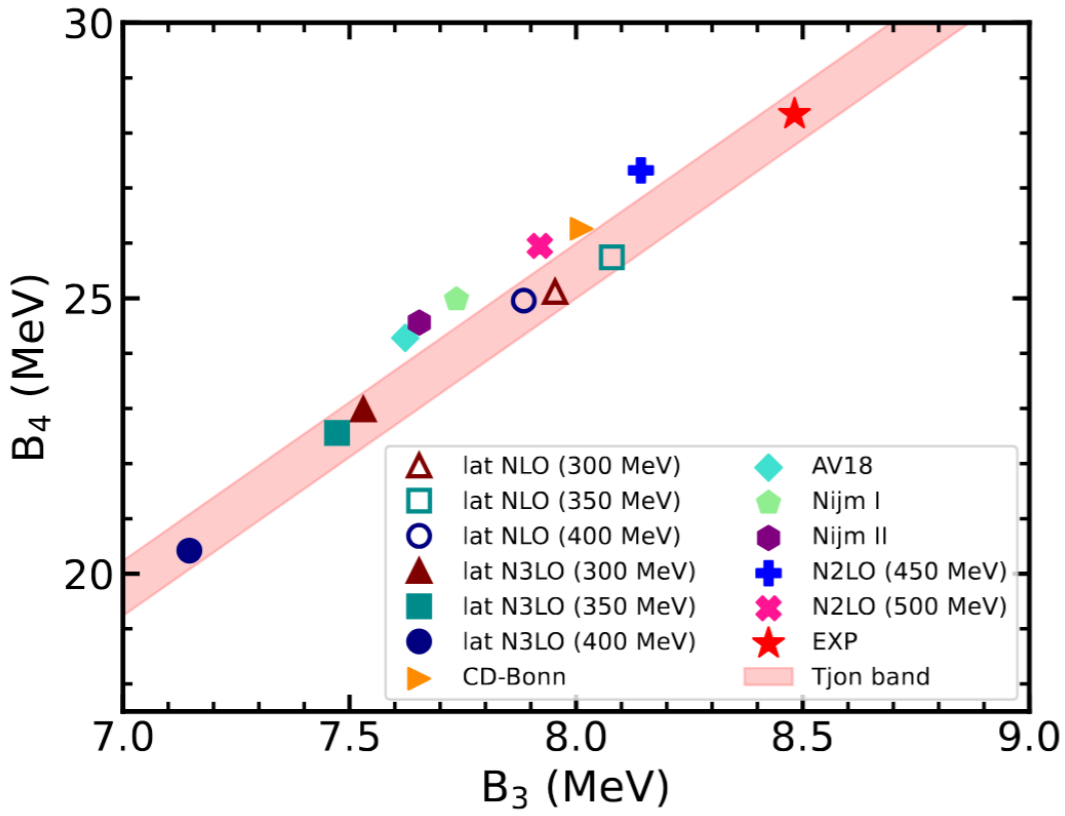
Perturbative expansion from random initial Hamiltonians





- The strength of the SU4 Interaction is rescaled by a constant kappa
- The convergence is universal, exact binding energies can be recovered with any initial guess!
- The precision can be enhanced by carefully finding a optimized H0

Tjon line from ptQMC calculations at N3LO



J. Liu, T. Wang, B.L., arXiv:2502.13565 (2025)

- He4 energies are calculated with ptQMC
- H3 energies are calculated with exact diagonalization

- Cancellations of various perturbative corrections locate the He4 energies on the Tjon line

300, 350 and 400 denotes the momentum cutoff in MeV

	E_{tot}	E_{SU4}	E_{λ^1}	E_{λ^2}	E_{μ^1}	$E_{\lambda^1\mu^1}$
NLO (300)	−25.5(1)	−23.36(4)	3.0	−5.1(1)	0	0
N^3LO (300)	−23.4(1)	−23.36(4)	3.0	−5.1(1)	2.7	−0.6
NLO (350)	−26.1(1)	−23.36(5)	3.2	−5.9(1)	0	0
N^3LO (350)	−22.9(1)	−23.36(5)	3.2	−5.9(1)	4.4	−1.2
NLO (400)	−25.3(1)	−23.37(4)	7.0	−9.0(1)	0	0
N^3LO (400)	−20.9(1)	−23.37(4)	7.0	−9.0(1)	6.3	−1.9

Summary and Perspective

- Perturbative Quantum Monte Carlo method is an efficient tool for solving nuclear many-body problems.
  - We need a high-quality zeroth order Hamiltonian without the sign problem, which can be constructed by fitting to finite nuclei.
  - We need a careful decomposition of the interaction, either by power counting or the feasibility for the Monte Carlo calculations.

- Things to do:
  - Uncertainty quantifications
  - Higher order perturbative corrections, especially for shallow bound states
  - Higher order corrections for density, radius, etc.
  - Benchmark with other *ab initio* methods
  - …

Thank you for you attention!