Recent progress in lattice effective field theory

Bing-Nan Lü[1]
吕炳楠
Nuclear Lattice EFT Collaboration

[1]Graduate School of China Academy of Engineering Physics, Beijing

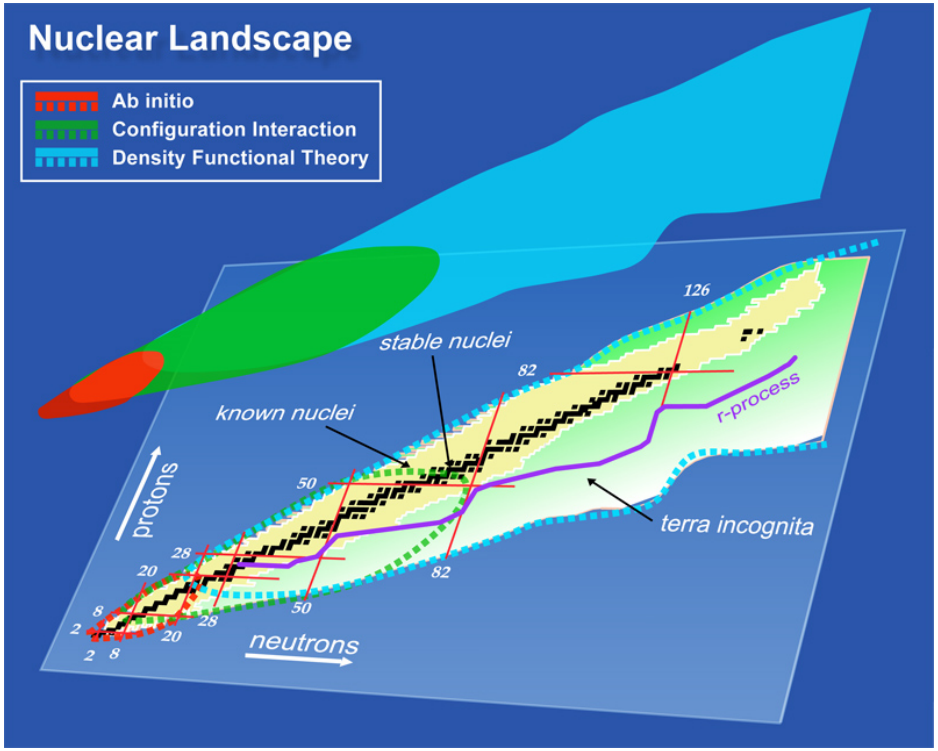
7th Symposium on Chiral Effective Field Theory (NanJing) Oct-17-2022

Road map - Towards a comprehensive description of the nucleus

- ***Ab initio* methods**:
  Microscopic interactions
  Lattice QCD (A = 0, 1, 2, ...)
  NCSM, F-Y, GFMC (A = 3-16)
  Coupled cluster, IMSRG (A = 16-100)

- **Configuration-interaction theories**:
  Phenomenological interactions
  Shell model

- **Density functional theories**:
  Phenomenological interactions
  mean field approximation
  Skyrme, Gogny, RMF, ...



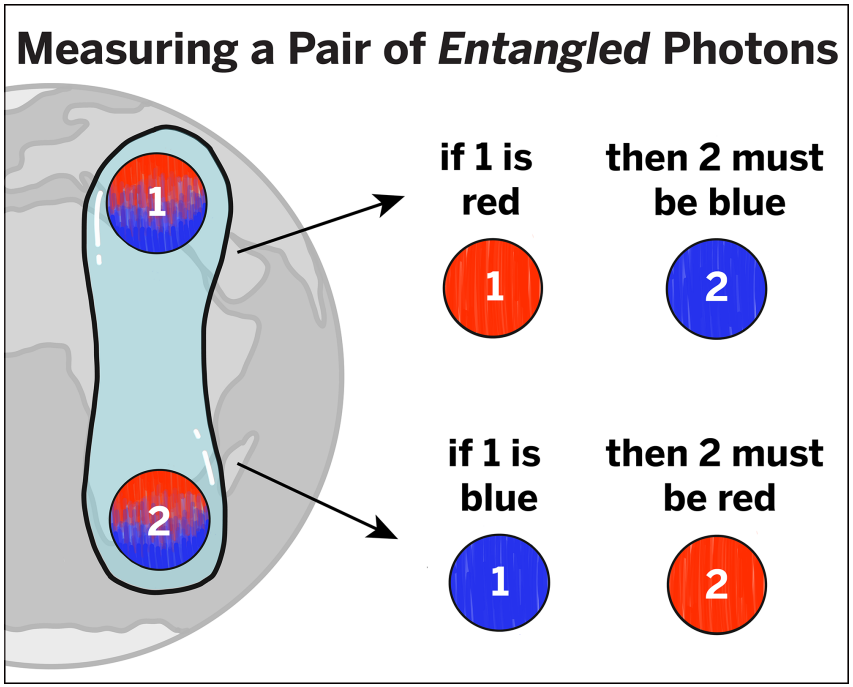
Lattice EFT: *Ab initio* method for A = 3-100

Why need nuclear ab initio methods

Mean field models are useful

but **quantum correlations** not included

$$|\Psi\rangle = 1/\sqrt{2}\,[|0\rangle|1\rangle + |1\rangle|0\rangle]$$



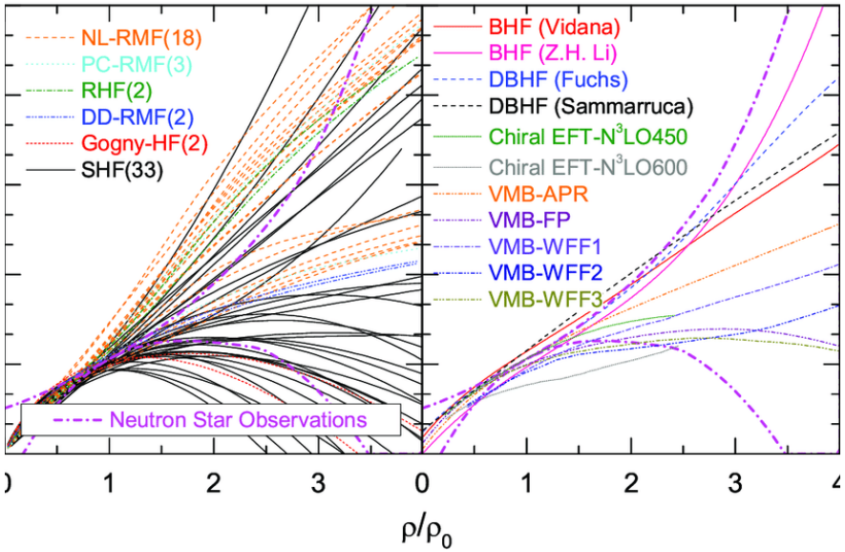
In mean field models, motion of particle 1

is independent of other particles

$$P(1,2) = P(1) \times P(2)$$

Predictions are model-dependent

Example: symmetry energy

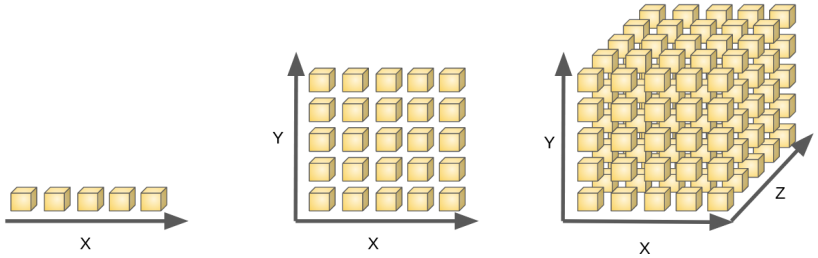


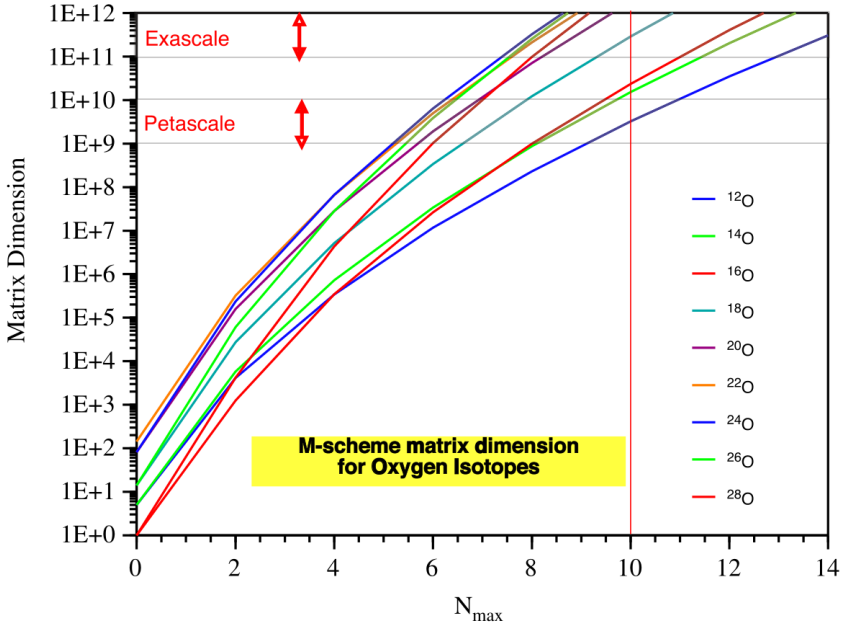
N.-B. Zhang and B.-A. Li, EPJA 55, 39 (2019)

Symptom 1: Lack of quantum correlations
Symptom 2: Imprecise nuclear forces
Recipe: **Exactly** solve many-body Schrödinger equation with **precise** nuclear force $\Longrightarrow$ **nuclear ab initio methods**

Dimensionality curse in nuclear many-body problems

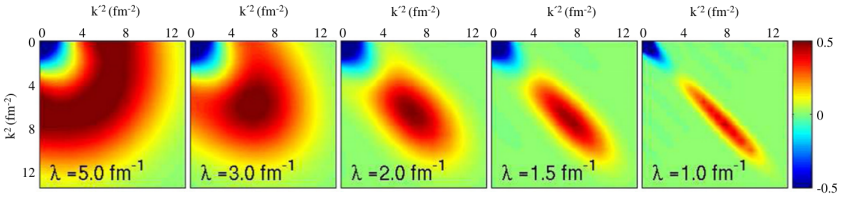
Exponential increase of resources



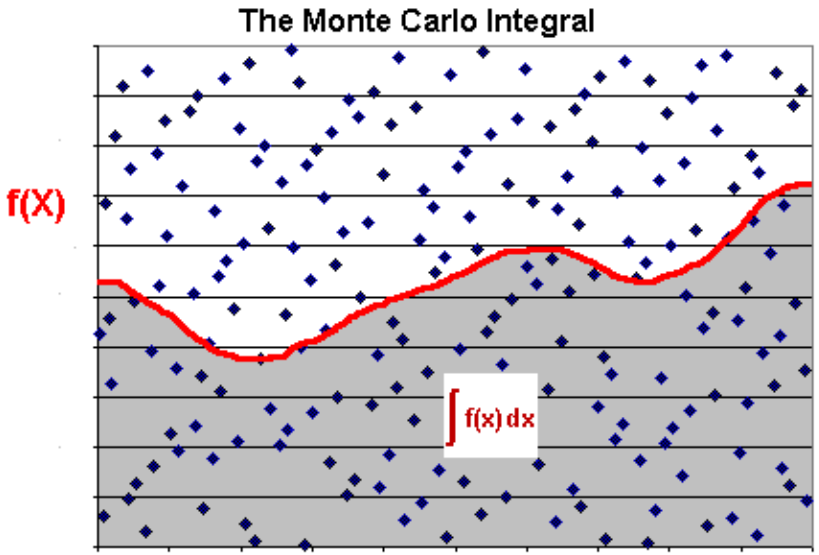


PRC 101, 014318 (2020)

Solution 1: Reduce effective Hilbert space with SRG evolution



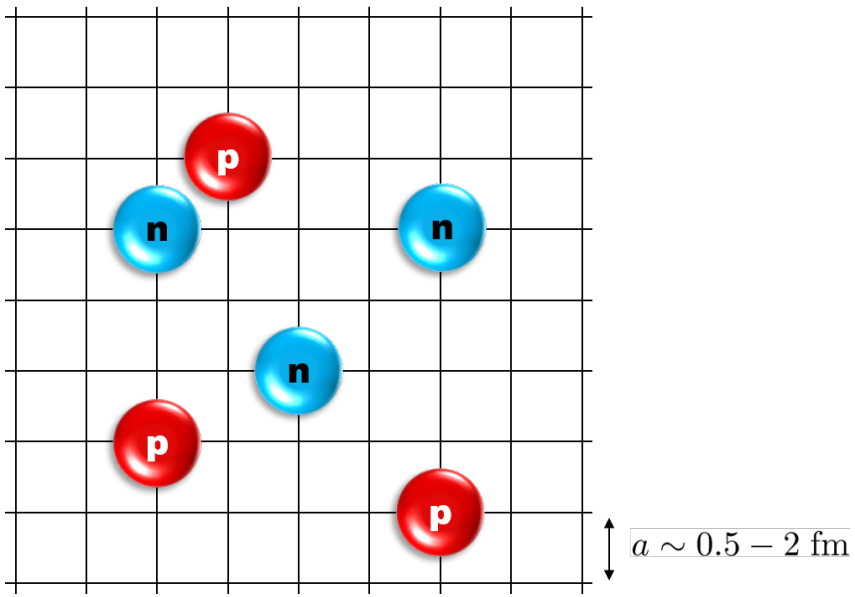
Solution 2: Monte Carlo algorithms



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 ($\sim$chiral symmetry breaking scale)
- Protons & neutrons interacting via **short-range, δ-like** and **long-range, pion-exchange** interactions
- Exact method, polynomial scaling ($\sim A^2$)

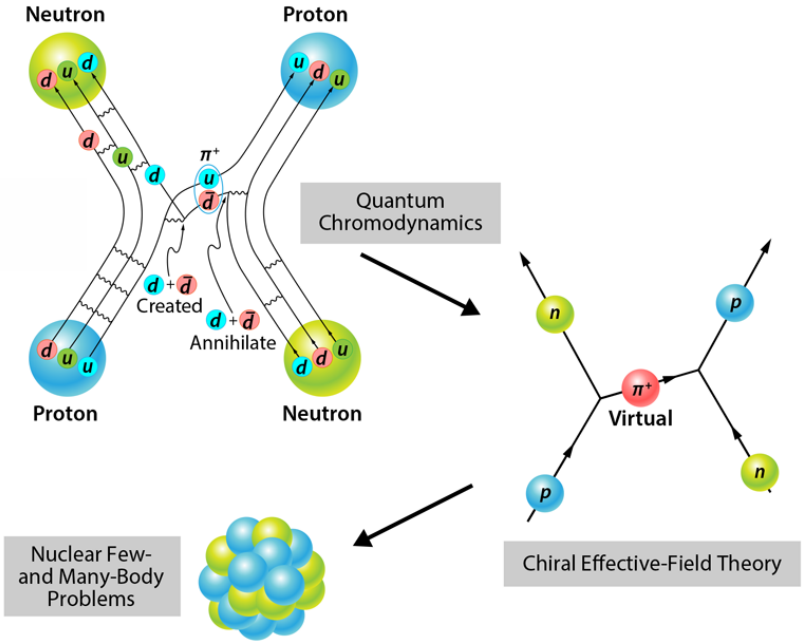


Lattice adapted for nucleus

Introduction: Chiral effective field theory

Chiral EFT: The low-energy equivalence of the QCD
Weinberg (1979,1990,1991), Gasser, Leutwyler (1984,1985)

- Proton (uud), neutron (udd), pion ($u\bar{d}$)
- Spontaneously broken chiral symmetry: $SU(2)_L \times SU(2)_R \rightarrow SU(2)_V$
- Goldstone theorem implies a light pion: Long-range part of the nuclear force
- Contact terms: Short-range part of the nuclear force
- Hard scale: $\Lambda_\chi \sim 1$ GeV: Chiral EFT works for momentum $Q \ll \Lambda_\chi$



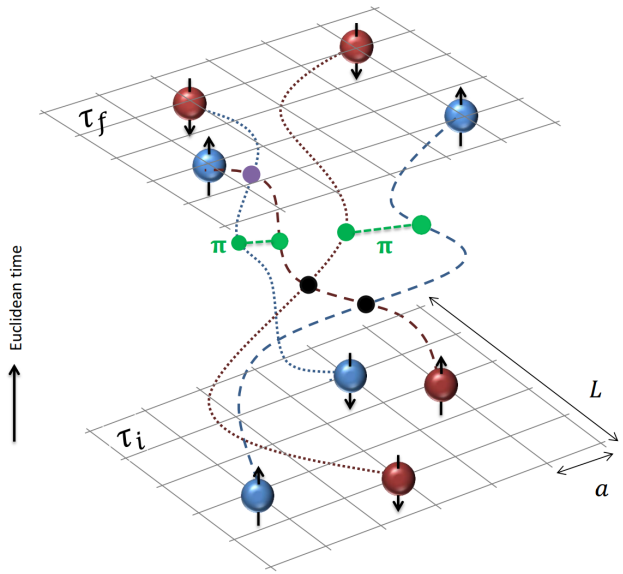
Quarks confined in nucleons and pions

Simulate many-body system in LEFT

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

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

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



- At finite temperature:

$$\langle O\rangle = \frac{\text{Tr}\left(e^{-\beta H}\hat{O}\right)}{\text{Tr}\left(e^{-\beta H}\right)}$$

For a two-body $\delta-$ function interaction on the lattice

$$H = \sum_{\boldsymbol{nn'}} -\psi^\dagger_{\boldsymbol{n}} \frac{\nabla^2_{\boldsymbol{nn'}}}{2M}\psi_{\boldsymbol{n'}} + C\sum_{\boldsymbol{n}} :(\psi^\dagger_{\boldsymbol{n}}\psi_{\boldsymbol{n}})^2:$$

$\psi^\dagger_{\boldsymbol{n}}(\psi_{\boldsymbol{n}})$ create (annihilate) a partice at mesh point $\boldsymbol{n}$.
N-N interactions decomposed with **Hubbard–Stratonovich transformation:**

$$:\exp(-a_t H):= \int \prod_{\boldsymbol{n}} ds_{\boldsymbol{n}} :\exp\left[\sum_{\boldsymbol{n}}\left(-\frac{s^2_{\boldsymbol{n}}}{2} + a_t\psi^\dagger_{\boldsymbol{n}}\sum_{\boldsymbol{n'}}\frac{\nabla^2_{\boldsymbol{nn'}}}{2M}\psi_{\boldsymbol{n'}} + \sqrt{-a_t C}\, s_{\boldsymbol{n}}\psi^\dagger_{\boldsymbol{n}}\psi_{\boldsymbol{n}}\right)\right]:$$

Imaginary time extrapolation to find ground state

Samples are generated by
Markov Chain Monte Carlo

Observables calculated as $\langle O \rangle = (1/N)\sum_{i=1}^{N} O_i$

Error scales as $\varepsilon \sim \mathscr{O}(1/\sqrt{N})$

Number of samples $N \sim 10^3 \sim 10^6$

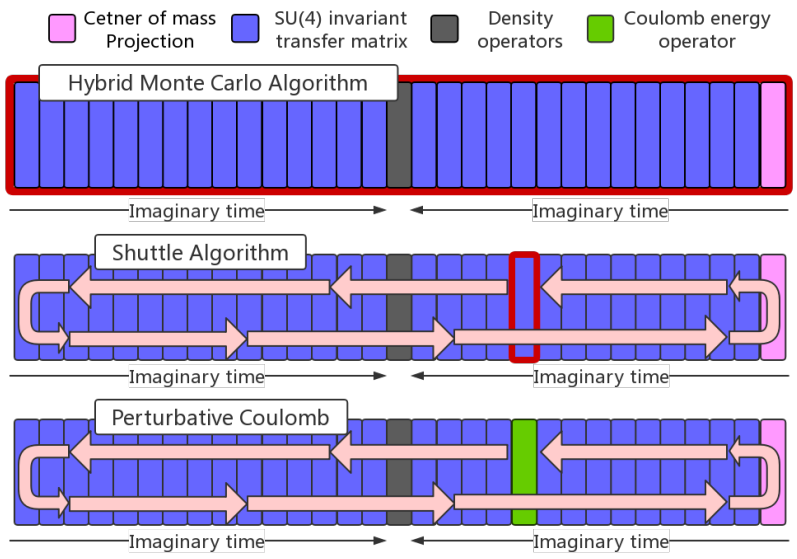
Total energies at large t follow

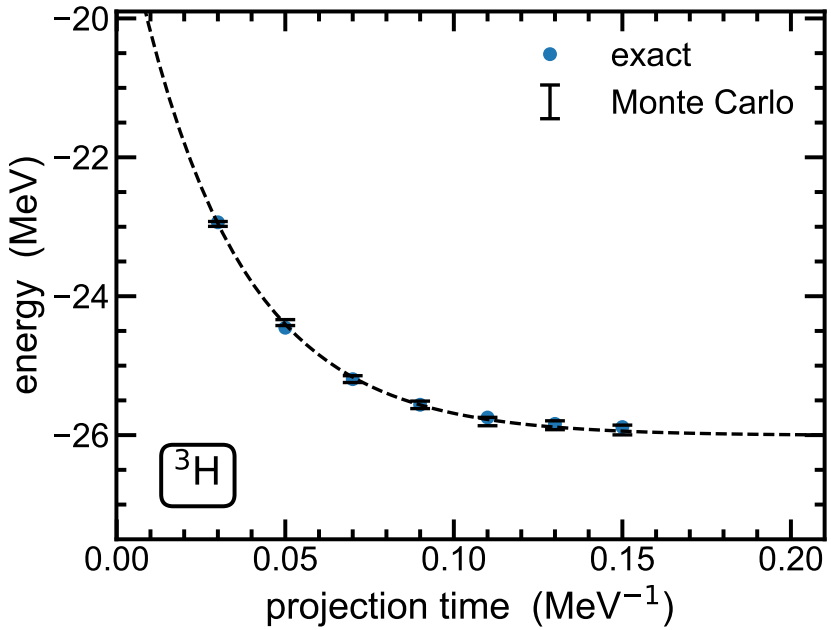
$$E_A(t) = E_A(\infty) + c\exp[-\Delta E \tau].$$

For any inserted operator $\mathscr{O}$,

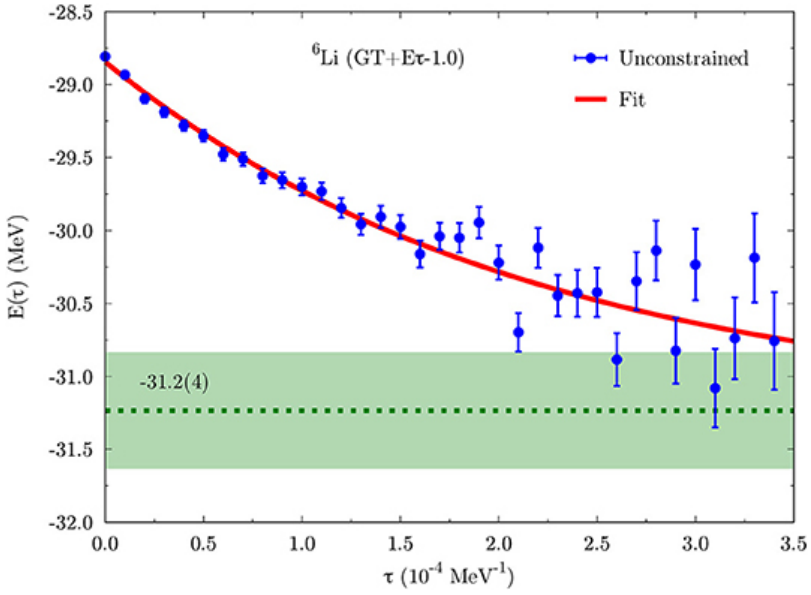
$$\mathscr{O}_A(\tau) = \mathscr{O}_A(\infty) + c'\exp[-\Delta E \tau/2],$$

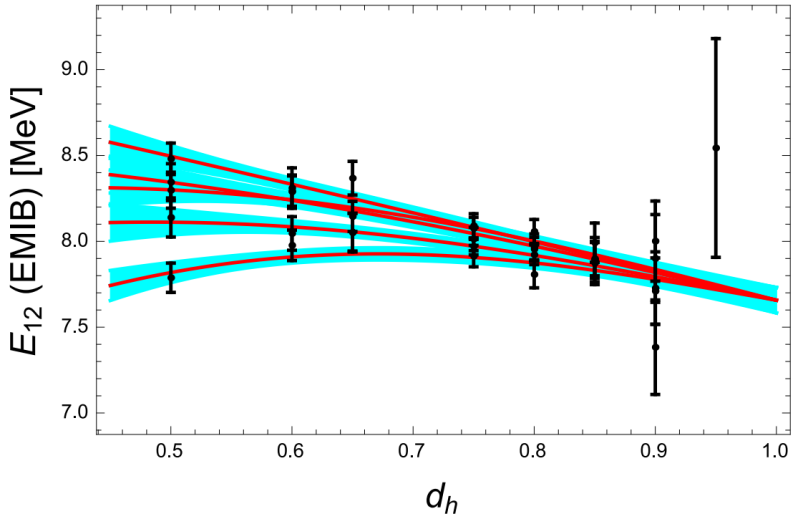
c, c', ΔE are fitting parameters.

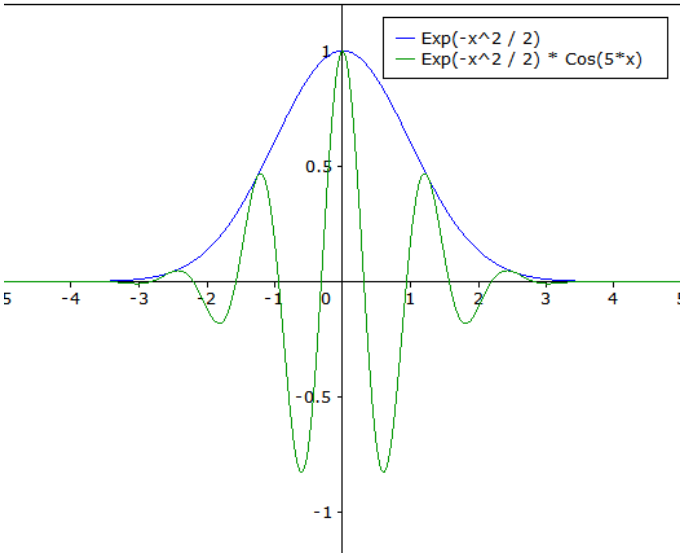




Monte Carlo sign problem







- Sign problem: Monte Carlo works well for well-behaved functions, however, sometimes the integral becomes highly oscillating.
- QMC sign problem comes from the fermion anti-symmetrization.
- Split $H = H_0 + \lambda V_C$. H_0: w/o sign problem; V_C: w/ sign problem.
- **Solution 1**: numerical extrapolation from $\lambda = 0$ to $\lambda = 1$.
- **Solution 2**: perturbative calculation near $\lambda = 0$.

Monte Carlo sign problem

Monte Carlo methods are powerful, but limited by sign problem
Fortunately, there are sign-problem-free systems with specific symmetries

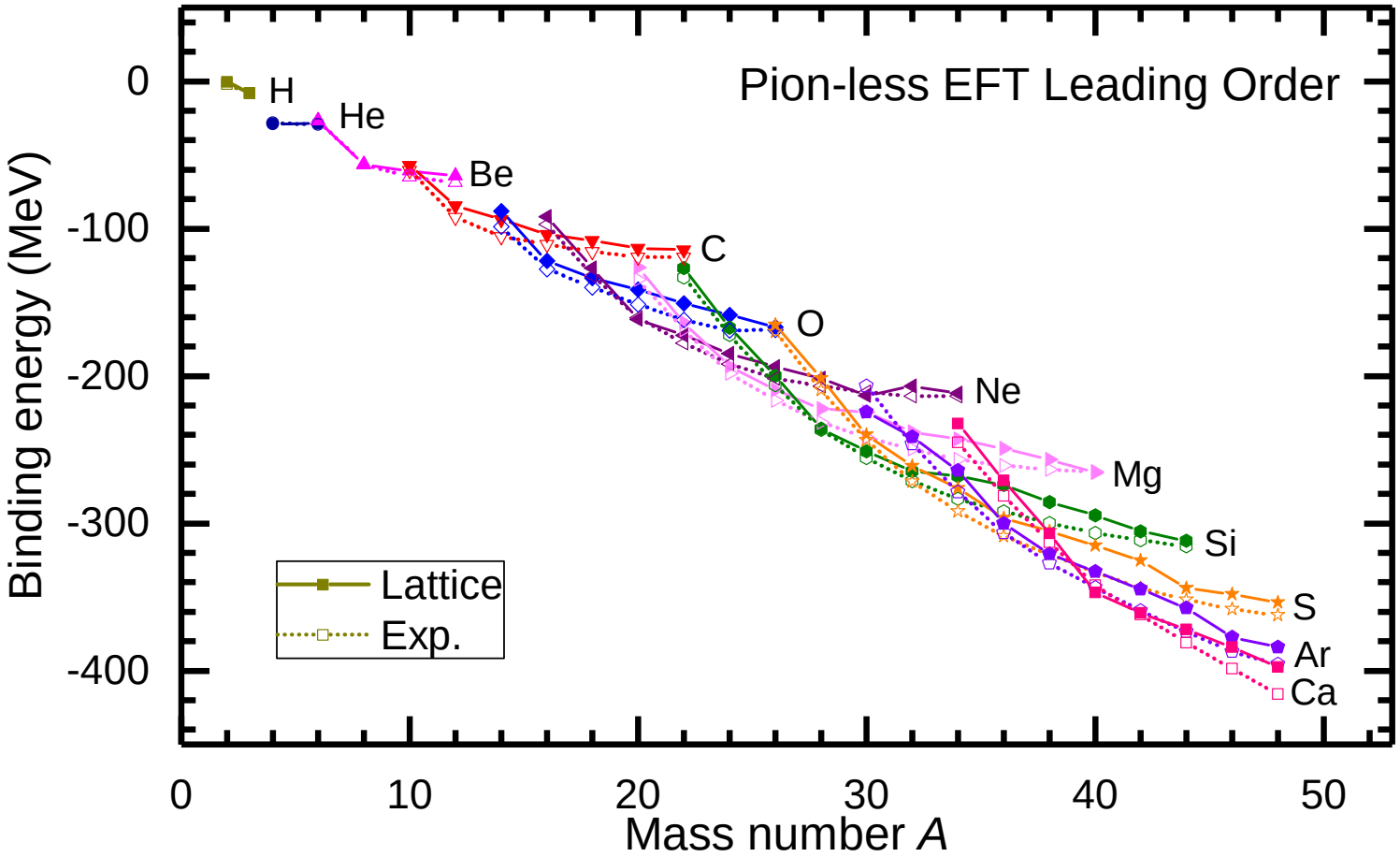
"For example, the **nuclear systems** can be simulated with a SU(4) symmetric interaction in lattice EFT[18], or with simplified interactions such as AV8' with Green's function Monte Carlo method[44]. In **condensed matter physics**, the square-lattice Heisenberg model can be free from sign problem for specific parametrizations[45], and unified principles for designing sign-problem-free actions for lattice fermionic models are proposed[46-48]. In these works it was revealed that the sign problem can be avoided by imposing certain symmetries, such as time-reversal symmetry[46], Majorana positivity[47] or Majorana-time-reveral symmetry[48]. For **ultracold atoms**, spin- 3/2 fermionic system with exact SO(5) symmetry can be sign-problem-free[49] and more general rules for finding such systems are discussed[50]. The **unitary Fermi gas** with equal number of spin-up and spin-down particles provides another important system that can be simulated with QMC without the sign problem[51, 52]. In **quantum chemistry**, it is shown that the sign problem can be alleviated by optimizing the wave functions[53], or introducing efficiently computable basis changes[54]."

Nuclear force has an approximate SU(4) symmetry
In this SU(4) limit the nuclear force is independent of spin-isospin and can be simulated without sign problem $\Longleftarrow$ **How good is this approximation?**

Nuclear binding from a SU(4) nuclear force

Ab initio calculation = **precise nuclear force** + **exactly solving Schrödinger equations**

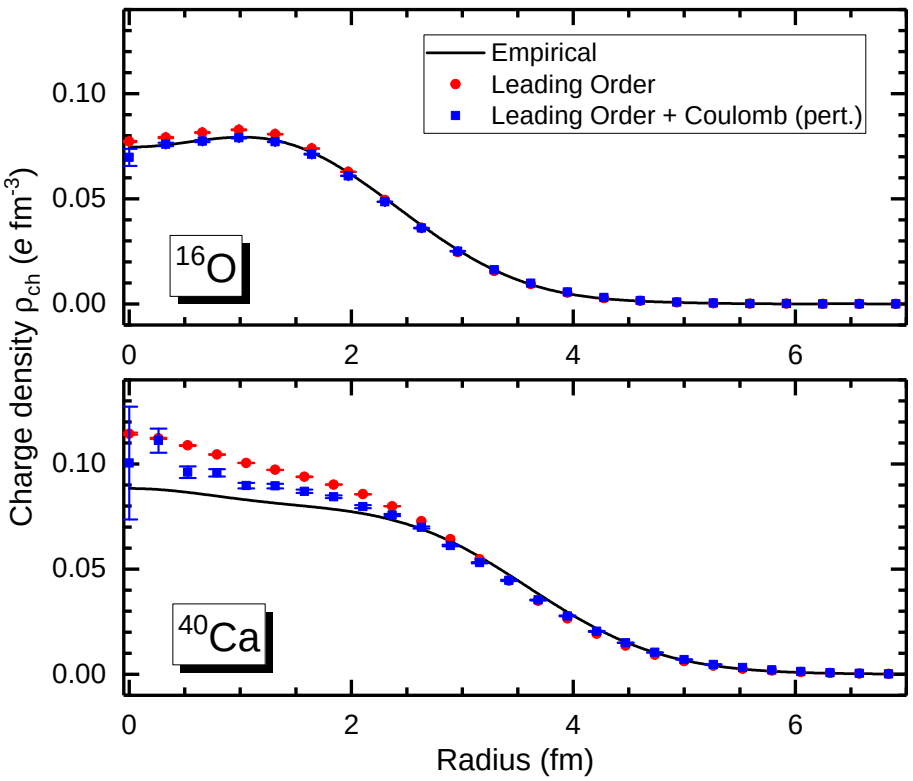
In full quantum Monte Carlo simulations, **equations are solved exactly**
A simple SU(4) interaction (central force only!) can describe the nuclear binding

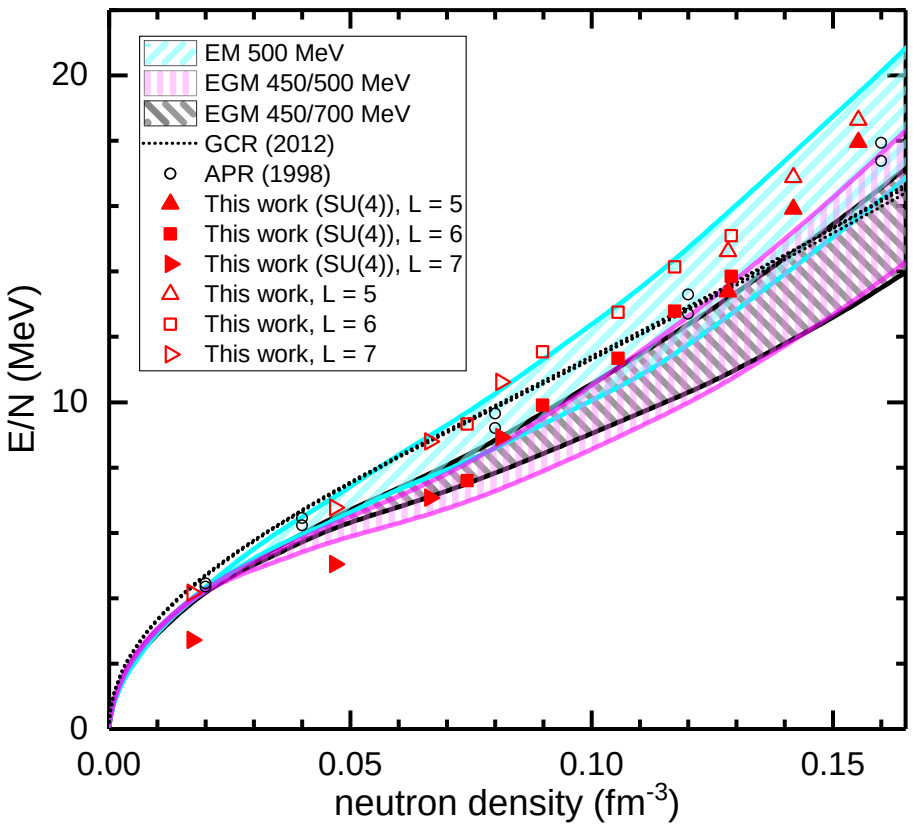


Lu et al., Phys. Lett. B 797, 134863 (2019)

Charge density and neutron matter from a SU(4) force

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





Lu et al., Phys. Lett. B 797, 134863 (2019)

Trade-off in Monte Carlo simulations

- Simplified interactions with high symmetry $\Longrightarrow$Sign-problem-free, exactly solvable with MC
- Realistic complex interactions $\Longrightarrow$Severe sign problem, can only be approximately solved with mean field methods

Is it possible to exactly solve a realistic interaction with MC?

Idea: Starting from a simplified sign-problem-free interaction add corrections with perturbation theory

- Much weaker sign problem in perturbative calculations
- Most quantum correlations included non-perturbatively
- Systematically improvable order by order, can check convergence

Higher order perturbation theory is complicated
(e.g., exponentially increasing number of Feynman diagrams)
Adaptation to MC is even more challenging!

Reyleigh-Schrödinger perturbation theory

For a Hamiltonian $H = H^{(0)} + \lambda V_C$,

- In conventional stationary perturbation theory:

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

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

- However, in projection Monte Carlo algorithms,

$$E_{\text{g.s.}} = \lim_{\tau \to \infty} \exp(-\tau H) |\Psi_T\rangle$$

  targets the ground states (or low-lying states) directly.
- In projection methods, excited states are very expensive. $\leftarrow$ required for 2nd order energy or 1st order wave function!
- All projection QMC calculations use at most first order perturbation theory.

Perturbative Monte Carlo (ptQMC) algorithm

We can expand $|\Psi\rangle$ against V_C,

$$|\Psi\rangle = \lim_{L_t\to\infty} M^{L_t/2}|\Psi_T\rangle = |\Psi_0\rangle + |\delta\Psi_1\rangle + \mathscr{O}(V_C^2), \tag{1}$$

with the wave functions defined as

$$|\Psi_0\rangle = \lim_{L_t\to\infty} M_0^{L_t/2}|\Psi_T\rangle, \qquad |\delta\Psi_1\rangle = \lim_{L_t\to\infty}\sum_{k=1}^{L_t/2} M_0^{L_t/2-k}(M-M_0)M_0^{k-1}|\Psi_T\rangle,$$

$$E = E_0 + \delta E_1 + \delta E_2 + \mathscr{O}(V_C^3),$$

where the partial energy contributions at each orders are

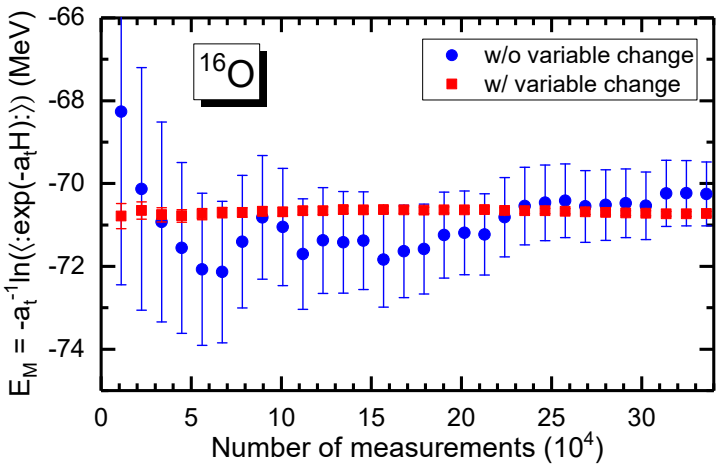
$$\begin{aligned} E_0 &= \langle\Psi_0|(K+V)|\Psi_0\rangle/\langle\Psi_0|\Psi_0\rangle, \\ \delta E_1 &= \langle\Psi_0|V_C|\Psi_0\rangle/\langle\Psi_0|\Psi_0\rangle, \\ \delta E_2 &= \left(\langle\Psi_0|V_C|\delta\Psi_1\rangle - \delta E_1 \mathrm{Re}\langle\delta\Psi_1|\Psi_0\rangle\right)/\langle\Psi_0|\Psi_0\rangle, \end{aligned} \tag{2}$$

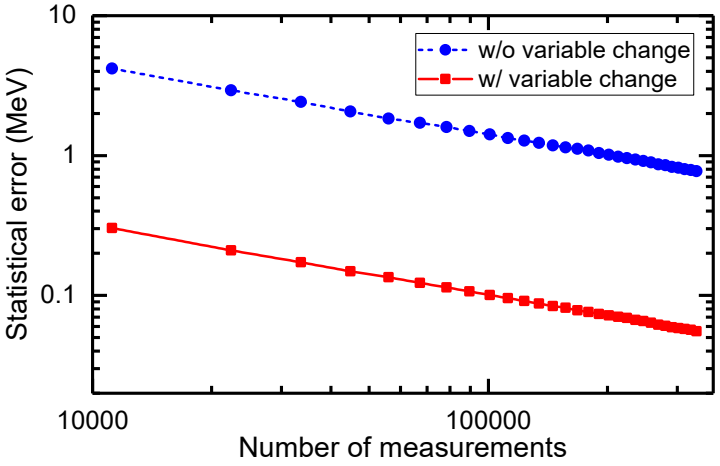
in which all matrix elements and overlaps can be expressed with,

$$\begin{aligned} \mathscr{M}(O) &= \langle\Psi_T|M_0^{L_t/2}OM_0^{L_t/2}|\Psi_T\rangle, \\ \mathscr{M}_k(O) &= \langle\Psi_T|M_0^{L_t/2}OM_0^{L_t/2-k}MM_0^{k-1}|\Psi_T\rangle. \end{aligned}$$

Lu *et al.*, PRL 128, 242501 (2022)

ptQMC with realistic chiral interaction





Perturbed amplitude can be transformed into an approximate Gaussian integral with a variable change. Note that

$$\langle \exp(\sqrt{-a_t C} s\rho)\rangle_T \approx \exp(\sqrt{-a_t C} s \langle\rho\rangle_T)$$

$$\begin{aligned}\mathscr{M}_k(O) &= \langle \Psi_T | M_0^{L_t/2} O M_0^{L_t/2-k} M M_0^{k-1} | \Psi_T\rangle \\ &= \int \mathscr{D}c P(c+\bar{c}) \langle \cdots O \cdots M(s_k, c+\bar{c}) \cdots \rangle_T \\ &= \mathscr{M}(s) \exp\left(\frac{\bar{c}^2}{2}\right) \int \mathscr{D}c \exp\left(-\frac{c^2}{2} + \varepsilon\right)\end{aligned}$$

$\bar{c}(\boldsymbol{n}) = \frac{\partial}{\partial c(\boldsymbol{n})} \ln\langle \cdots M(s_k, c) \cdots \rangle_T \Big|_{c=0}$ is a constant field easy to calculate

Integral over c calculated with MC

Left panel: Test calculation of the transfer matrix energy $E = -\ln\langle : \exp(-a_t H) : \rangle / a_t$
Lu *et al.*, PRL 128, 242501 (2022)

Benchmark Hamiltonian: N^{2}LO chiral Hamiltonian

We benchmark the ptQMC algorithm with a N^{2}LO chiral Hamiltonian
$H = K + V_{2\mathrm{N}} + V_{3\mathrm{N}} + V_{\mathrm{cou}}$

$$
\begin{aligned}
V_{2N} = & \Big[B_1 + B_2(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2) + C_1 q^2 + C_2 q^2(\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2) + C_3 q^2(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2) + C_4 q^2(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)(\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2) \\
& + C_5\frac{i}{2}(\boldsymbol{q}\times\boldsymbol{k})\cdot(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2) + C_6(\boldsymbol{\sigma}_1\cdot\boldsymbol{q})(\boldsymbol{\sigma}_2\cdot\boldsymbol{q}) + C_7(\boldsymbol{\sigma}_1\cdot\boldsymbol{q})(\boldsymbol{\sigma}_2\cdot\boldsymbol{q})(\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)\Big] e^{-\Sigma_{i=1}^{2}\left(p_i^6+p_i'^6\right)/\Lambda^6} \\
& - \frac{g_A^2 f_\pi(q^2)}{4F_\pi^2}\left[\frac{(\boldsymbol{\sigma}_1\cdot\boldsymbol{q})(\boldsymbol{\sigma}_2\cdot\boldsymbol{q})}{q^2+M_\pi^2} + C_\pi'\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\right](\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2) \\
V_{3\mathrm{N}} = & \frac{c_E}{2F_\pi^4\Lambda_\chi} e^{-\Sigma_{i=1}^{3}\left(p_i^6+p_i'^6\right)/\Lambda^6}
\end{aligned}
$$

with C_{1-7}, g_A, c_E etc. **low energy constants** fitted to N-N scattering or π-N scattering data, $\Lambda = 340$ MeV is the **momentum cutoff**

LEC	B_1	B_2	C_1	C_2	C_3
	-2.443	-0.125	0.143	-0.012	-0.013
LEC	C_4	C_5	C_6	C_7	c_E
	-0.020	0.273	0.0	-0.078	0.712

Table: Fitted LECs' in lattice unit

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

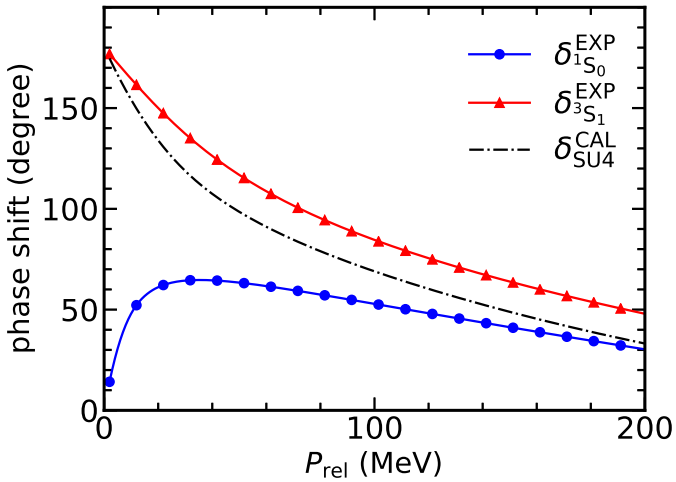
$$\tilde{\rho}(\boldsymbol{n}) = \sum_i \tilde{a}_i^\dagger(\boldsymbol{n})\tilde{a}_i(\boldsymbol{n}) + s_L \sum_{|\boldsymbol{n}'-\boldsymbol{n}|=1} \sum_i \tilde{a}_i^\dagger(\boldsymbol{n}')\tilde{a}_i(\boldsymbol{n}'), \tag{3}$$

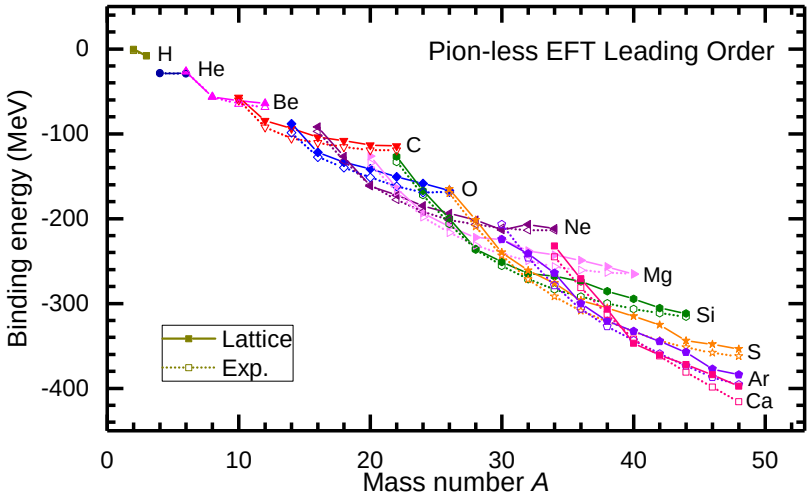
where i is the joint spin-isospin index

$$\tilde{a}_i(\boldsymbol{n}) = a_i(\boldsymbol{n}) + s_{NL} \sum_{|\boldsymbol{n}'-\boldsymbol{n}|=1} a_i(\boldsymbol{n}'). \tag{4}$$

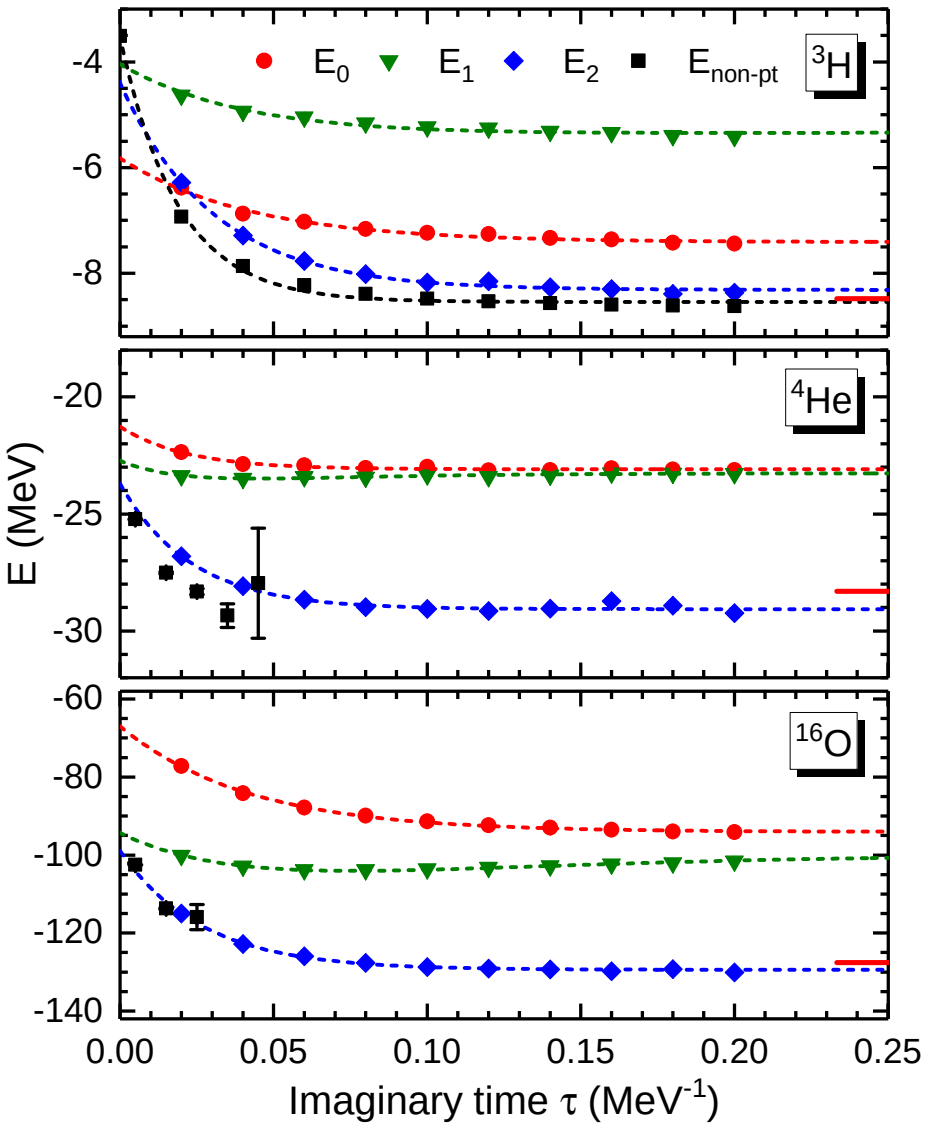
In this work we use a lattice spacing $a = 1.32$ fm and the parameter set

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





ptQMC with realistic chiral interaction

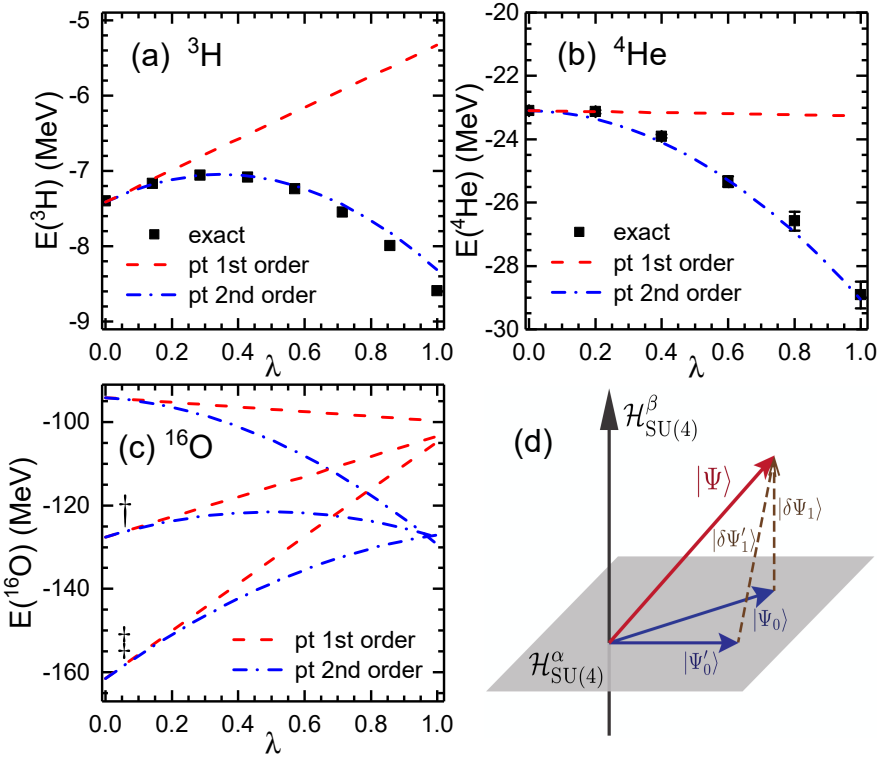


- We split $H = H_0 + (H - H_0)$ and perform perturbative calculations
- E_0 is the ground state of H_0
- $E_1 = E_0 + \delta E_1$ is the first order corrected energy
- $E_2 = E_1 + \delta E_2$ is the second order corrected energy
- $E_{\mathrm{non-pt}}$ is the exact solution (~infinite order)
- Red bars on the right: Experiments Lu *et al.*, PRL 128, 242501 (2022)

For ^{4}He and ^{16}O, sign problem prevent us from going to large τ, resulting in large statistical errors. But no need to worry,

Perturbation theory can save us!

Abnormally large second order corrections



- Though consistent with the exact solutions, we found abnormally large second order energy corrections
- We write $H = H_0 + \lambda(H - H_0)$ and study the λ-dependence of energies $(0 \leq \lambda \leq 1)$
- $E_1 = E_0 + \lambda \delta E_1$ is a straight line
- $E_2 = E_1 + \lambda^2 \delta E_2$ is a parabola
- $E_{\mathrm{non-pt}}$ is the exact solution
- For ^{16}O we use three different H_0 Lu *et al.*, PRL 128, 242501 (2022)

As H_0 respects the SU(4) symmetry, the wave function $|\Psi_0\rangle$ must belong to one of its irreducible representations (irreps). The full Hamiltonian H breaks the SU(4) symmetry, thus its ground state $|\Psi\rangle$ is a mixture of different SU(4) irreps. The components of $|\Psi\rangle$ that mixes the SU(4) irreps can only be seen in $|\delta\Psi_1\rangle$ or δE_2

Reminder: A **symmetry breaking** perturbative Hamiltonian usually implies a large 2nd order energy correction!

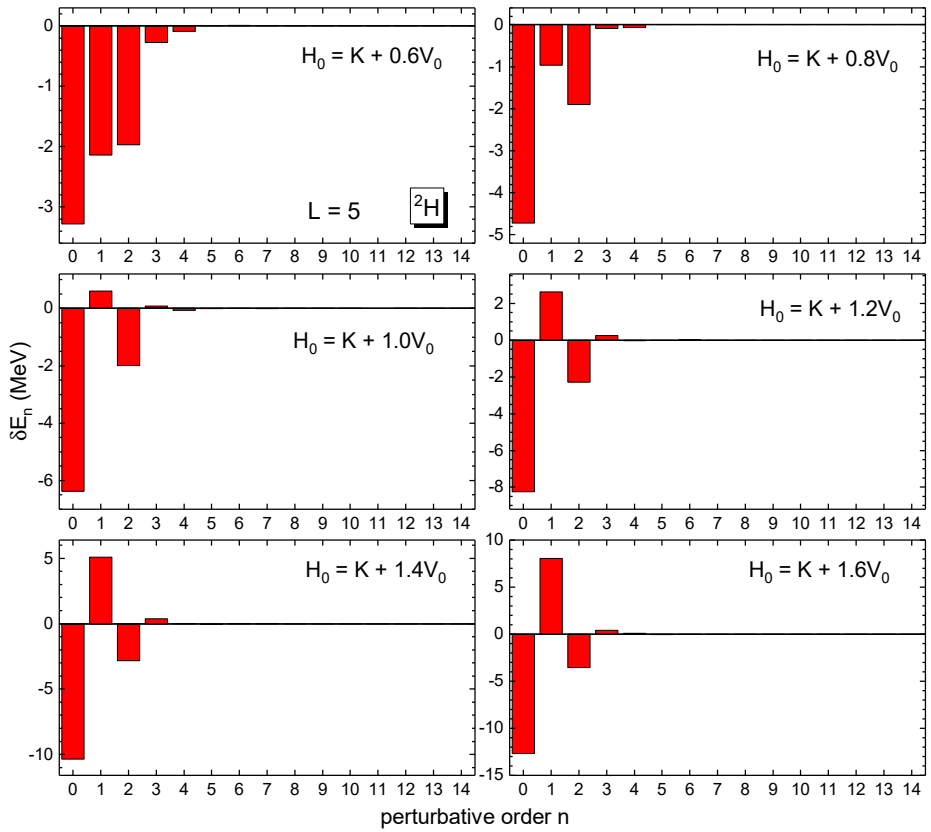
Numerical results for several light nuclei

Table: The nuclear binding energies at different orders calculated with the ptQMC. $E_{\rm exp}$ is the experimental value. All energies are in MeV. We only show statistical errors from the MC simulations.

	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

Realistic N^{2}LO chiral Hamiltonian fixed by few-body data + perturbative quantum MC simulation = nice agreement with the experiments
Excellent predicative power $\Longrightarrow$ Demonstration of both **nuclear force model** and **many-body algorithm**

Perturbative calculations beyond the second order



Perturbative energy correction δE_n of the deuteron at each order. For the zeroth order we show E_0.

- We calculated deuteron energy $E(^2\mathrm{H})$ in a small box $L = 6.6$ fm with a chiral Hamiltonian
- H is split as $H = (K + \mu V_0) + (V - \mu V_0)$, V_0 is the SU(4) interaction and V is the full chiral interaction
- $\mu = 0.6, \cdots, 1.6$ is a constant

E_0, δE_1 and δE_2 are always significant. δE_3 and higher order contributions are negligible, regardless of what H_0 we choose as the unperturbed Hamiltonian

The second order correction is large due to the symmetry breaking effect. There is no such mechanism for higher-order corrections, thus the higher-order corrections follow the usual power-counting hierachy.

Summary & Perspective

- Ab initio nuclear physics grows rapidly in **last two decades**.
  - No core shell model, In-medium SRG, lattice EFT, Green's function Monte Carlo, Coupled cluster, ...
  - mass 4-100, ground state, excited states, finite -T, etc.
- Monte Carlo methods are powerful but plagued by the sign problem.
- Combining MC methods with the perturbation theory may solve the sign problem in many useful senarios.
- We developed an efficient algorithm for doing perturbative calculations in MC methods beyond the first order.
- When combined with a realistic nuclear chiral force, the results reproduce the experimental binding energies very well.
- Works in progress:
  - Efficient methods for calculating the third order corrections, or estimating the truncation errors of the perturbative series;
  - Applications to other interesting systems, e.g., bosons, finite-temperature systems, density distributions, etc.;

Thank you for your attention