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Full Configuration-Interaction Quantum Monte Carlo

for accurate nuclear structure calculations

Rongzhe Hu

Peking University

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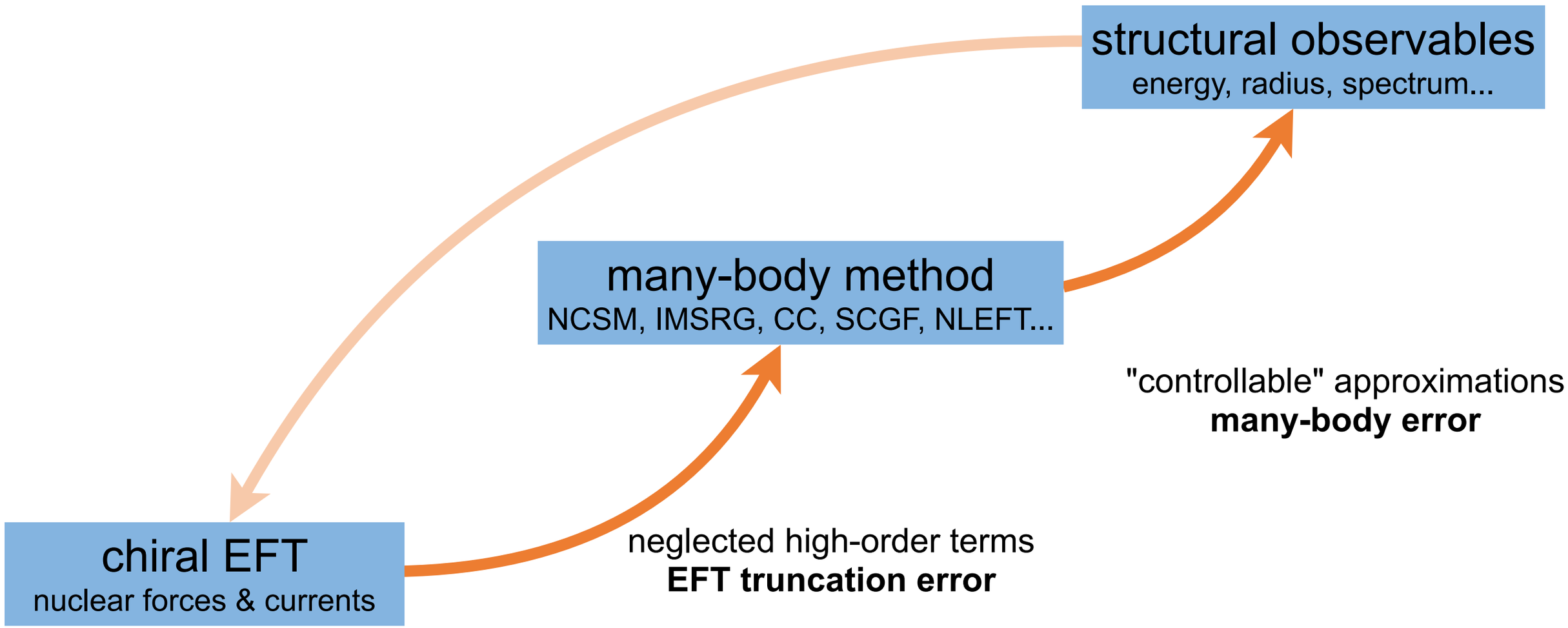
Nuclear *Ab Initio* Pipeline



Need to well-control these errors for reliable predictions.

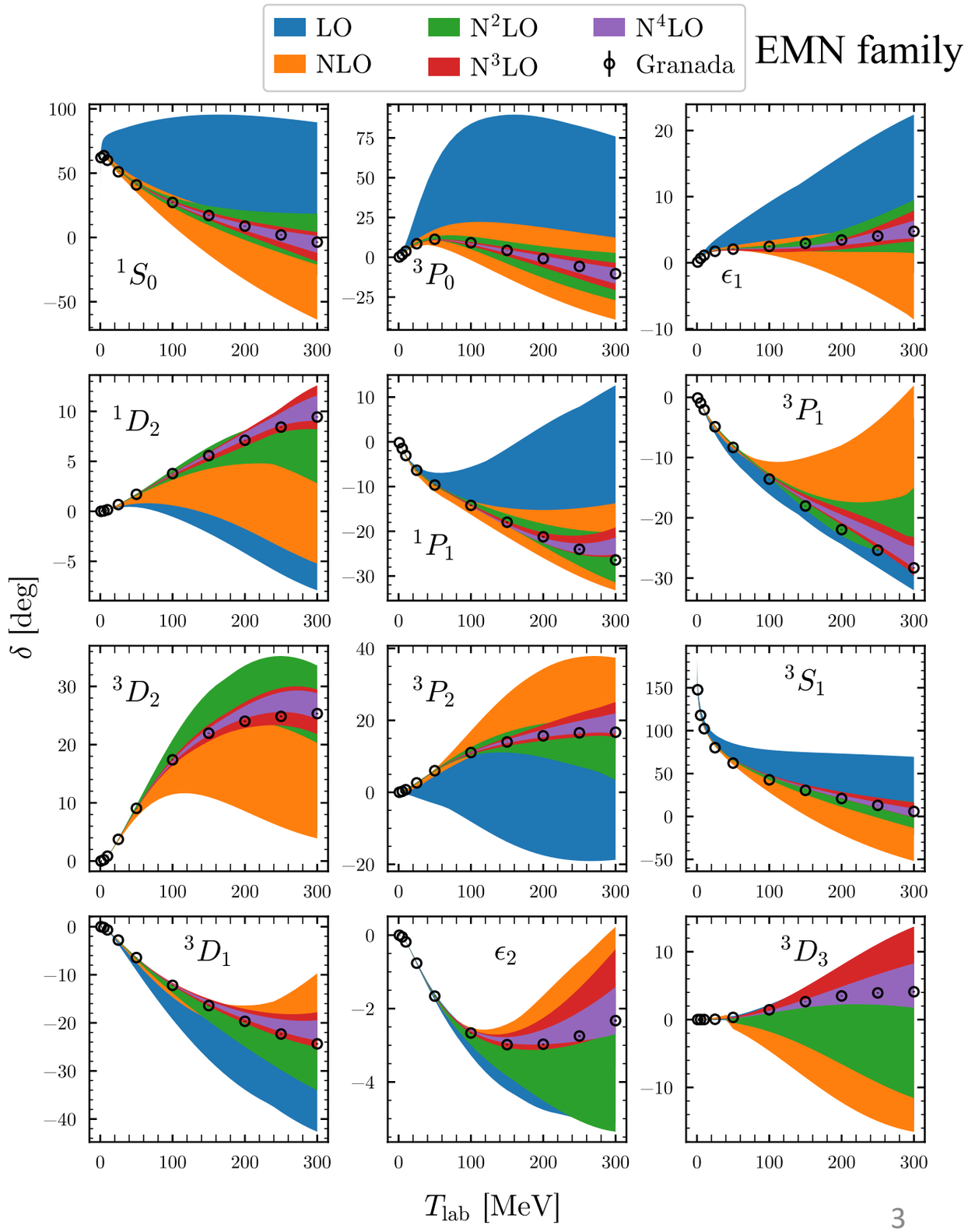
EFT Truncation Error

$$X^{(\nu)}(p) = \sum_{i=0}^{\nu} a_i Q^i,$$

$$Q = \max\left(\frac{M_\pi}{\Lambda_b}, \frac{p}{\Lambda_b}\right).$$

Bayesian analysis...

Not so hard to estimate
EFT truncation error



Many-Body Error

Super hard to estimate many-body errors

Deterministic: Many-body expansion

- MBPT: MBPT(2,3,4)
- IMSRG: IMSRG(2, $3f_2$)
- SCGF: ADC(2, 3)
- CC: CCSD, CCSD(T)
- …

very few truncation orders to compare

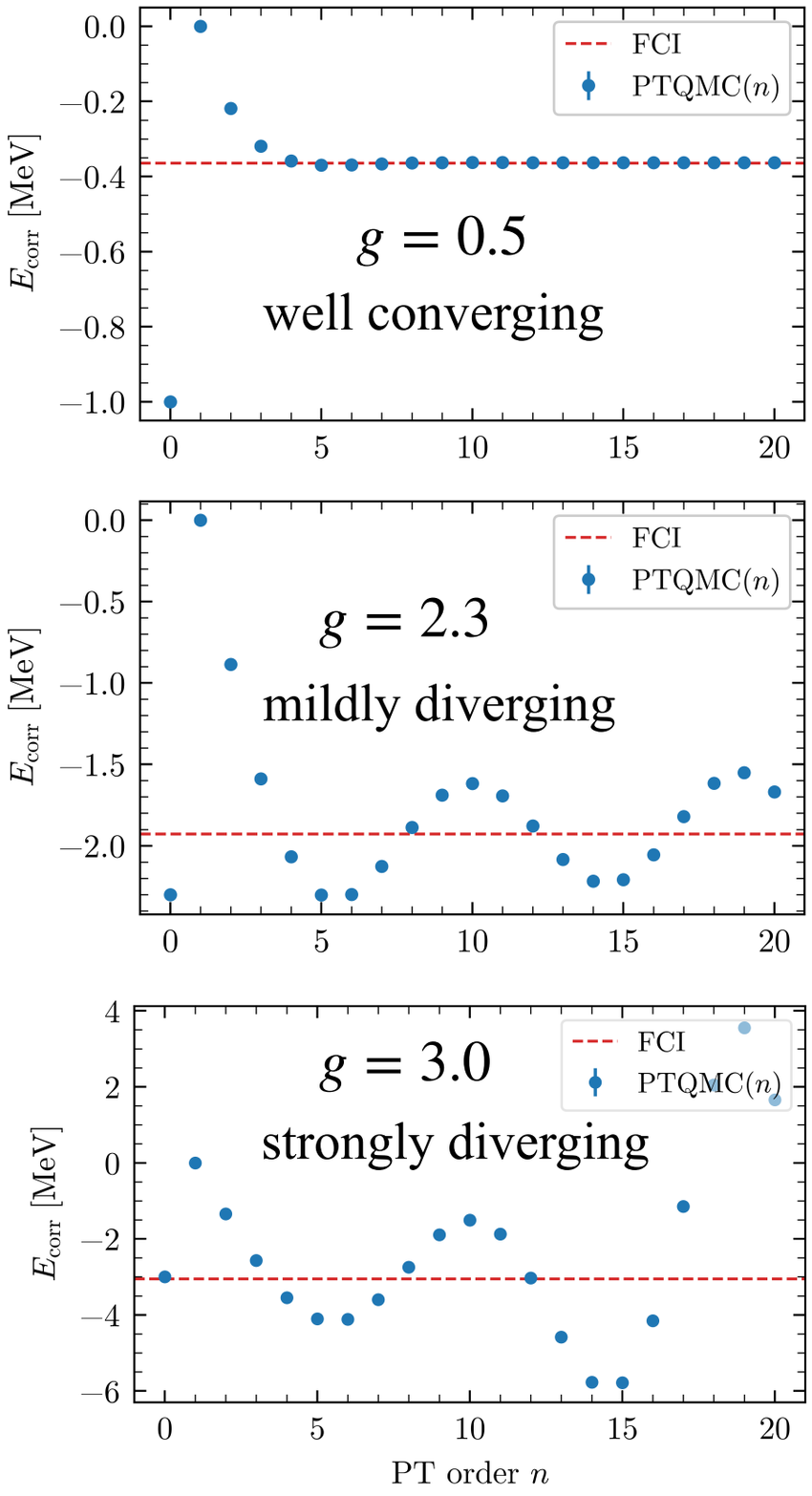
Stochastic: Quantum Monte Carlo

- VMC
- AFQMC
- CIMC
- …

hard to improve accuracy

(WFM)

MBPT Convergence



Richardson pairing model

$$\hat{H} = \delta \sum_{p\sigma} (p-1)\hat{a}^{\dagger}_{p\sigma}\hat{a}_{p\sigma} - \frac{1}{2} g \sum_{pq} \hat{a}^{\dagger}_{p+}\hat{a}^{\dagger}_{p-}\hat{a}_{p-}\hat{a}_{p+}$$

Convergence of MBPT heavily depends on interaction strength

- diverge for **high-density** nuclear matter
- diverge for **high-cutoff** nuclear forces

PRC Letter, 113 L051302 (2026)

CC&IMSRG Convergence

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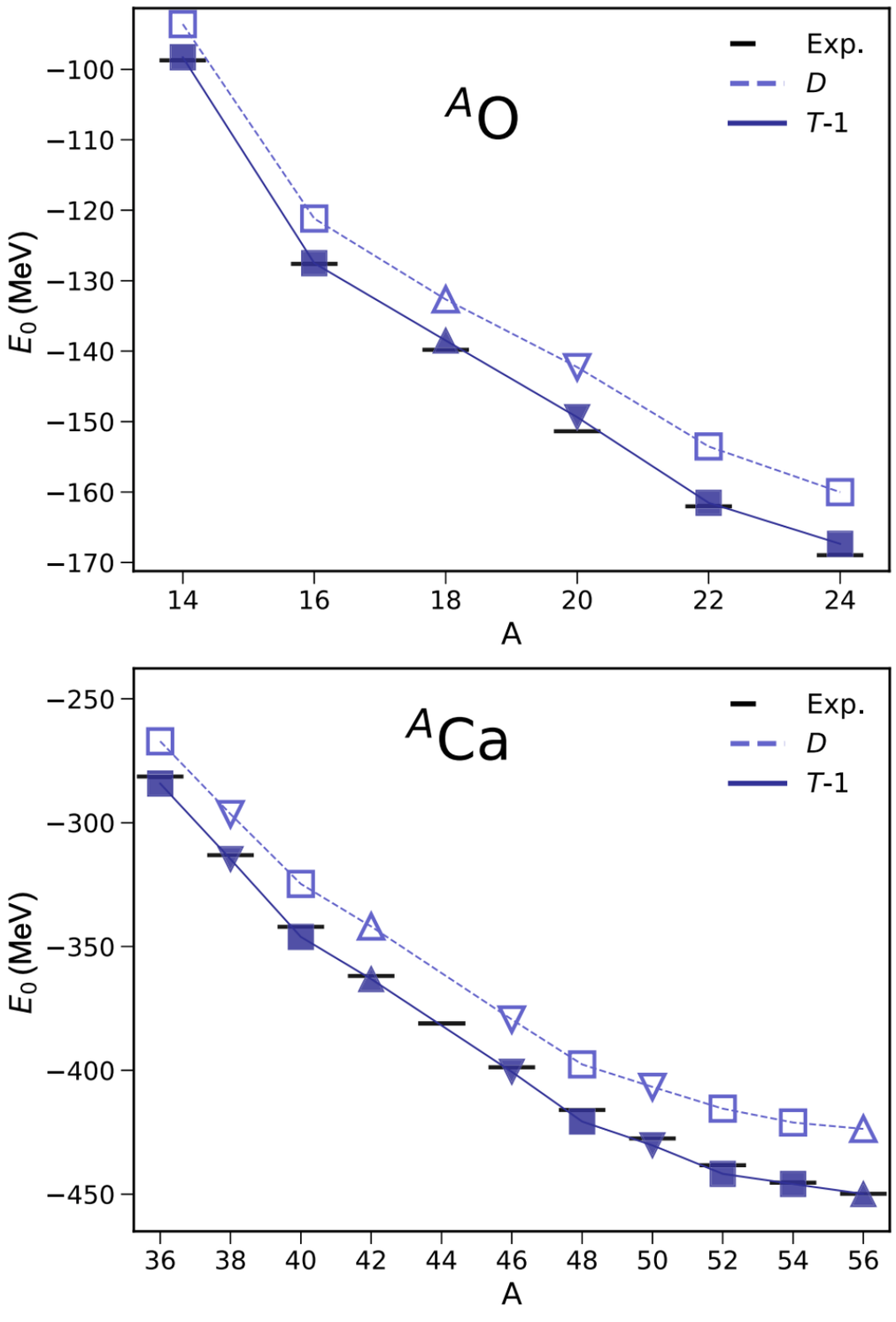
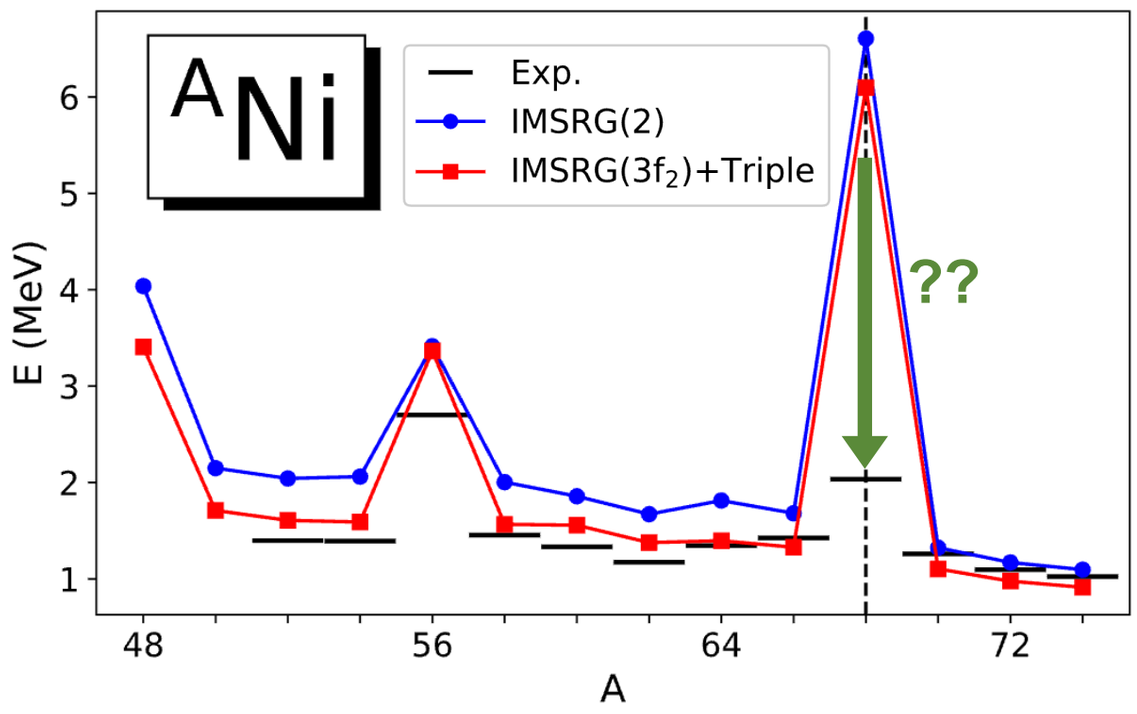
PRC 112, 014315 (2025)



PRC 110, 044317 (2024)



CCSD → CCSDT-1, IMSRG(2) →IMSRG(3f$_2$)

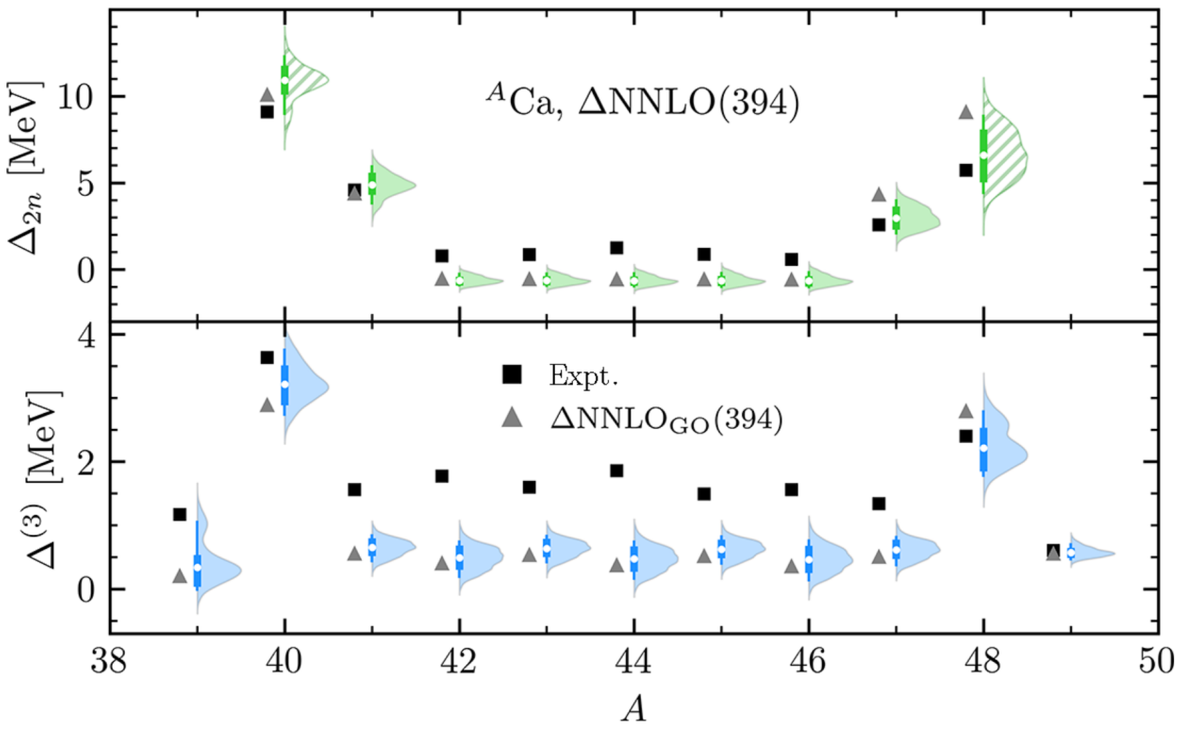
- **5%∼10%** ground-state energy corrections.
- may larger corrections for other properties.

- almost impossible to estimate these many-body uncertainties.

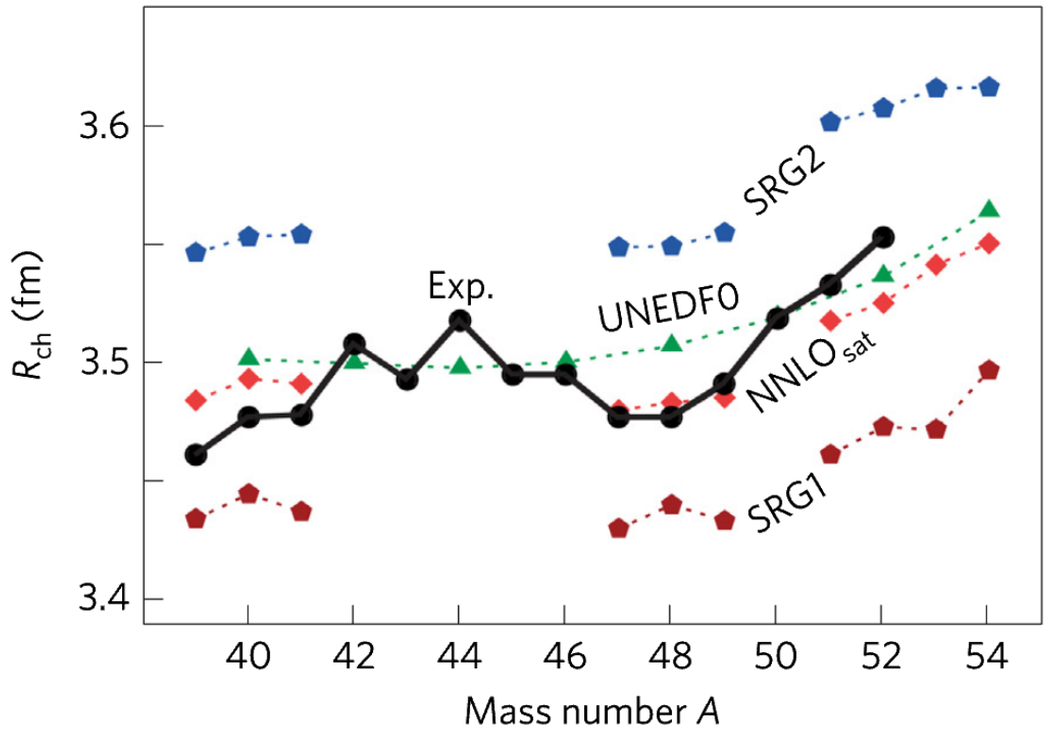
Many-Body Inefficiency

There are many puzzles in nuclear theory that is due to the missing many-body correlations.

PRC 113, L051303 (2026)



Nature Physics 23, 594 (2016)



It is important to either get better accuracy or estimate residual many-body uncertainty.

FCIQMC: Brief History

- 2009: first introduced in quantum chemistry, **J Chem Phys 131, 054106 (2009)**.

- 2010-now: widely applied in electronic, molecular, solid and condense matter systems...

- HEG: **PRB 85, 081103 (2012).**
- Solids: **Nature 493, 365 (2013), PRL 114, 033001 (2014).**
- Finite-Temperature: **PRL 115, 050603 (2014).**
- ...

- ~2020: begin to work in PKU…
- 2025: nuclear shell-model calculations, **NST 36, 212 (2025).**
- 2025: first *ab initio* calculation for infinite nuclear matter, **PRL 137, 062503 (2026).**
- 2026: first *ab initio* calculation for finite-nuclei, **arXiv 2606.22341, 2607.05525.**

...

in collaboration with quantum chemistry groups

FCIQMC: Overview

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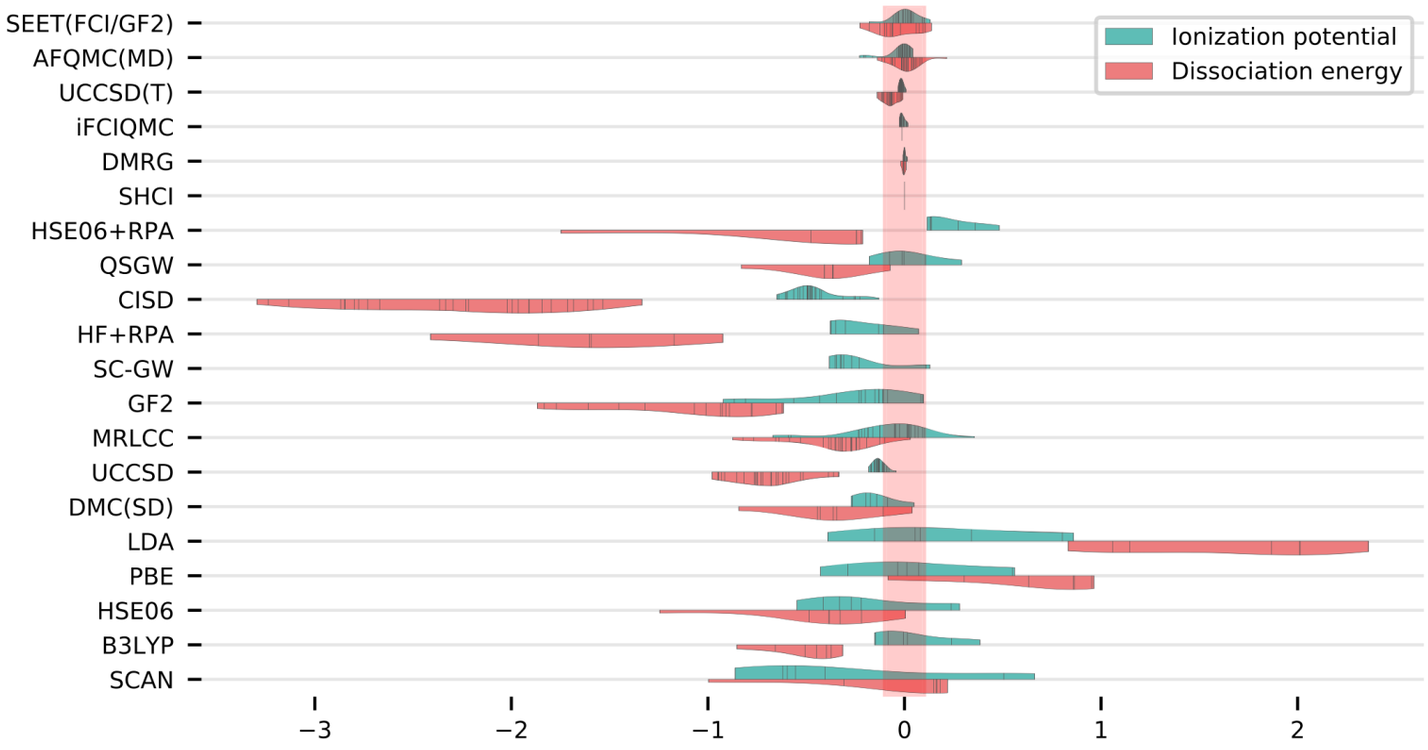
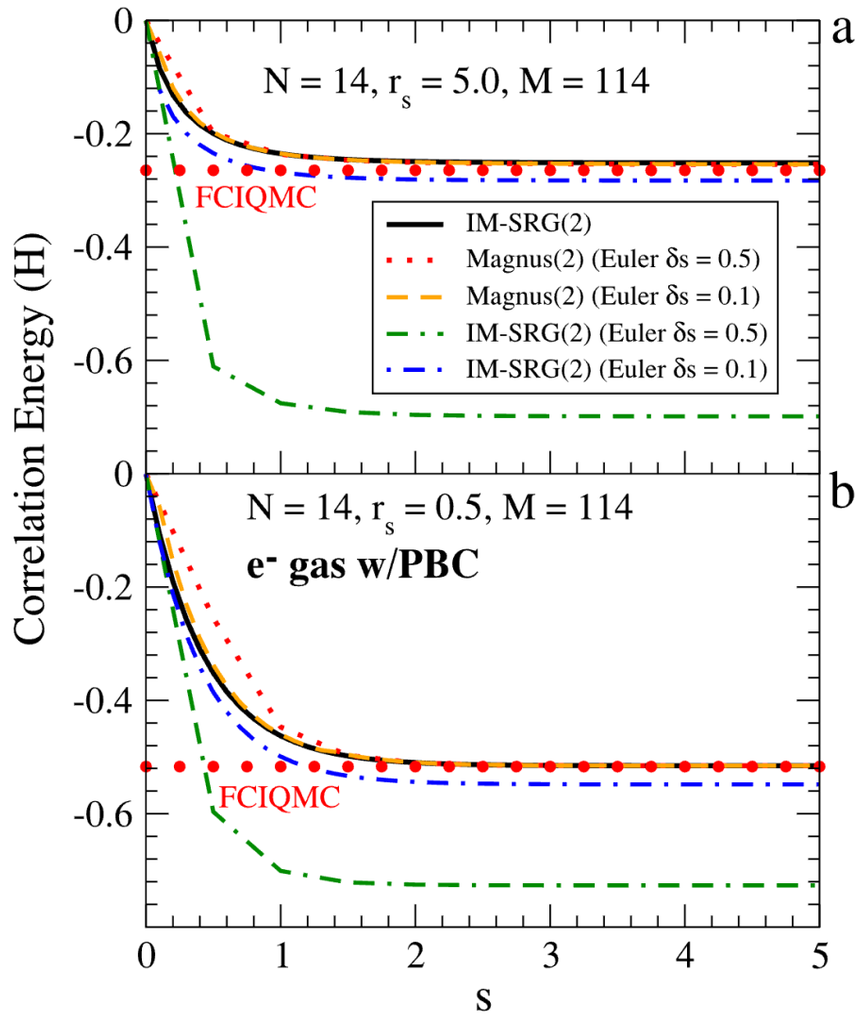
Full Configuration-Interaction Quantum Monte Carlo
FCIQMC ≃ FCI + QMC



PRX 10, 011041 (2020)



H. Hergert et al., Physics Reports 621 (2016)

- (One of) the most accurate many-body method in quantum chemistry.
- Usually serves as a benchmark for other methods.

FCIQMC: Main Idea

projector-QMC in determinant space

- imaginary-time projection

$$\hat{P}(\tau) = e^{-\tau(\hat{H}-E_0)}$$

- ground-state appears in the large-τ limit

$$|\Phi_0\rangle \propto \lim_{\tau\to\infty} |\Psi(\tau)\rangle = e^{-\tau(\hat{H}-E_0)}|\Psi(\tau=0)\rangle$$

- written in configuration space

$$|\Psi(\tau)\rangle = \sum_i C_i(\tau)\,|D_i\rangle$$

$$-\frac{\mathrm{d}C_i(\tau)}{\mathrm{d}\tau} = \sum_j (H_{ij} - E_0\delta_{ij})C_j(\tau)$$

- use stochastic “walkers” to sample these C_i

FCIQMC: Walkers

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Definition of walkers

1. Each walker *a* is put on a $|D_i\rangle$ with a sign $s_a = \pm 1$.

2. Number of walkers of $|D_i\rangle$

$$N_i = \sum_{a \in |D_i\rangle} s_a$$

3. Total walker number

$$N_{\mathrm{w}} = \sum_i |N_i|$$

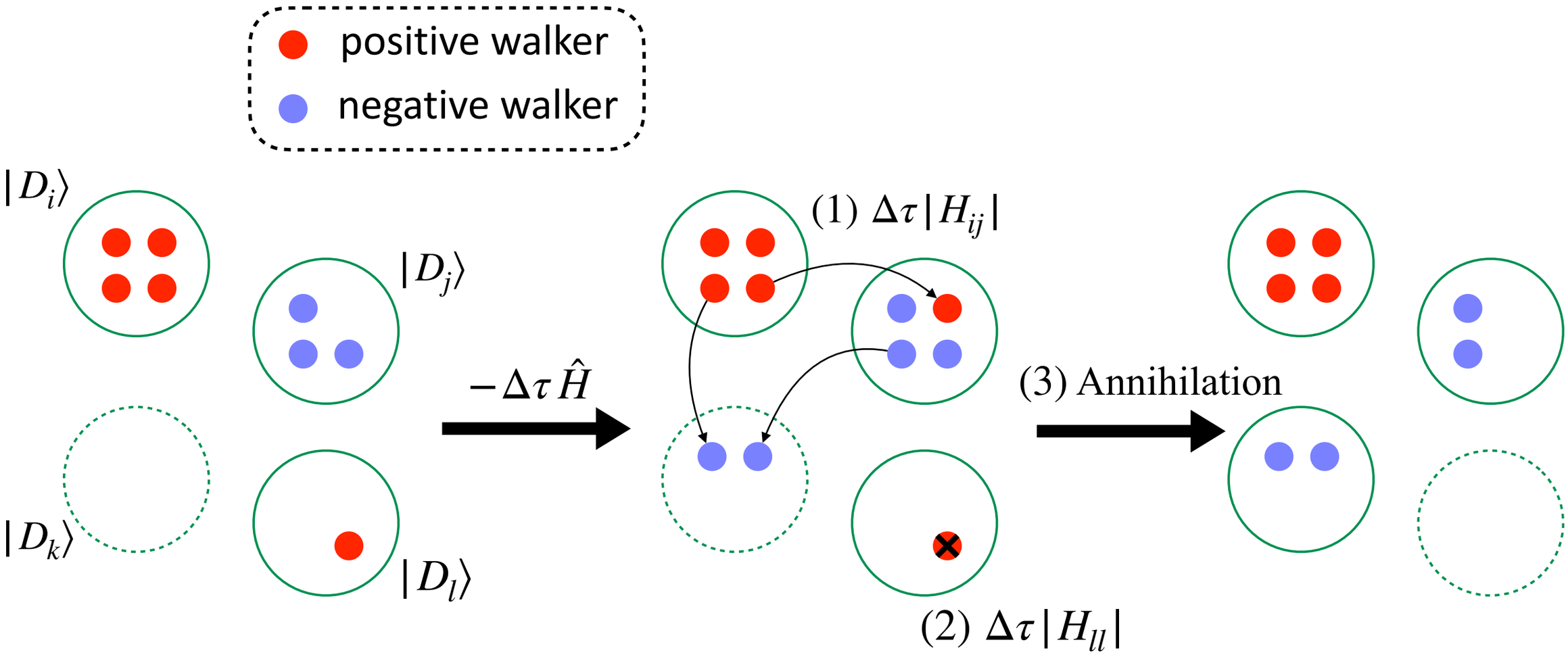
Designing appropriate stochastic algorithms for walkers is the key in FCIQMC method!

4. Evolution of walkers obey the **master equation**

$$N_i(\tau + \Delta\tau) - N_i(\tau) = -\Delta\tau(H_{ii} - S)N_i(\tau) - \Delta\tau \sum_{j \neq i} H_{ij}N_j(\tau)$$

$|\Psi(\tau)\rangle \simeq \sum_i N_i(\tau)\,|D_i\rangle$ sample the FCI wavefunction directly

FCIQMC: Simple Picture



$$|\Psi(\tau)\rangle = 4|D_i\rangle - 3|D_j\rangle + |D_l\rangle$$

$$|\Psi(\tau+\Delta\tau)\rangle = 4|D_i\rangle - 2|D_j\rangle - 2|D_k\rangle$$

$$|\Psi(\tau+\Delta\tau)\rangle = \hat{P}(\Delta\tau)|\Psi(\tau)\rangle$$

FCIQMC: Algorithm

$$N_i(\tau+\Delta\tau)-N_i(\tau)=-\Delta\tau(H_{ii}-S)N_i(\tau)-\Delta\tau\sum_{j\neq i}H_{ij}N_j(\tau)$$

1) spawning step

- for each walker (on $|D_i\rangle$), randomly choose a connected $|D_j\rangle$ with probability $p_{\mathrm{gen}}(j\,|\,i)$, try to spawn a new walker on $|D_j\rangle$ with probability

$$p_{\mathrm{spawn}}(j\,|\,i)=\frac{\Delta\tau\,|H_{ij}|}{p_{\mathrm{gen}}(j\,|\,i)}$$

- the sign of the new walker is $-\mathrm{sign}(H_{ij}N_i)$

2) diagonal death/clone step

- for each walker (on $|D_i\rangle$), calculate probability

$$p_{\mathrm{death}}(i)=\Delta\tau(H_{ii}-S)$$

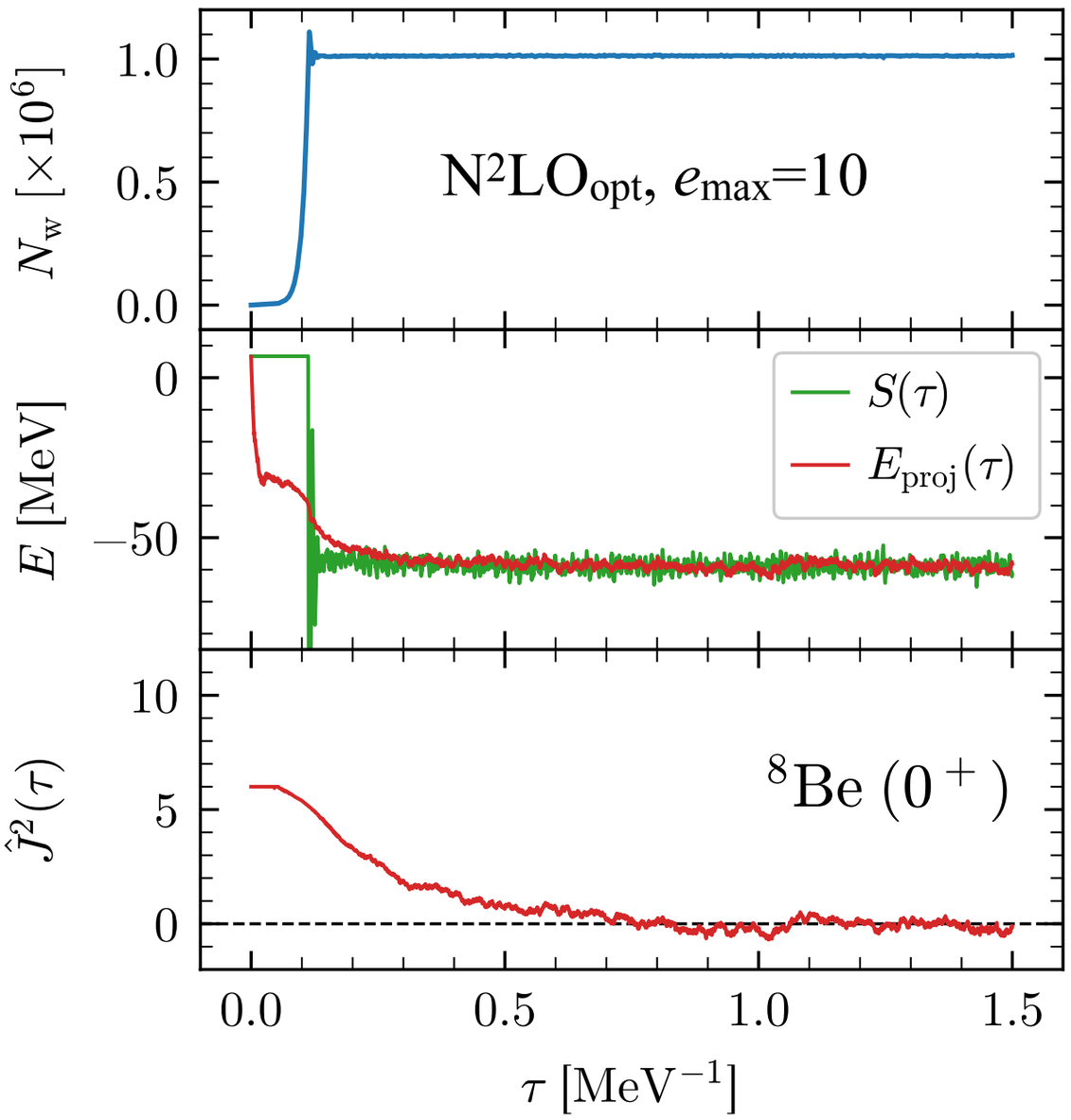
if $p_{\mathrm{death}}(i)>0$, it dies with probability $p_{\mathrm{death}}(i)$;

if $p_{\mathrm{death}}(i)<0$, it clones with probability $-p_{\mathrm{death}}(i)$

3) annihilation step

- all walkers on the same $|D_i\rangle$ with different signs annihilate with each other.

FCIQMC: Example



arXiv 2607.05525

1. Warm up period

- begin with a single walker on HF determinant $|D_0\rangle$
- fix $S = \langle D_0 | \hat{H} | D_0 \rangle$ and perform the evolution, until total walker number N_w

2. Projection period

- the shift is self-adjusted every A steps by

$$S(\tau) = S(\tau - A\Delta\tau) - \frac{\xi}{A\Delta\tau} \ln \frac{N_w(\tau)}{N_w(\tau - A\Delta\tau)}$$

- projected energy estimation:

$$E(\tau) = \frac{\langle D_0 | \hat{H} | \psi(\tau) \rangle}{\langle D_0 | \psi(\tau) \rangle} = \sum_i H_{0i} \frac{N_i(\tau)}{N_0(\tau)}$$

3. Statistic period

- When $S(\tau)$, $E(\tau)$ stabilize, the mean and uncertainty of ground-state energy are extracted.

FCIQMC: Initiator Approximation

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- The original FCIQMC algorithm is **accurate** without any systematic error.

- However, for large systems, a very large number of total walkers N_{w} is usually needed to suppress sign problem, making calculations difficult.

The initiator approximation (i-FCIQMC)

- In the evolution, we define important determinants $|D_i\rangle$ to be "**initiators**"

$$|N_i| > n_{\mathrm{init}}$$

- We forbid non-intiators to spawn new walkers on unoccupied determinants

- It is a **dynamic truncation** of the Hamiltonian

$$\tilde{H}_{ij} = \begin{cases} 0, & |N_j| \le n_\alpha \text{ and } N_i = 0 \\ H_{ij}, & \text{otherwise} \end{cases}$$

- The initiator error is the only systematic error of i-FCIQMC method, which can be efficiently eliminated by increasing N_{w}

$$\lim_{N_{\mathrm{w}} \to \infty} \textbf{i-FCIQMC} = \textbf{FCI}$$

FCIQMC: Estimators

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- projected estimator

$$\langle \hat{O}(\tau) \rangle_{\text{proj}} = \frac{\langle \psi_T | \hat{O} | \Psi(\tau) \rangle}{\langle \psi_T | \Psi(\tau) \rangle}$$

for $[\hat{H}, \hat{O}] = 0$, such as $\hat{J}^2$; and we usually take $|\psi_T\rangle = |D_0\rangle$
the projected estimator is **not variational**

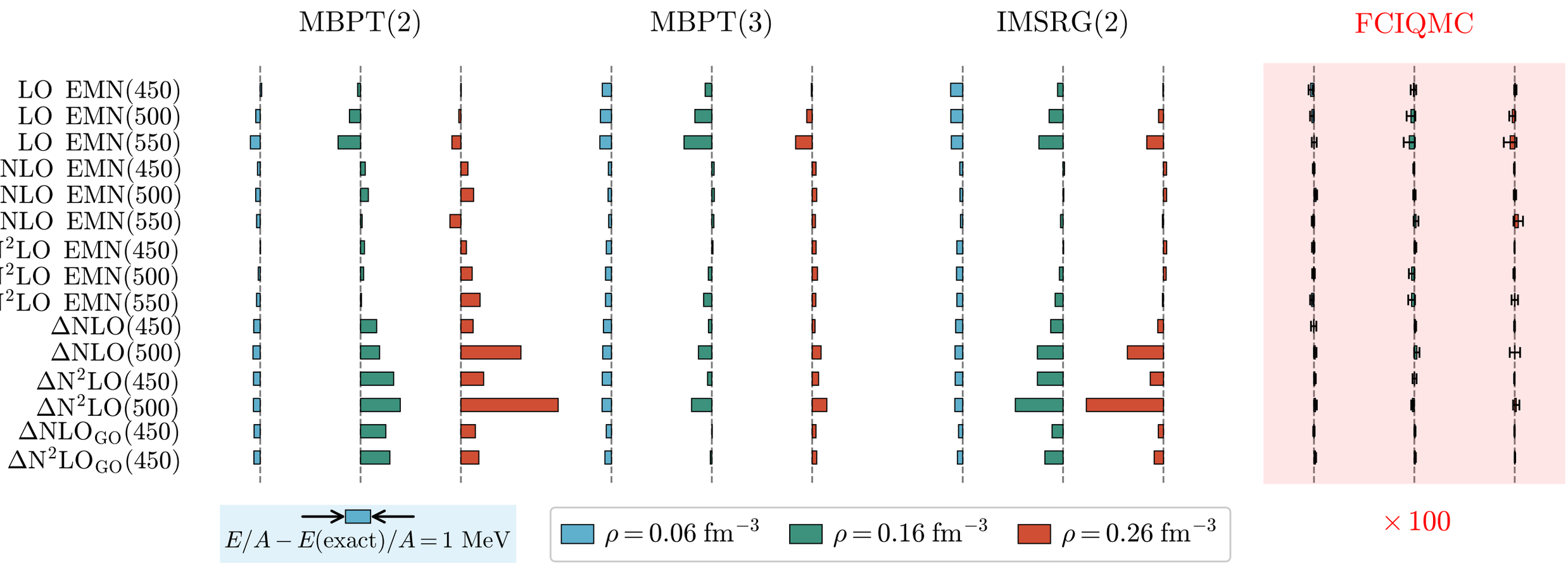
- pure estimator (RDM-estimator)

$$\langle \hat{O}(\tau) \rangle_{\text{pure}} = \frac{\langle \Psi(\tau) | O | \Psi(\tau) \rangle}{\langle \Psi(\tau) | \Psi(\tau) \rangle}$$

for any operators: $\hat{H}$, $\hat{r}^2$, ...
the pure estimator is variational upper limit for energy: $E_{\text{pure}} \geq E_0$

- for energy in FCIQMC, shift S is also another estimator

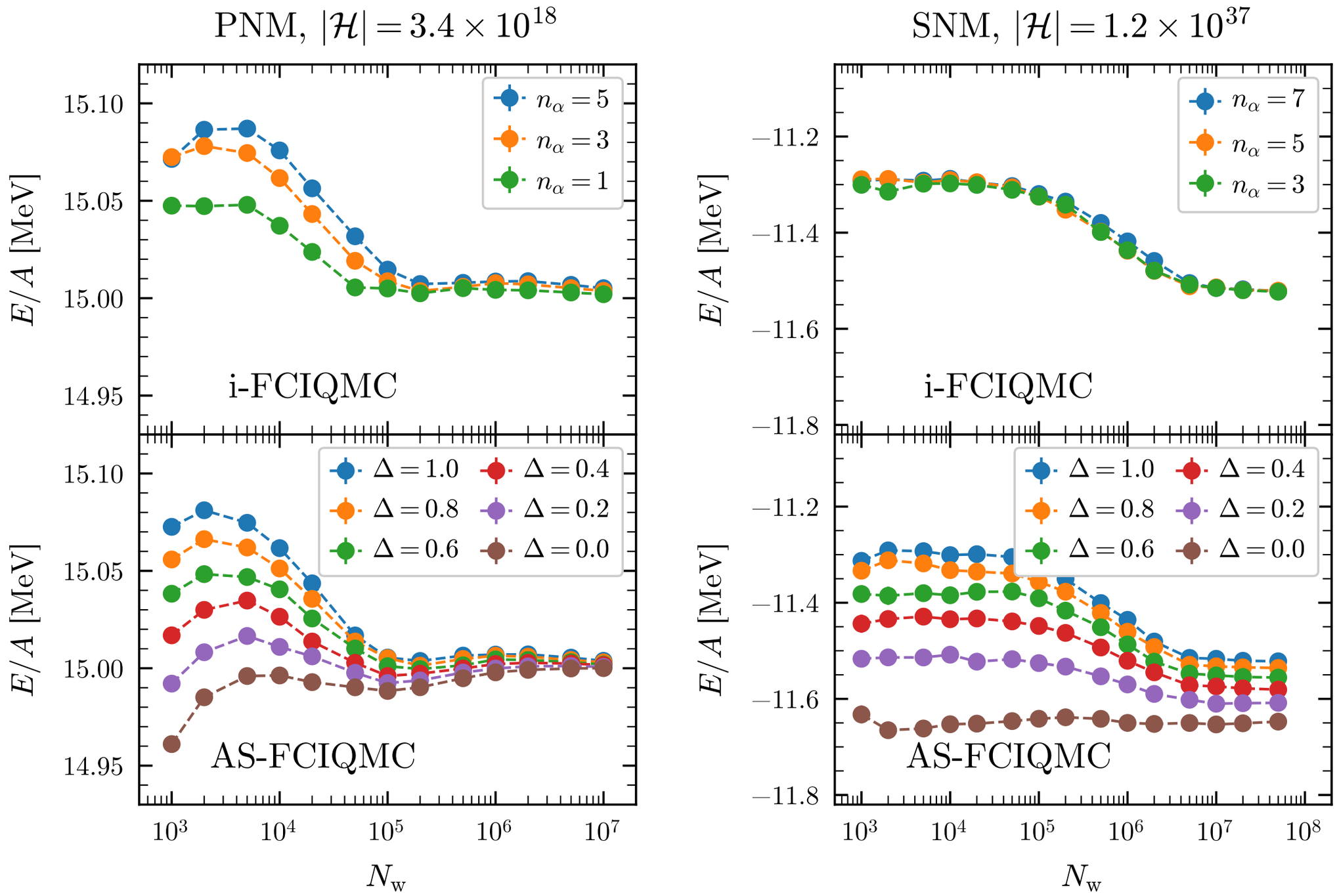
FCIQMC: Benchmark



PRL 137, 062503 (2026)

- Calculations for SNM in a small model space (4 nucleons, 28 s.p. orbits).
- FCIQMC gives accurate solutions in all cases.

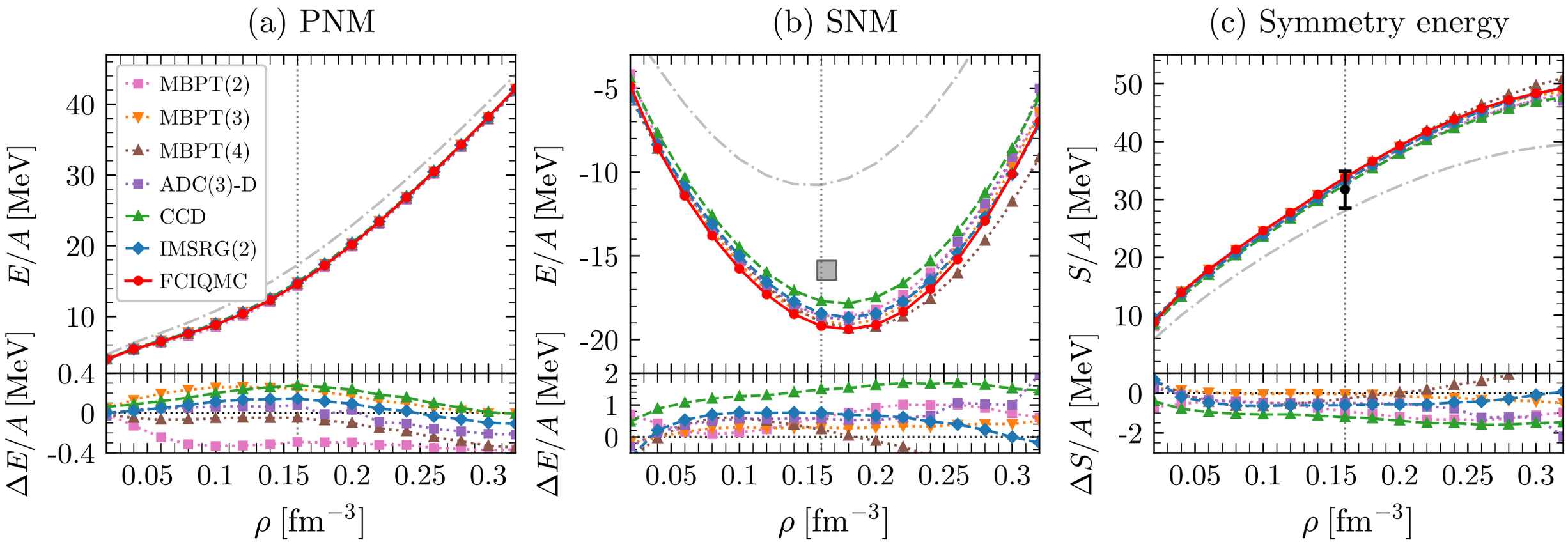
FCIQMC: Convergence



accurate for pure neutron matter

~0.15 MeV error for SNM

FCIQMC: Nuclear-Matter



PRL 137, 062503 (2026)

- interaction: ΔN^2LO_{GO}
- model space: A=66(76) and M=682(1364)

1. generally agree with post-HF methods for this soft interaction.
2. FCIQMC directly samples wave function in the full configuration space.

FCIQMC: Nuclear-Matter

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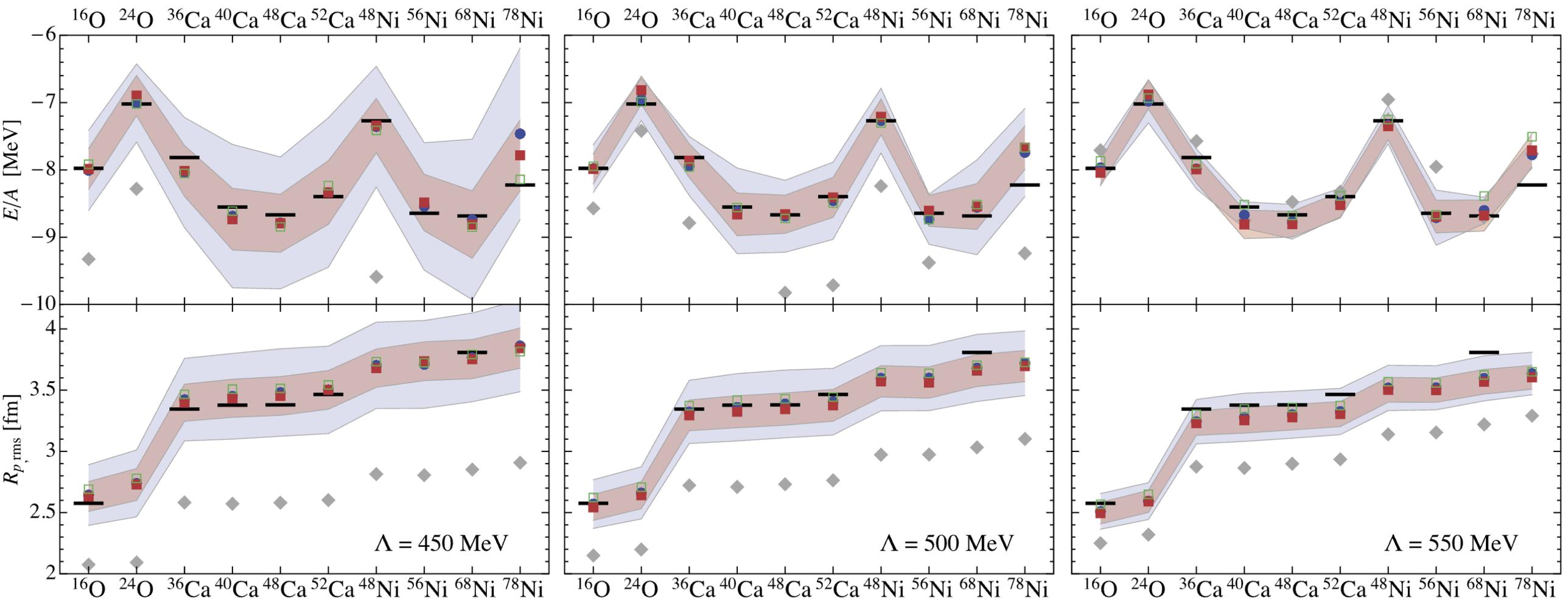
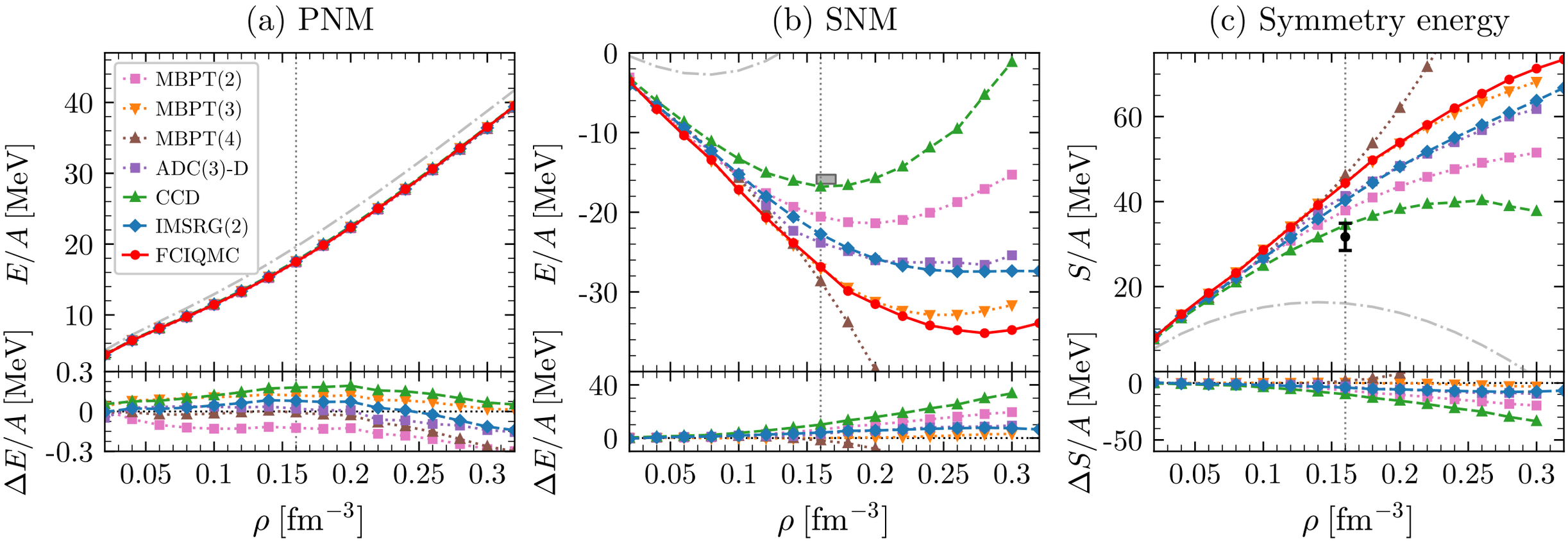
PLB 808, 135651 (2020)



- N^2LO_{Heuther} interaction (SRG-evolved) is reported to accurately describing ground-state energies and charge-radii for finite-nuclei.
- what about nuclear matter? (We use the bare one)

FCIQMC: Nuclear-Matter

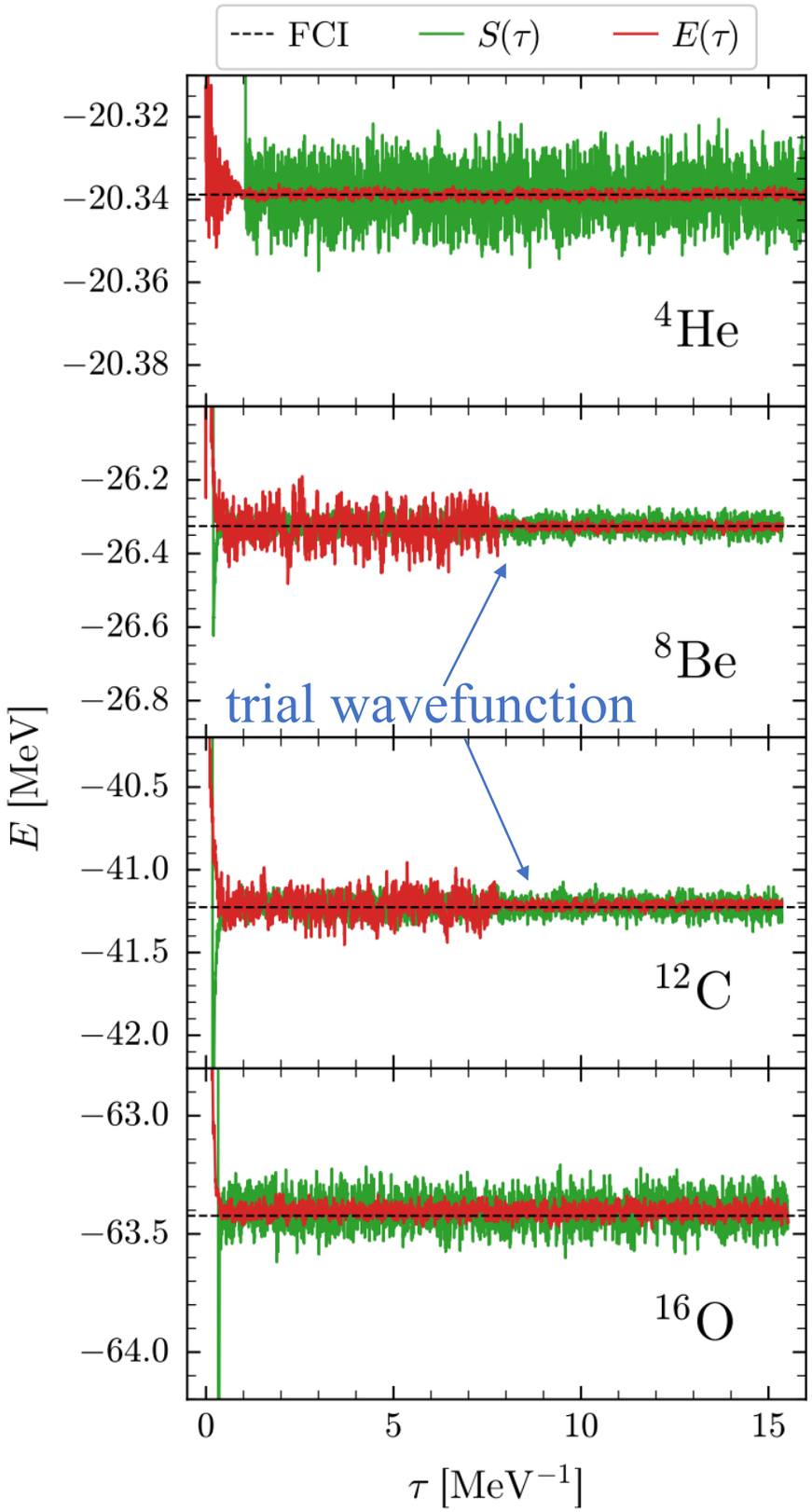


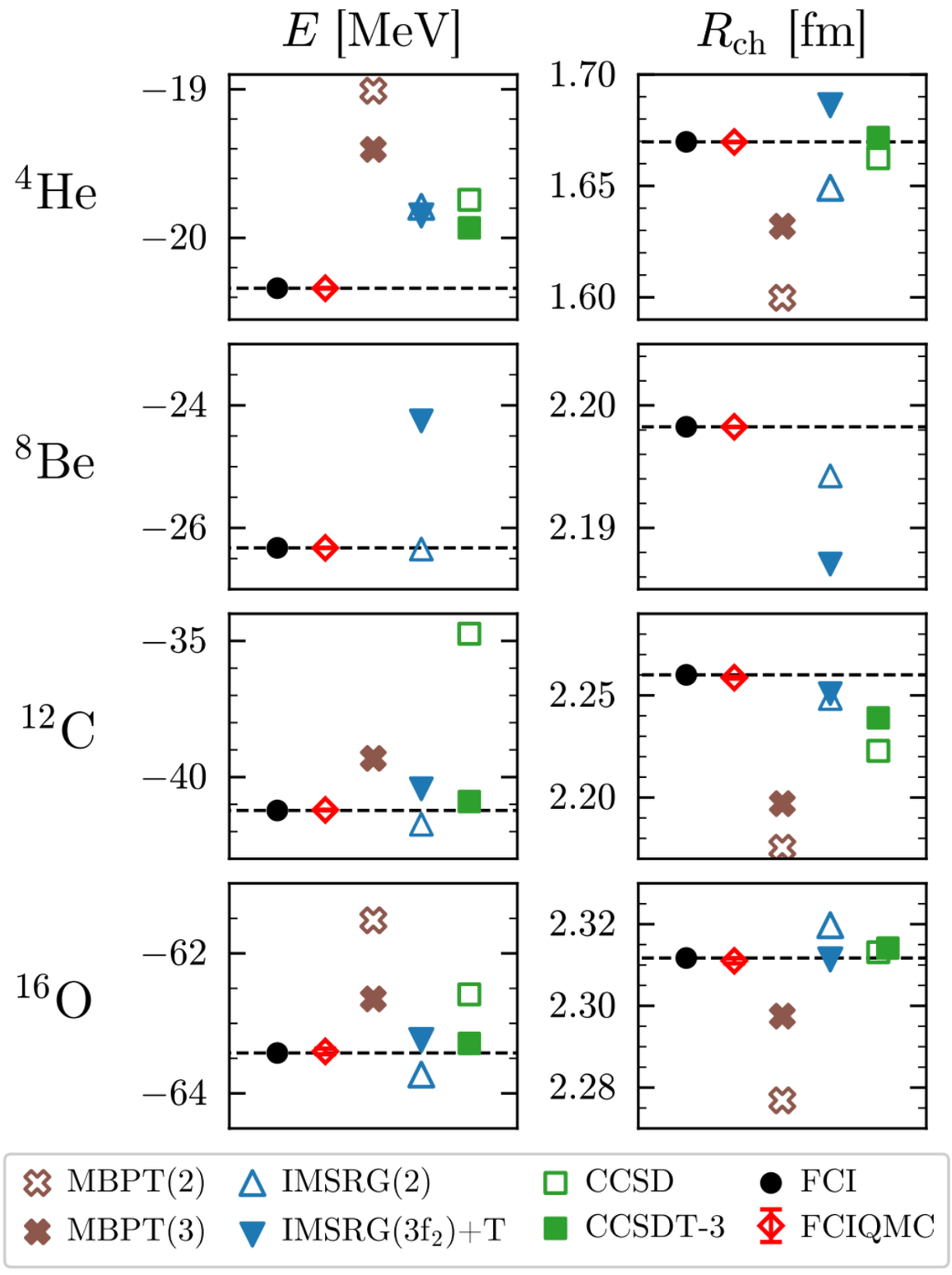
PRL 137, 062503 (2026)

1. generally agreement for PNM.
2. very large differences for SNM → strongly-correlated.
3. FCIQMC concludes it can't reproduce reasonable saturation.

High-order correlations can be important in describing nuclear matter saturation, especially for hard nuclear forces.

FCIQMC: Finite-Nuclei

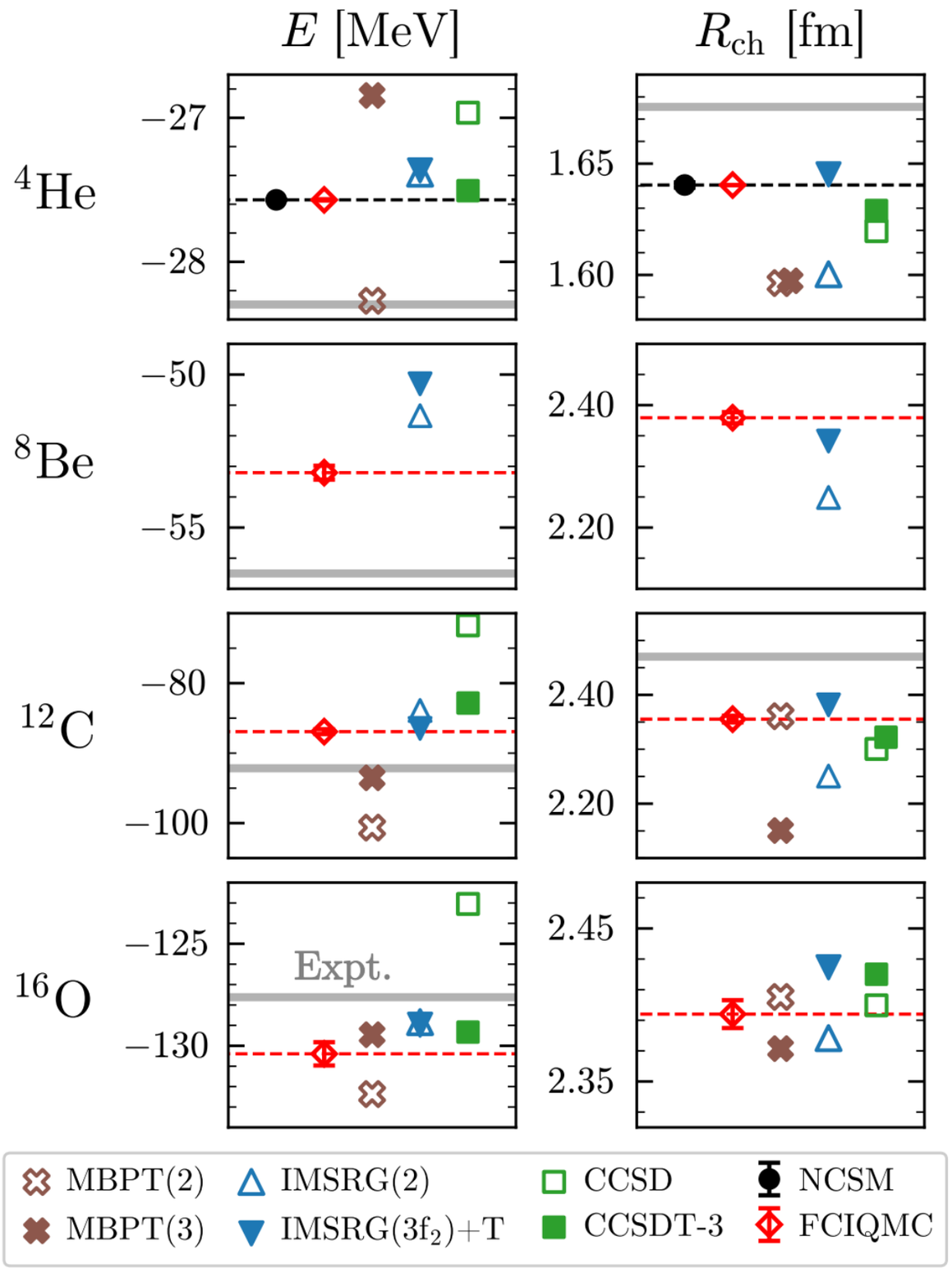




$\mathrm{N^2LO_{opt}}$, $e_{\max} = 2$

arXiv 2606.22341

FCIQMC: Finite-Nuclei

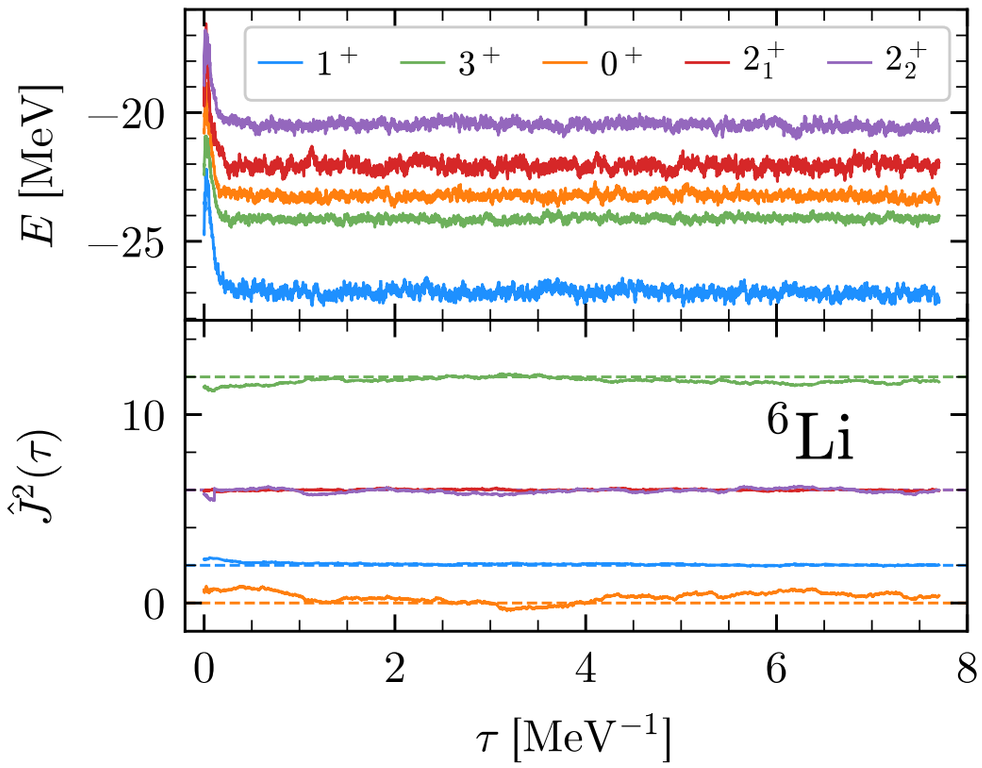


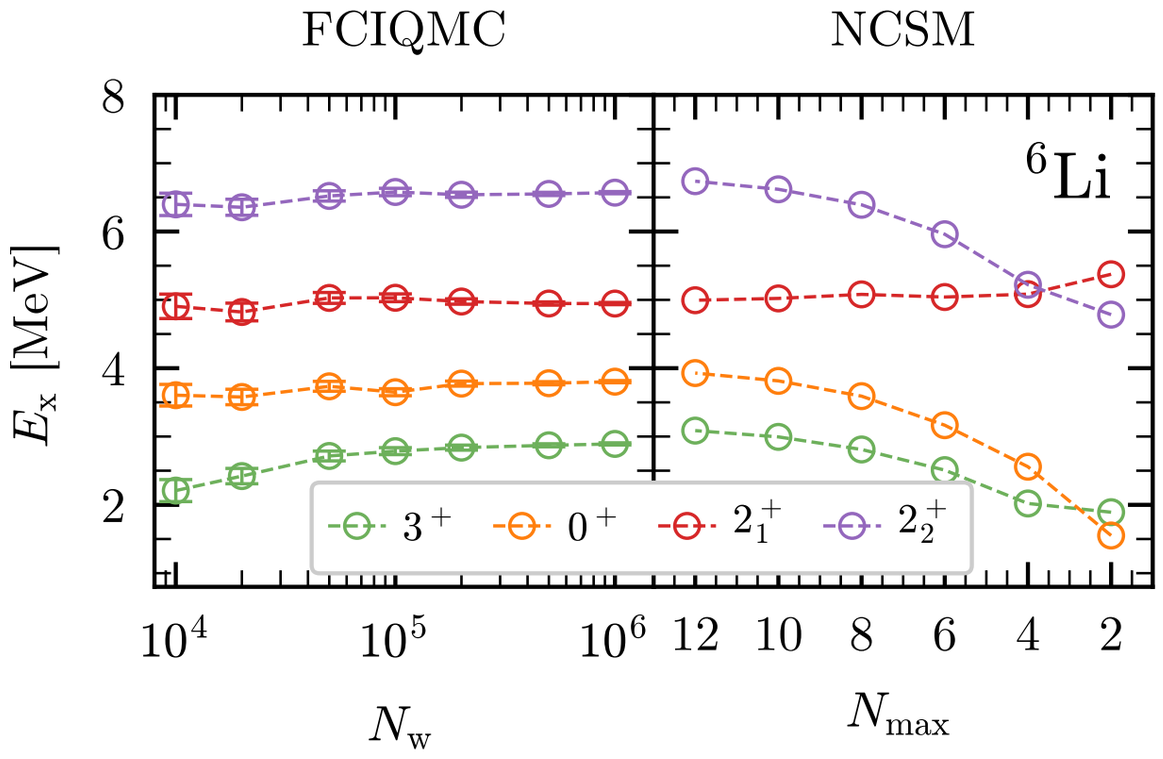
arXiv 2606.22341

$\mathrm{N^2LO_{opt}}, e_{\max} = 10$

- FCIQMC is able to give accurate ground-state energies and charge-radii with many-body uncertainties **under 1%**.
- reveal the critical role of high-order correlations in other truncated methods.
- exact calculation for 16O is particular important, because many interactions are optimized using this nuclei.

FCIQMC: Excited-States





arXiv 2607.05525

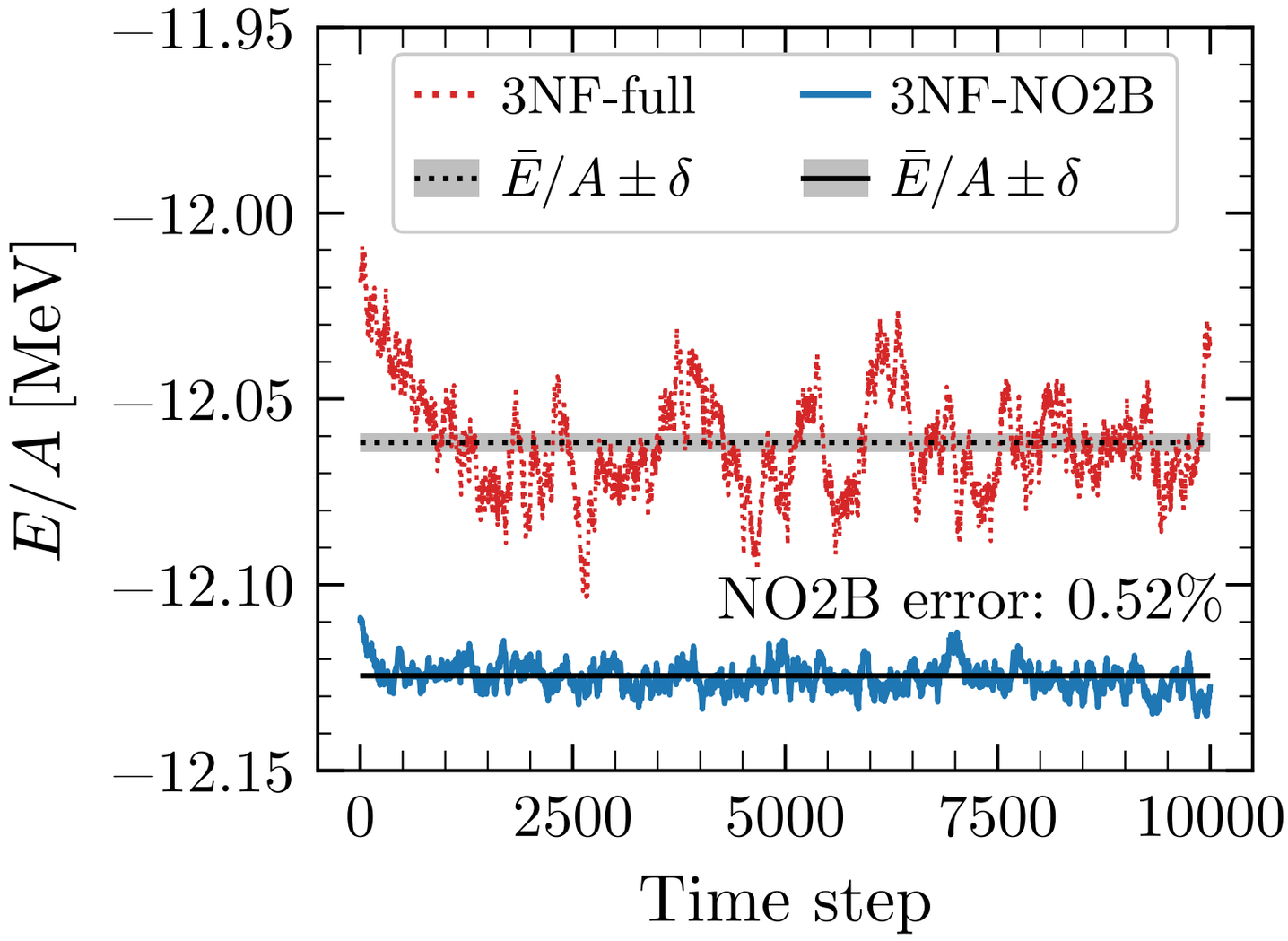
Excited-state calculation

- Gram-Schmidt orthogonalization on-the-fly

$$|\Psi_\nu\rangle \leftarrow |\Psi_\nu\rangle - \sum_{\mu<\nu} \frac{\langle\Psi_\mu|\Psi_\nu\rangle}{\langle\Psi_\mu|\Psi_\mu\rangle}|\Psi_\mu\rangle$$

- FCIQMC converges faster than NCSM.

FCIQMC: no need to normal-order



Quantify the error of NO2B approximation

FCIQMC: Summary

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Advantages

- very simple and “easy” to code
- highly parallel using MPI+OPENMP
- extremely memory friendly
- directly get the wavefunction
- don’t rely on imaginary-time extrapolation
- no $\Delta\tau$ bias, no fixed-node approximations
- systematically get improved by a single N_{w}
- …

Disadvantage

- expensive and heavily rely on massive HPC.
  ($\sim 10^7$ CPU hours spent for nuclear matter calculations)

Summary

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Two ways to approach the exact many-body limit

small space *large space*

FCI → FCIQMC

Hybrid with QMC

MBPT(2,3,4)
IMSRG(2,3f2)
CCSD(T)
ADC(2,3)

→ PTQMC(n)
SRGQMC(n)
CCMC(n)
diagMC(n)

low order *high order*