Advancing (Non)perturbative Many-Body Methods For Strongly Correlated Nuclear Matter

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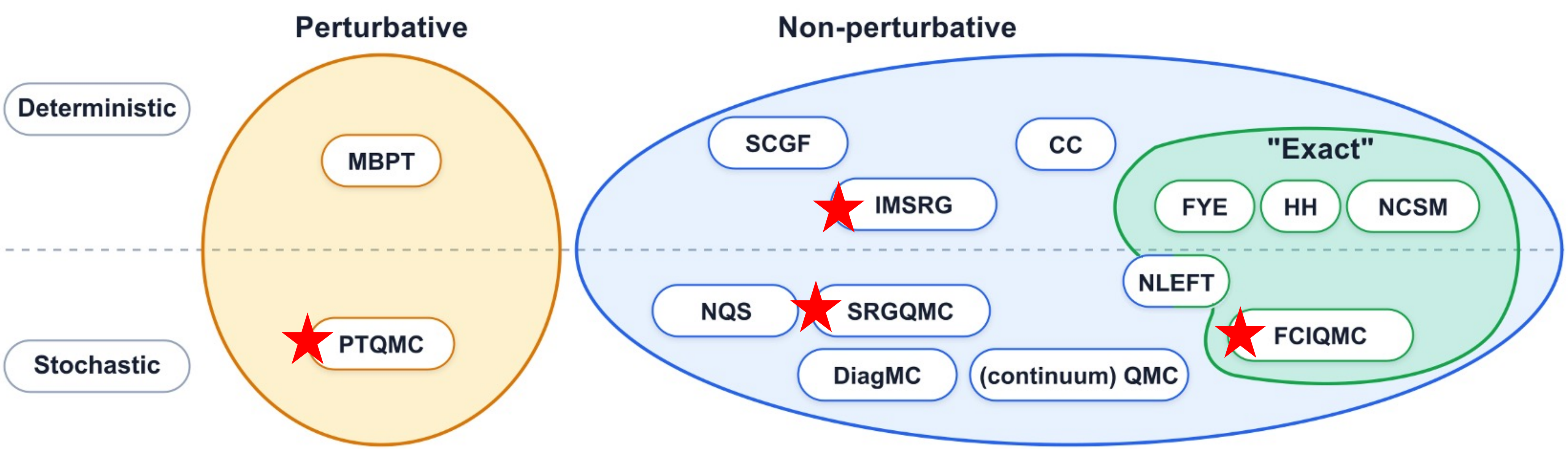
Many-Body Theory: *Nuclear Physics Meets Quantum Chemistry*

Deterministic and Stochastic Routes to Many-Body Correlations

$$\hat{H} = E_0 + \sum_{pq} f_{pq}\, a^\dagger_p a_q + \frac{1}{4}\sum_{pqrs} \overline{\Gamma}_{pq,rs}\, a^\dagger_p a^\dagger_q a_s a_r + \frac{1}{36}\sum_{pqrstu} \overline{W}_{pqr,stu}\, a^\dagger_p a^\dagger_q a^\dagger_r a_u a_t a_s .$$

→ Normal-ordered with respect to a reference state, typically **Hartree–Fock**.

The challenge: *capturing higher-order correlations beyond mean-field*.

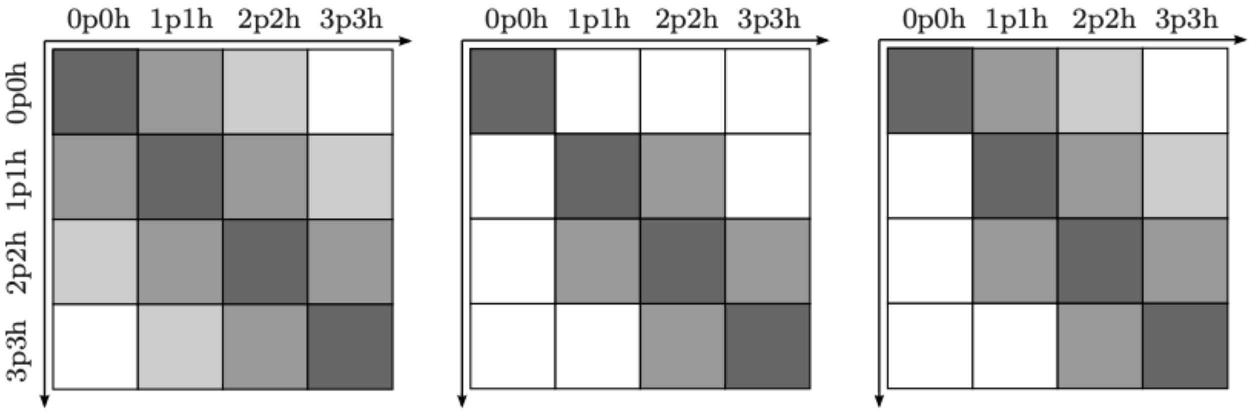


Complementary Routes: IMSRG & FCIQMC

IMSRG: Truncated Continuous Unitary Transformations (Scalable and Productive)

$$H(s) = U(s)H(0)U^{\dagger}(s)$$

$$\frac{\mathrm{d}H(s)}{\mathrm{d}s} = [\eta(s), H(s)] \longrightarrow \frac{\mathrm{d}O(s)}{\mathrm{d}s} = [\eta(s), O(s)]$$

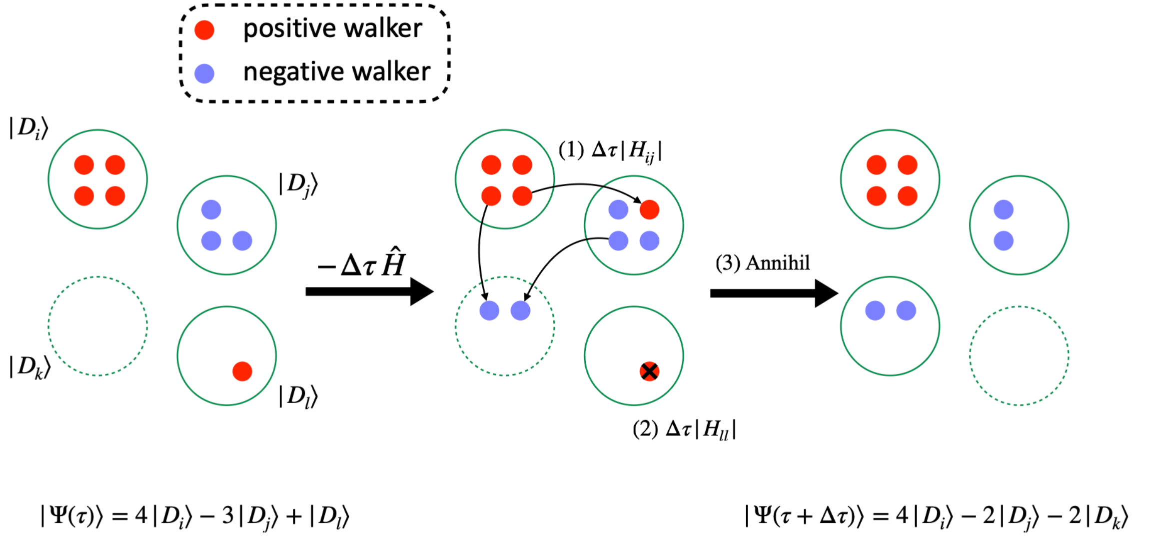


$\langle i|\, H_0 \,|j\rangle$ $\langle i|\, H_{\text{IM-SRG}} \,|j\rangle$ $\langle i|\, H_{\text{CC}} \,|j\rangle$

Off-diagonal couplings suppressed.

FCIQMC: Stochastic Imaginary-Time Projection (Accurate as a Benchmark)

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



Signed walkers stochastically project out the exact ground state.

 H. Hergert, *et al. Phys. Rep.*, **621**, 165(2016).

For the Equation of State: More Correlations ... ?

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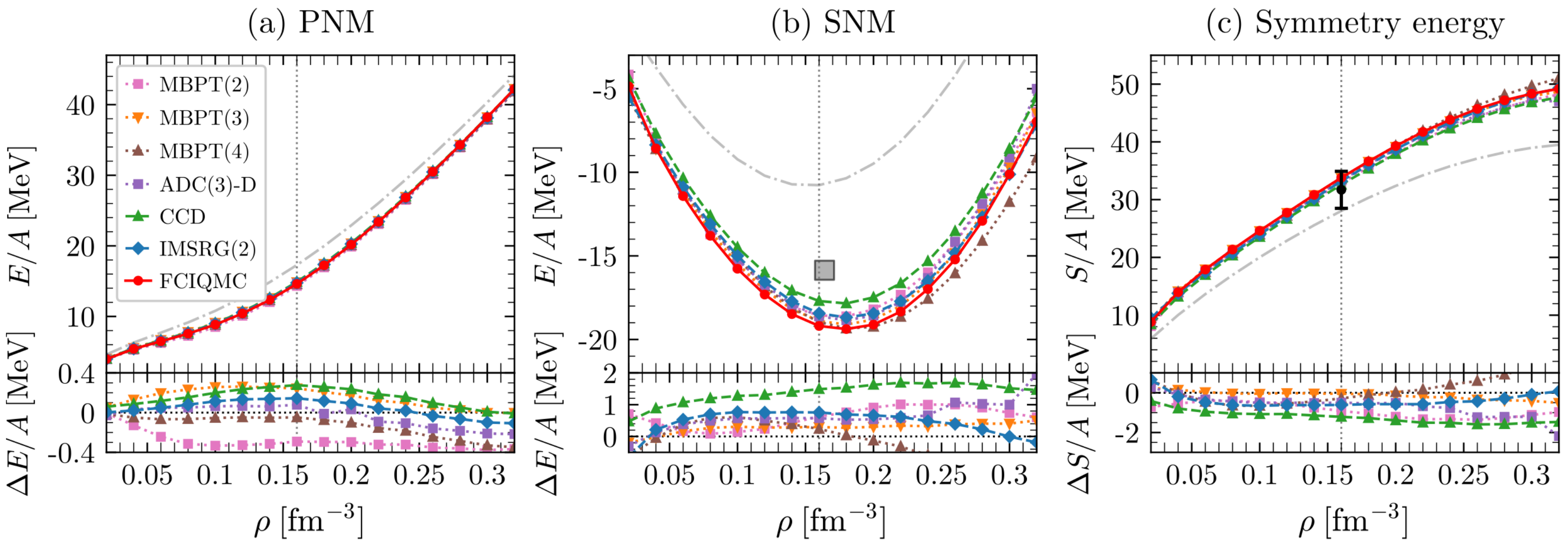


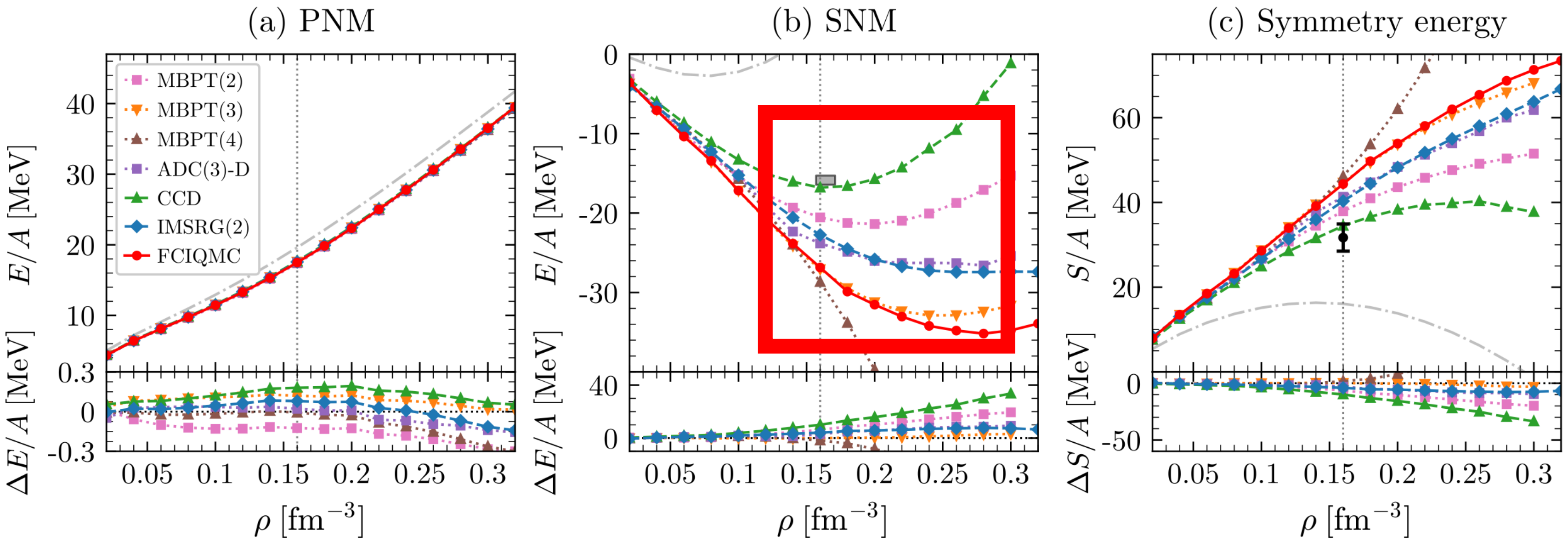
X. Zhen, **R. Hu**, *et al.*
Phys. Lett. B, **862**, 139350 (2025).

R. Hu, S. Jin, **X. Zhen**, *et al.*
Phys. Rev. Lett., **137**, 062503 (2026).

Similar Results for Softer Forces...

But for Harder forces ...

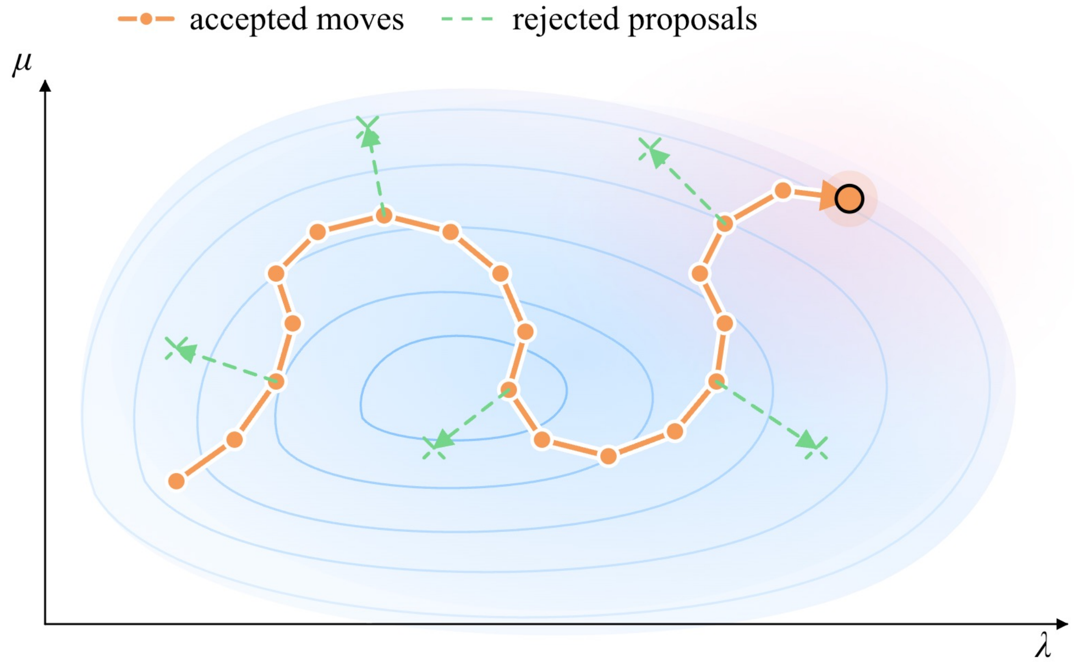
Systematically Underestimated!



思想自由 兼容并包

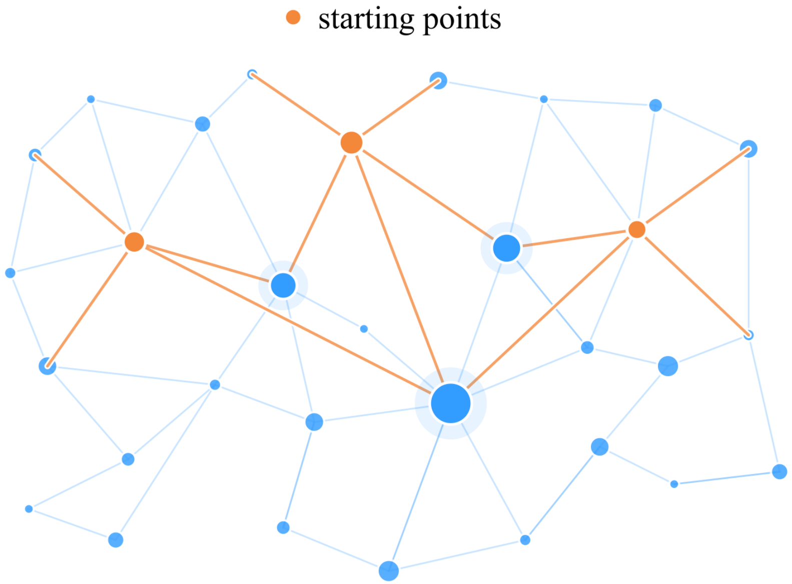
Quantum Monte Carlo : Continuity and Discreteness

Continuous Sampling:
Single point in high-dimensional space



Examples (~MC):
- **V**ariational
- **G**reen's **F**unction
- **D**iffusion
- **A**uxiliary **F**ield

Discrete Sampling:
Distribution of discrete objects



Examples (~MC):
- **D**iagrammatic
- **F**ull **C**onfiguration **I**nteraction
- **P**erturbation **T**heory
- **S**imilarity **R**enormalization **G**roup

PT : Why do we need Monte Carlo ?

$$H(\lambda) \equiv H_0 + \lambda H_1,$$
$$E(\lambda) \equiv E^{(0)} + \lambda E^{(1)} + \lambda^2 E^{(2)} + ...,$$
$$|\Psi(\lambda)\rangle \equiv |\Psi^{(0)}\rangle + \lambda|\Psi^{(1)}\rangle + \lambda^2|\Psi^{(2)}\rangle + ...$$

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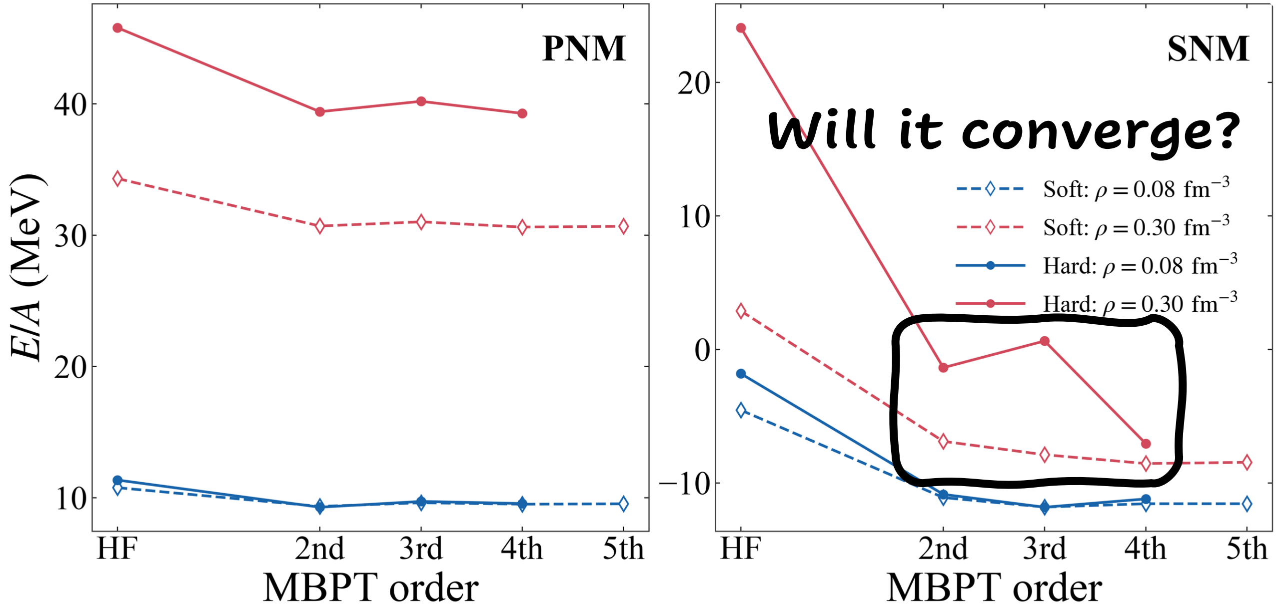
$$E^{(0)}|\Phi\rangle + \sum_{p=1}^{\infty}\lambda^p\Big(H_1|\Psi^{(p-1)}\rangle + H_0|\Psi^{(p)}\rangle\Big) = E^{(0)}|\Phi\rangle$$
$$+ \sum_{p=1}^{\infty}\lambda^p\Big(\sum_{j=0}^{p}E^{(j)}|\Psi^{(p-j)}\rangle\Big).$$

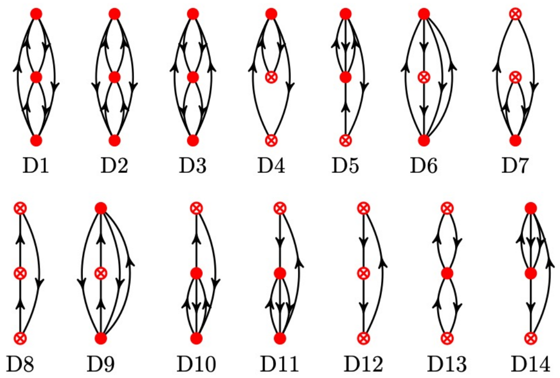
collect terms at the same order…

Configuration Space (computationally prohibitive) :

$$C_{m0}^{(p)} = \frac{1}{E^{(0)} - E_m^{(0)}}\left[\sum_q \langle\Phi_m|H_1|\Phi_q\rangle C_{q0}^{(p-1)} - \sum_{j=1}^{p} E^{(j)} C_{m0}^{(p-j)}\right]$$



Operator Space (currently up to fifth order) :



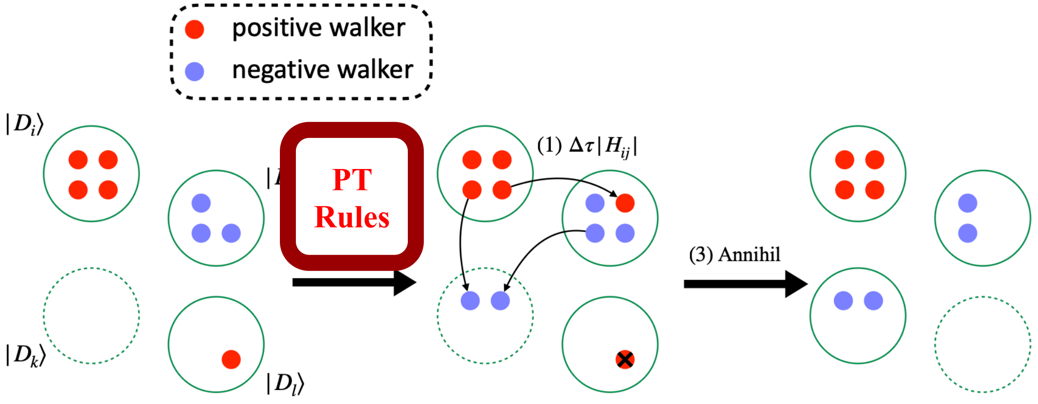
level	MBPT(n)	N_{diag} [a]	$N_{\mathrm{diag}}^{(\mathrm{eff})}$	N_{dim}	N_{grp}
two-body	HF	1	1	6	1
	2	1	1	9	1
	3	3	3	18	2
	4	39	24	24	4
	5	840	375	30	5
	6[b]	27300	11269	36	6
three-body	2	1	1	18	1
	3	19	14[c]	21; 24; 27	14

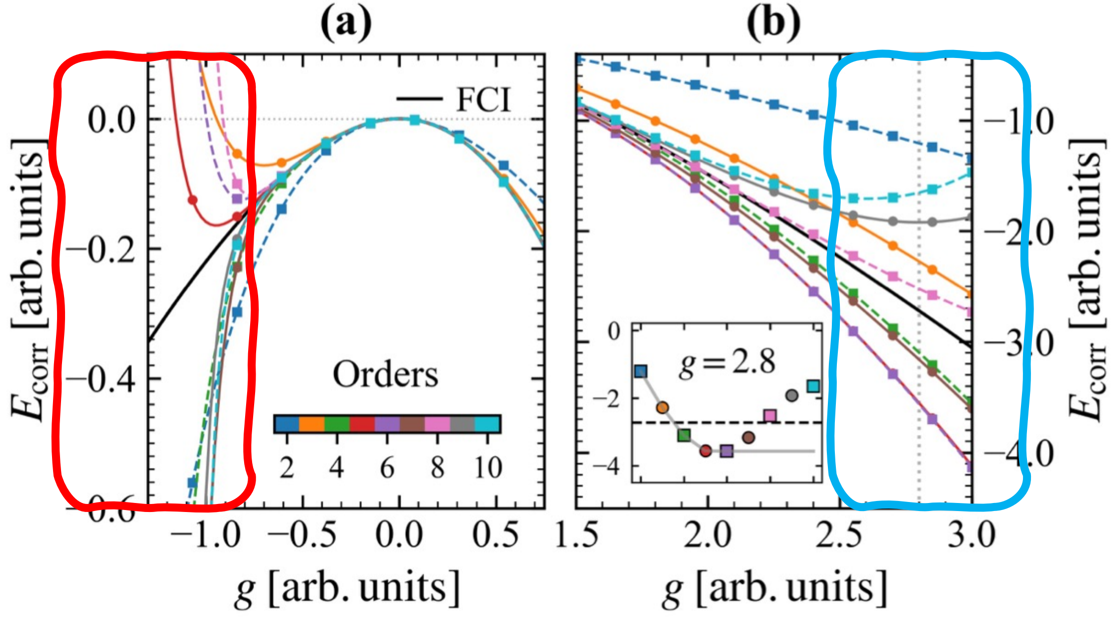
Can we go to even higher orders together with many-nucleon forces?

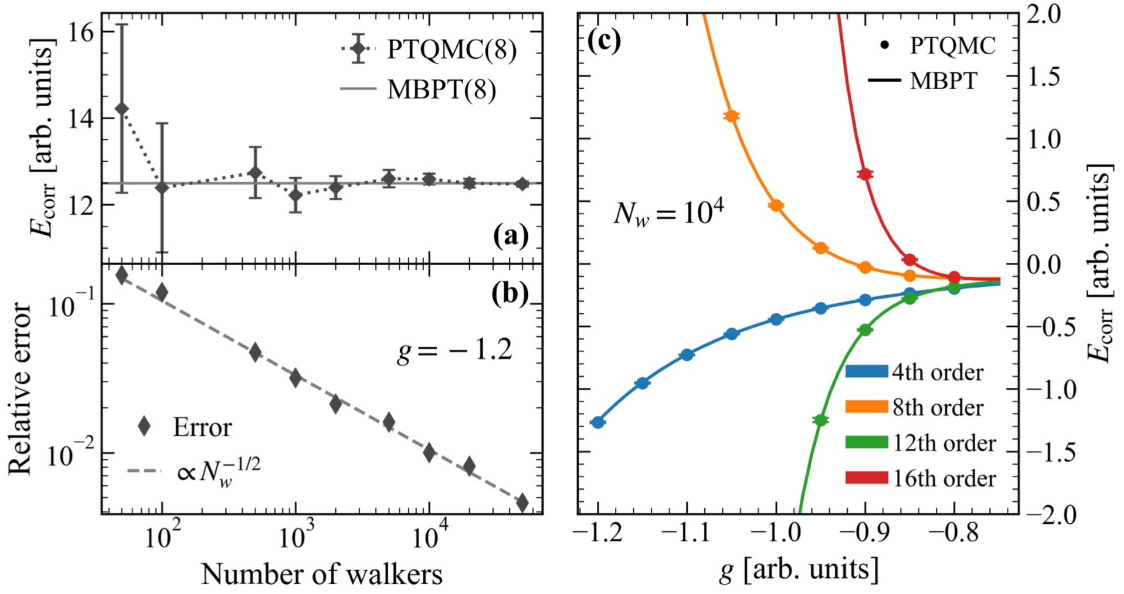
A. Tichai, R. Roth, *et al. Front. Phys.*, 8, **164** (2020).
C. Drischler, K. S. McElvain, *et al. arXiv:*2603.24532 (2026).
Z. Li, A. Tichai, *et al. arXiv:*2607.00119 (2026).

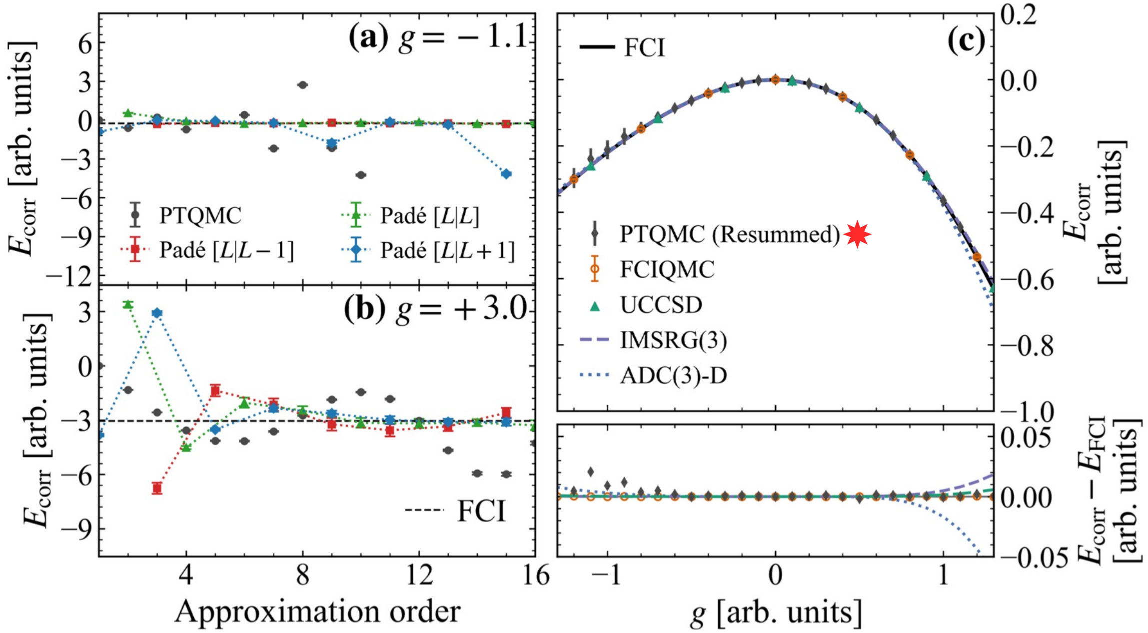
Perturbation Theory Quantum Monte Carlo (PTQMC)

- **Recursive spawning among configurations**









X. Zhen, **R. Hu**, *et al.* Editors' Suggestion.
Phys. Rev. C, **113**, L051302 (2026).

IMSRG : Can we go to higher orders?

H. Hergert, *et al*. *Phys. Rep.*, **621**, 165–222 (2016).
M. Heinz, *et al*. *Phys. Rev. C*, **103**, 044318 (2021).
B. C. He, S. R. Stroberg, *Phys. Rev. C*, **110**, 044317 (2024).

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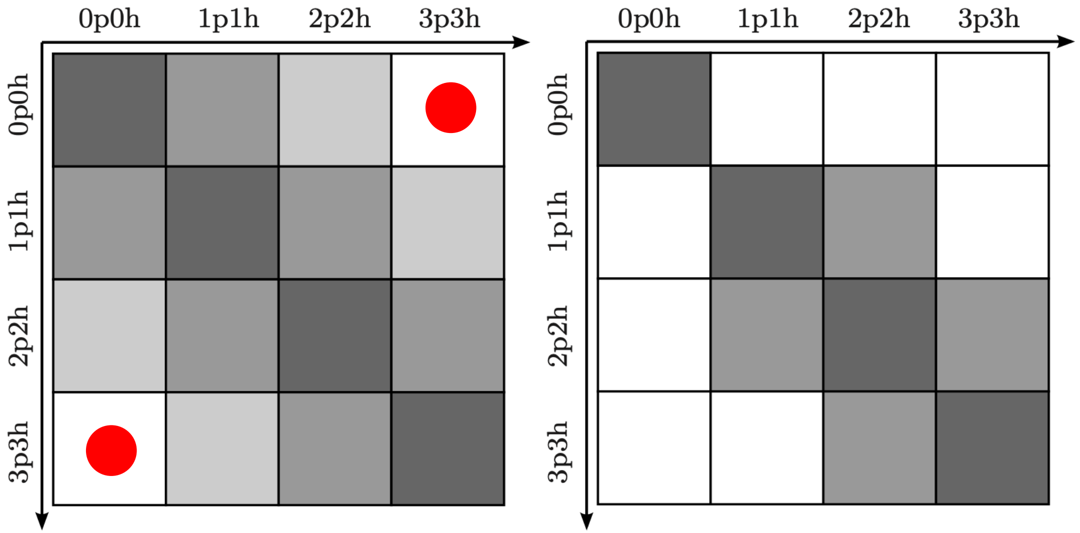


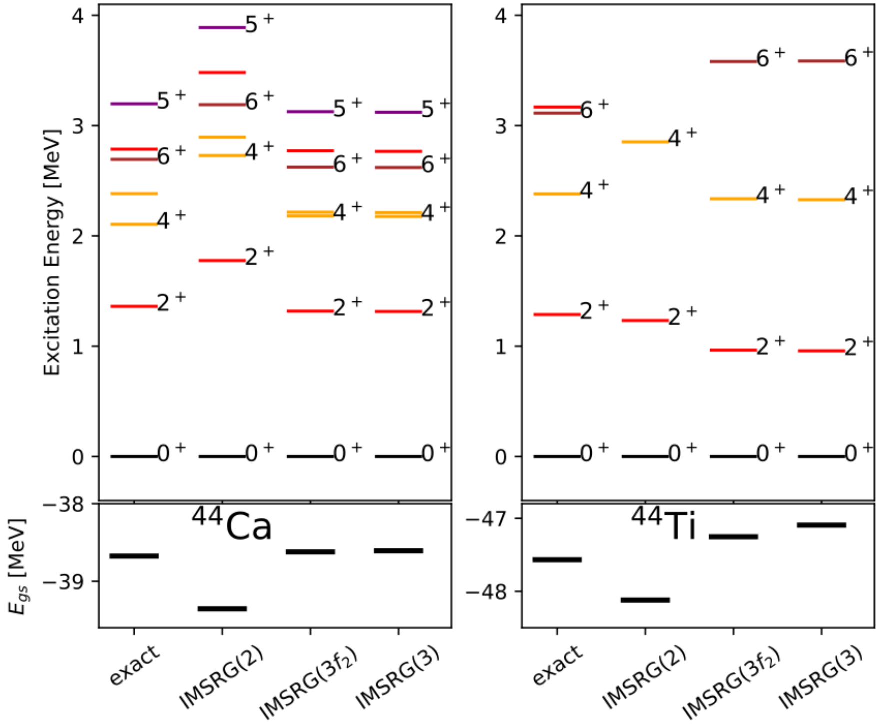
$\langle i|\, H(0)\, |j\rangle$ $\langle i|\, H(\infty)\, |j\rangle$

Three-Body Forces:
Important in nuclear physics but extremely expensive.

IMSRG(3f2) $O(N^6)$

$[2,[2,2]\rightarrow 3]\rightarrow 1,2$

Factorization for higher-order two-body correlations ! But…



Commutator	Cost	Included in …				
		IMSRG(3)-MP4	IMSRG(3)-N^7	IMSRG(3)-N^8	IMSRG(3)-g^5	IMSRG(3)
$[2,2]\rightarrow 3$	$O(N^7)$	✓	✓	✓	✓	✓
$[2,3]\rightarrow 2$	$O(N^7)$	✓	✓	✓	✓	✓
$[1,3]\rightarrow 3$	$O(N^7)$	✓	✓	✓	✓	✓
$[3,3]\rightarrow 0$	$O(N^6)$	✓	✓	✓	✓	✓
$[2,3]\rightarrow 1$	$O(N^6)$		✓	✓	✓	✓
$[1,3]\rightarrow 2$	$O(N^6)$		✓	✓	✓	✓
$[3,3]\rightarrow 1$	$O(N^7)$		✓	✓		✓
$[2,3]\rightarrow 3$	$O(N^8)$			✓	✓	✓
$[3,3]\rightarrow 2$	$O(N^8)$			✓	✓	✓
$[3,3]\rightarrow 3$	$O(N^9)$					✓

Polynomial Scaling

4 MBPT(2) ADC(2)
CCSD MBPT(3) ADC(3) IMSRG(2)
CCSD(T)
CCSDT MBPT(4)
9! CCSDT(Q) IMSRG(3)
CCSDTQ MBPT(5)

Similarity Renormalization Group Monte Carlo (SRGQMC)

R. Hu*, X. Zhen*, *et al. arXiv:*2607.08830 (2026).

- **Stochastic evolution of flow equations**

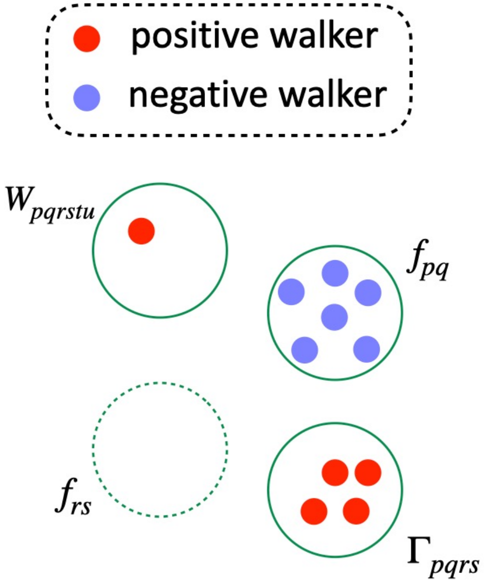
$$\frac{\mathrm{d}C}{\mathrm{d}\tau} = L(H)C$$

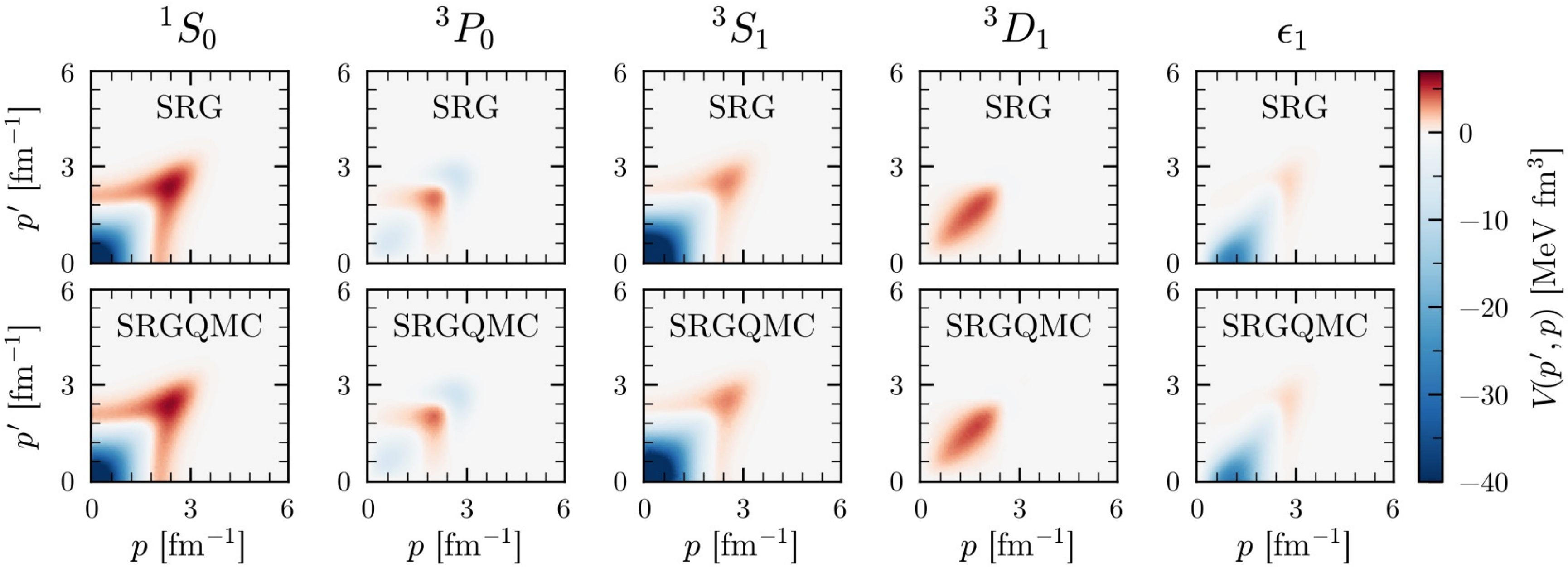
master equation ($\alpha = 1$)

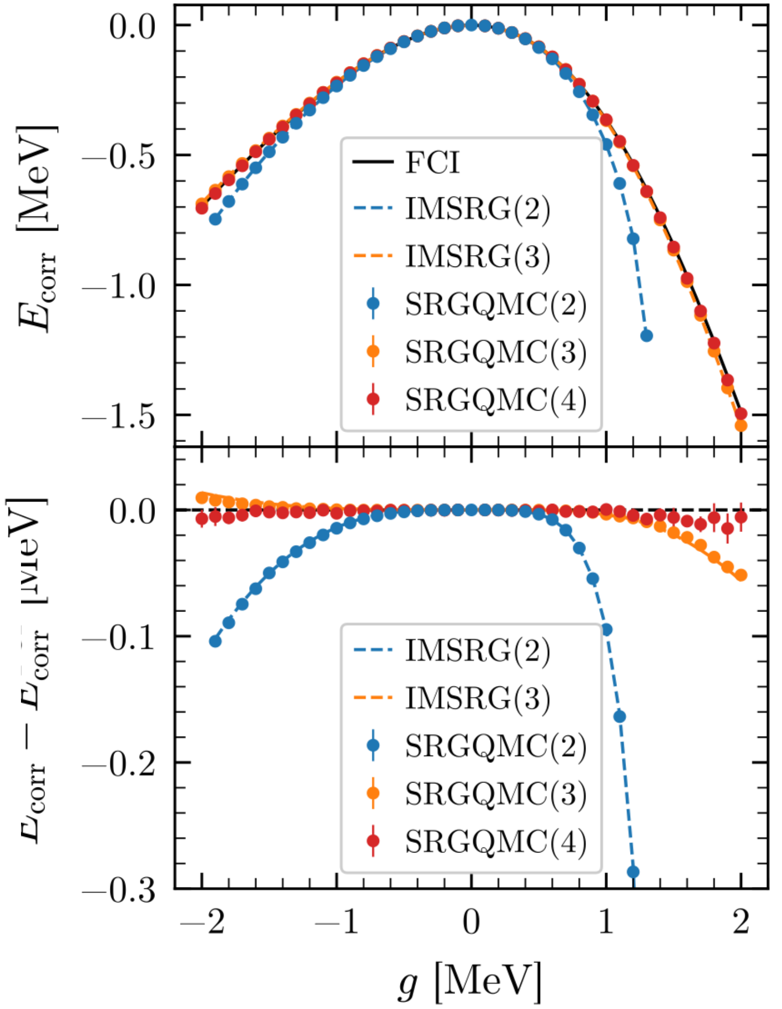
Source-free, homogeneous first-order ODEs !

flow equation ($\alpha = q + 1$)

$$\frac{\mathrm{d}H_s}{\mathrm{d}s} = \eta(H_s)H_s - H_s\eta(H_s),\ \eta(\lambda H_s) = \lambda^q \eta(H_s)$$







More on the way !

We are closing the loop !

Requirements

Physics Targets

Controlled equation of state:
Predict symmetric and neutron matter with cross-benchmarked calculations.

Separated uncertainties:
Quantify errors from nuclear interactions and many-body truncations.

Many-body forces:
Investigate the impact of three- and higher-body forces, especially at high densities.

Many-body Techniques

FCIQMC — Exact benchmarks:
Establish reliable anchors for strongly correlated systems.

PTQMC — High-order perturbative:
Access very high orders and diagnose convergence statistically.

SRGQMC — High-order nonperturbative:
Recover higher-rank correlations through stochastic flow evolution.

Next — ?

Brutal high-order, hybrid methods, multi-reference versions …

Validations

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