

Sign-problem-free quantum Monte Carlo simulation towards heavy nuclei

Bing-Nan Lu
吕炳楠

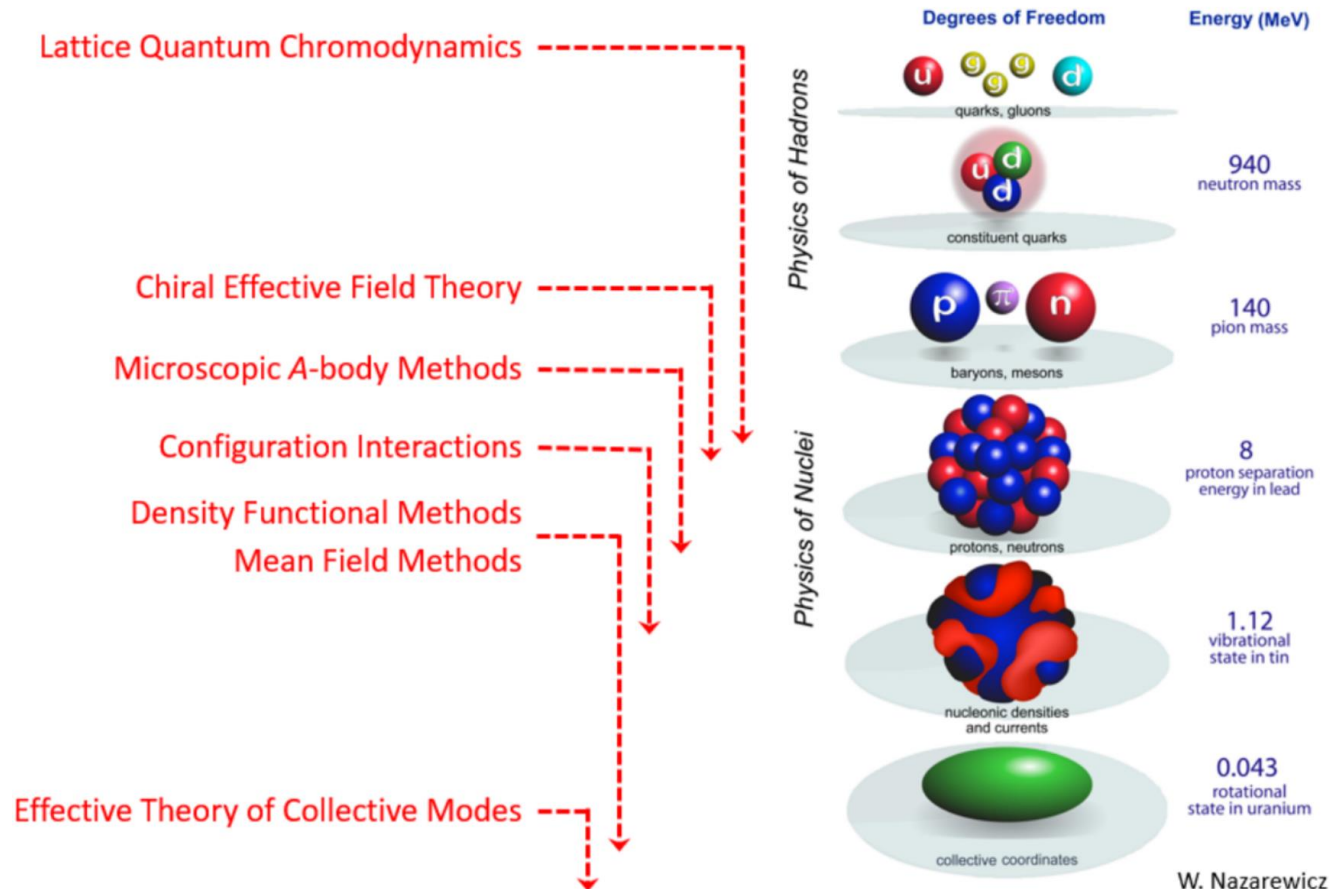
Graduate School of China Academy of Engineering Physics
中物院研究生院

Nuclear Physics Across Energy Scales Conference

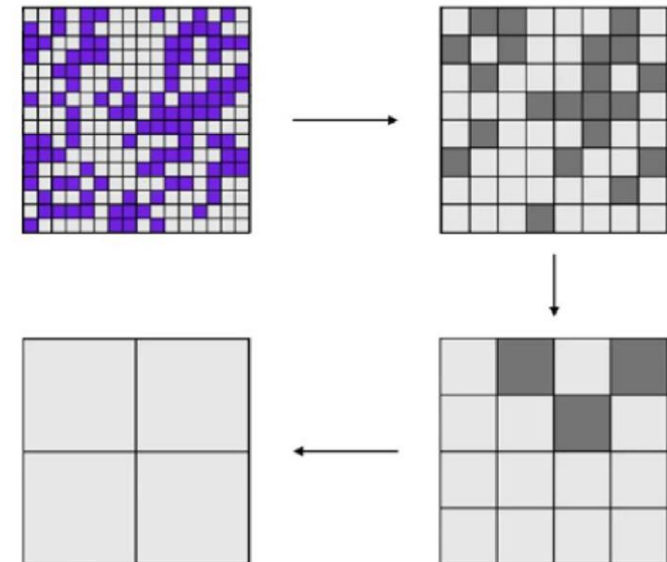
Sep 19, 2025



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

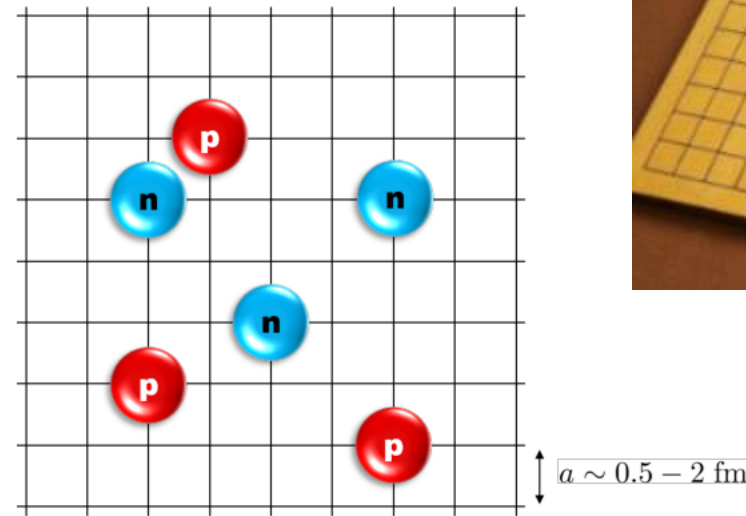


Lattice EFT: A many-body EFT solver

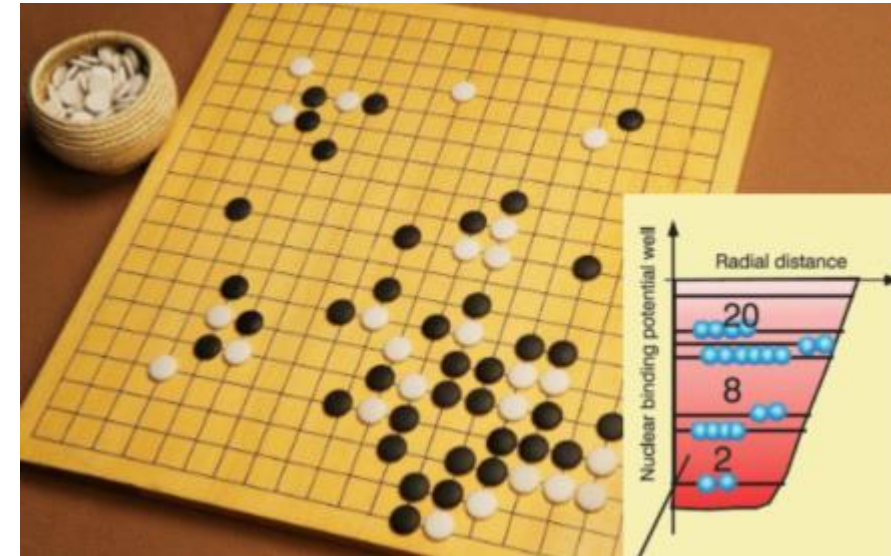
$$\text{Lattice EFT} = \text{Chiral EFT} + \text{Lattice} + \text{Monte Carlo}$$

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 $a \approx 1 \text{ fm} = 620 \text{ MeV}$
($\sim$ 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



- 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:

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

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

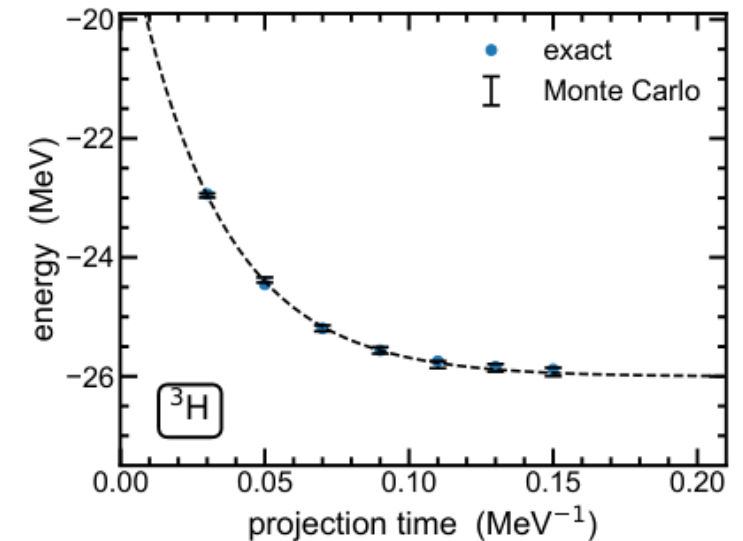
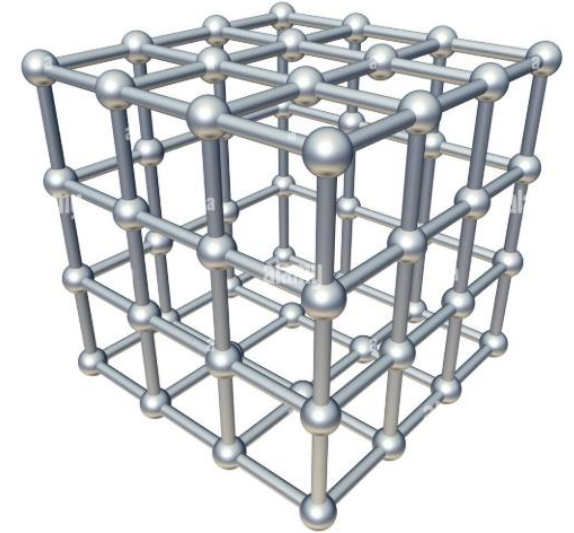
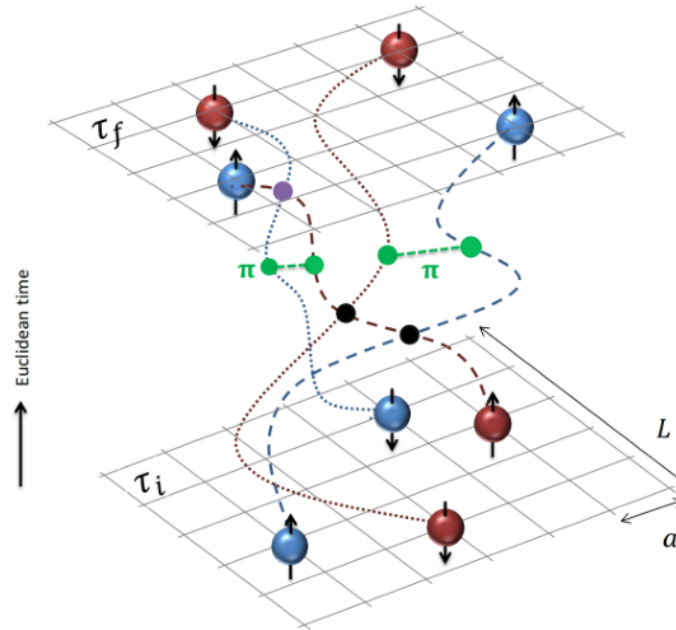
- Expectation value of any operator $\mathcal{O}$:

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

- τ is discretized into time slices:

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

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

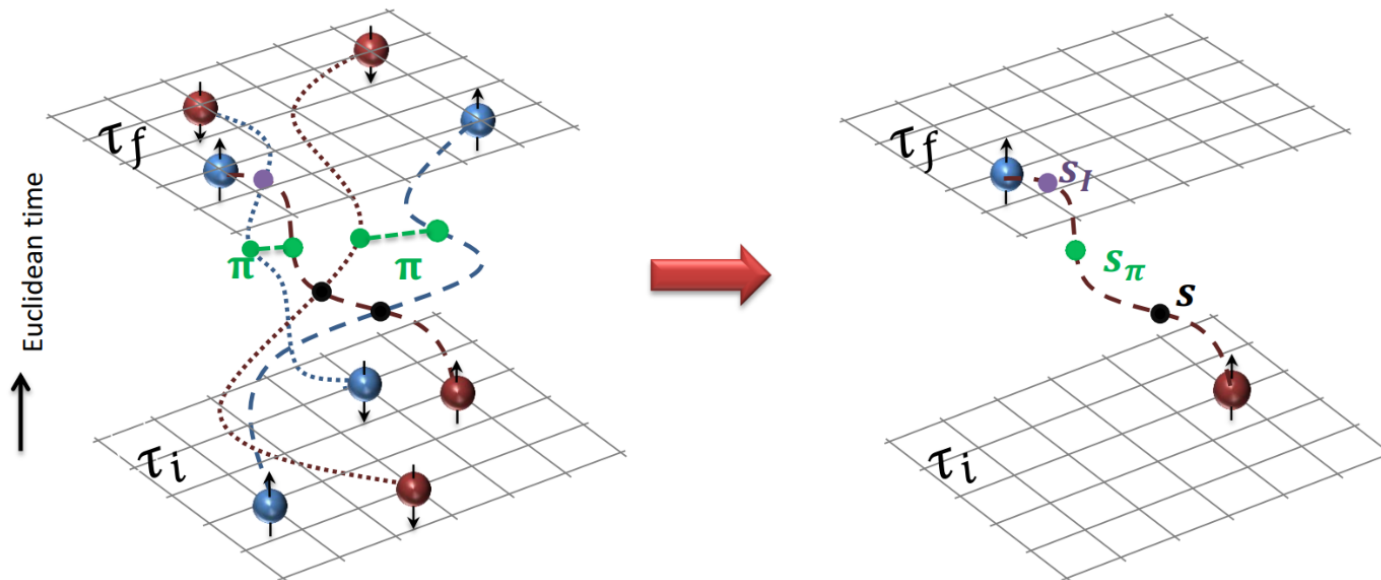


Lattice EFT: A many-body EFT solver

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

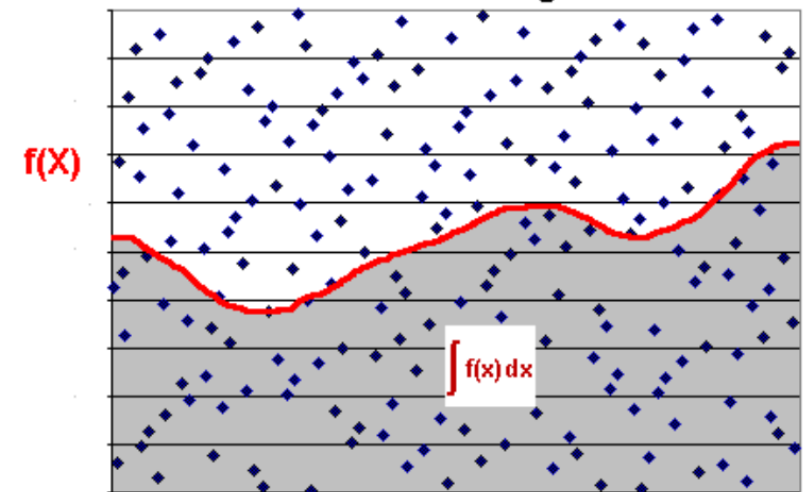
$$: \exp \left[-\frac{a_t C}{2} (\psi^\dagger \psi)^2 \right] := \frac{1}{\sqrt{2\pi}} \int ds : \exp \left[-\frac{s^2}{2} + \sqrt{-a_t C} s (\psi^\dagger \psi) \right] :$$

- 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. $\Leftarrow$ **No N-N interaction**



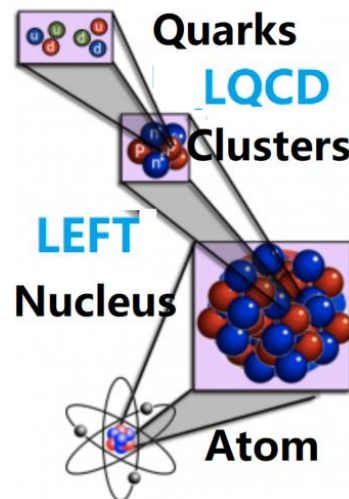
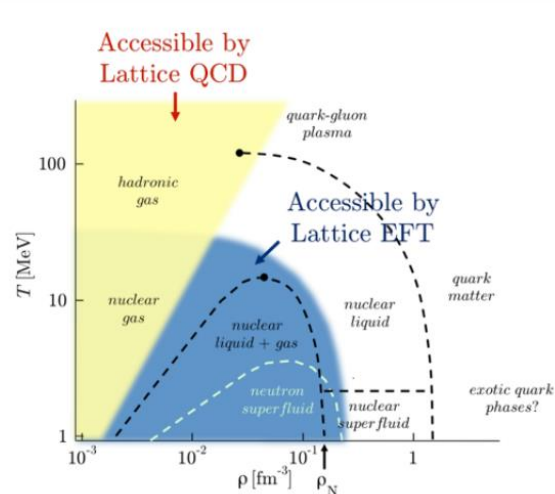
In lattice EFT, solving a general Hamiltonian consists of 5 steps:

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 $\tau \rightarrow \infty$ to find the true ground state.
5. Take the limit $L \rightarrow \infty$ to eliminate the finite volume effects.



Compare Lattice EFT and Lattice QCD

	LQCD	LEFT
degree of freedom	quarks & gluons	nucleons and pions
lattice spacing	~ 0.1 fm	~ 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 / ρ_{sat}
sign problem	severe for $\mu > 0$	moderate

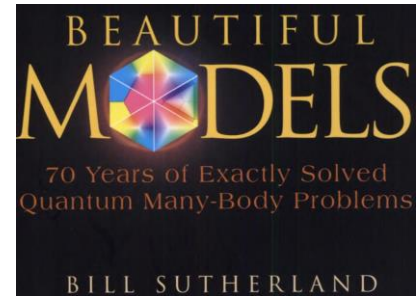
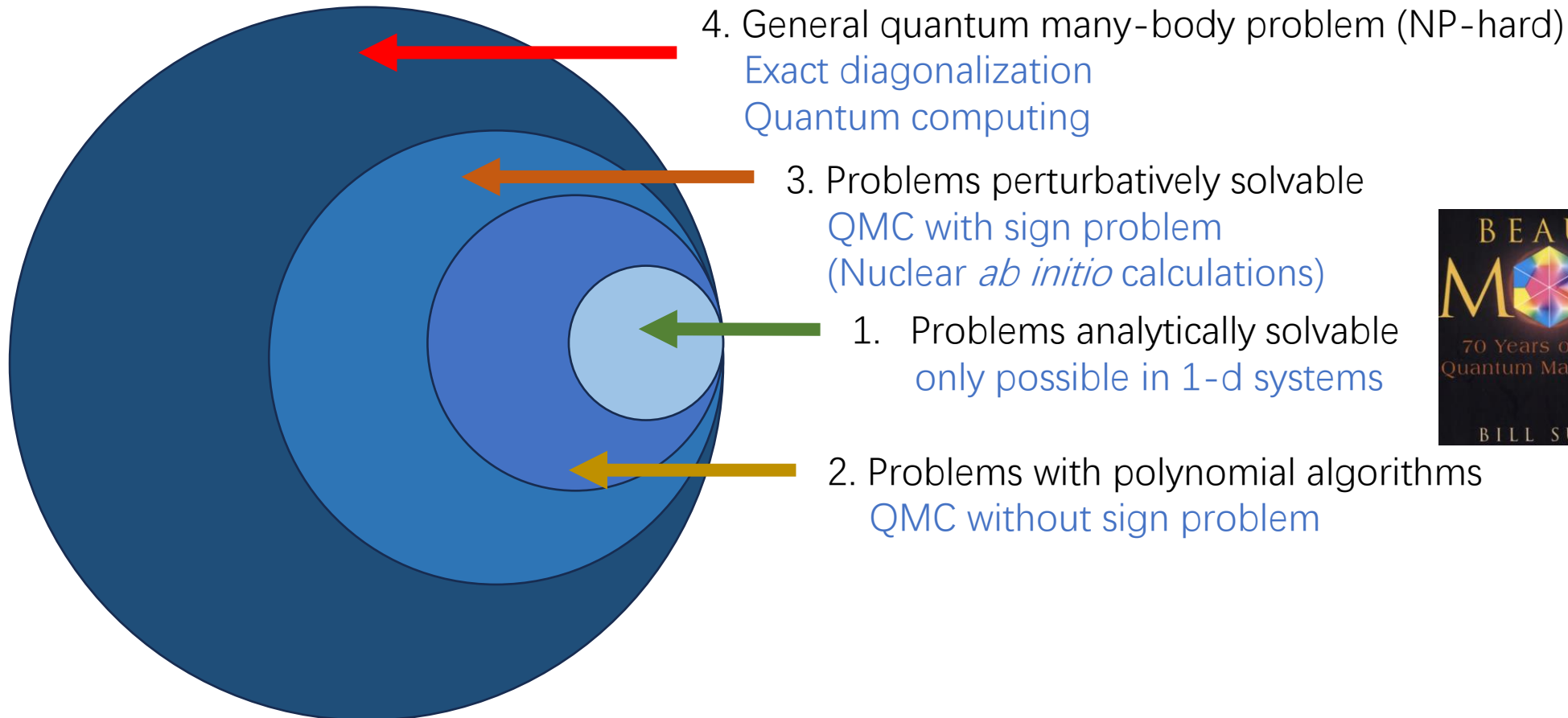


- Lattice EFT share a lot of common features with Lattice QCD. However,
 - Non-rel. $\rightarrow$ particle number conservation
 - Quadratic dispersion relation $\rightarrow$ no Fermion doubling problem
 - EFT contains non-renormalizable terms $\rightarrow$ no continuum limit

	Two-nucleon force	Three-nucleon force
LO	 2 LECs	—
NLO	 7 LECs	—
N ² LO	 2 LECs	 2 LECs
N ³ LO	 15 LECs	

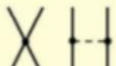
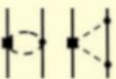
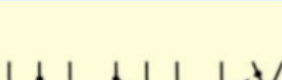
Quantum many-body problem classification

- Models with strong interactions present great challenges



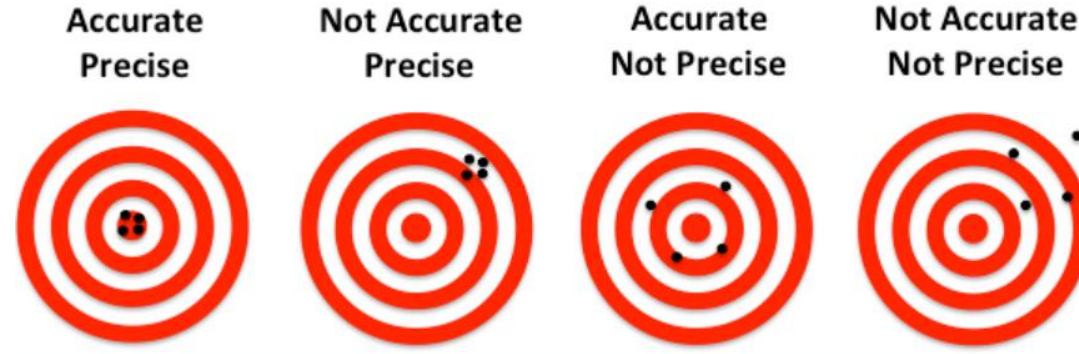
Nuclear many-body problem

- Given general nucleon-nucleon interactions, we consider the solution of many-body Schrodinger equations.
- **Challenges:**
 - Modern nuclear forces are complicated
 - Many-body forces
 - Hard core in NN potential
 - Large number of spin-isospin components
 - ...
 - High experimental accuracy
 - Binding energies, [exp. error ~eV](#) [theo. error ~MeV](#)
 - Request high-quality predictions

	Two-nucleon force	Three-nucleon force
LO	 2 LECs	—
NLO	 7 LECs	—
N ² LO		 2 LECs
N ³ LO	 15 LECs	

Computationally accessible models

- Is there any nuclear force model that can be solved with following requirements?
 - Request 1: exact polynomial complexity ← **easy to solve**
 - Request 2: no truncation needed (unbiased solutions) ← **high precision**
 - Request 3: reproduce experiments ← **high accuracy**



- Existing quantum many-body models satisfying request 1, 2 are typically **toy-models** or only work in **low-dimensions**
Not quite useful for nuclear physics

Toy-models vs. realistic models

- Toy-models typically capture the **essential elements** of the system. Used to study **qualitative** behaviors such as phase transitions.
- However, the **quantitative** predictions are **not accurate**
- Recently such models are introduced to resolve the tensions in **nuclear *ab initio* calculations**
 - Nuclear binding near a quantum phase transition, Elhatisari et al., PRL117, 132501 (2016)
 - Essential elements for nuclear binding, BL et al., PLB797, 134863 (2019)
 - Correlations imposed by the unitary limit between few-nucleon systems, nuclear matter, and neutron stars, Kievsky et al., PRL121, 072701 (2018)
 - Distilling the essential elements of nuclear binding via neural-network quantum states, Gnech et al., PRL133, 142501 (2024)



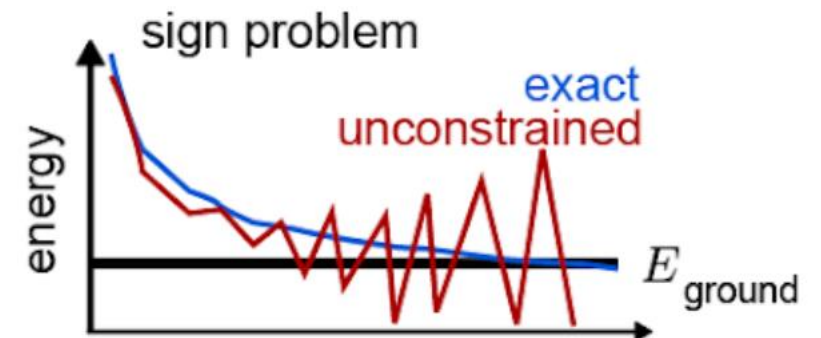
Typically 4-5 parameters, attempting to reconcile phase shifts, few-body data, many-body data and nuclear matter
Can we improve their accuracy to make them more useful?

Sign problem in quantum Monte Carlo

- **Quantum Monte Carlo** approaches transform the **quantum many-body problems** into high-dimensional integrals that can be evaluated stochastically
- Statistical error $\sim O(N^{-1/2})$
- **Sign problem** occurs when the integrand is NOT positive definite $\leftarrow$ can not be viewed as a **probability distribution**
- Sign problem is severe for **fermionic systems** due to the anti-symmetrization nature of the fermion wave functions
- **Sign-problem-free QMC** exists but confined to toy-models $\leftarrow$ can be solved with exactly polynomial complexity
 1. Sign problem might be tolerable for light nuclei. **However**, any sign problem increases exponentially with the particle number $\leftarrow$ **exponential complexity returns!**
 2. Sign problem might be partially solved by constrained path / perturbation theory. **However**, these require systematic expansion and induces **systematic biases**.

Sign-problem-free QMC allows us to solve the nuclear many-body problem from light to heavy nuclei with remarkably high numerical precision.

Yet its potential has not been fully exploited.



Examples of sign-problem-free QMC

- **Lattice QCD** with two identical quark species

$$Z = \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}[U] e^{-S_G[U]} \det[D[U]], \quad \det[D[U]] = \det[D_u[U]] \det[D_d[U]] = \det[D_u[U]]^2 > 0$$

- **Nuclear Lattice EFT** with Wigner-SU(4) interactions (even-even nuclei)

$$Z = \int \mathcal{D}s e^{-s^2/2} \det[Z(s)], \quad \det[Z(s)] = \det[Z_{\uparrow}(s)] \det[Z_{\downarrow}(s)] = \det[Z_{\uparrow}(s)]^2 \geq 0$$

- Repulsive Fermi-Hubbard model at half-filling
- Kane-Mele-Hubbard model
- Half-filled Kondo lattice model

Positivity of the fermionic determinant is protected by the time-reversal symmetry

Sufficient condition for absence of the sign problem in the fermionic quantum Monte Carlo algorithm, C.-J. Wu and S.-C. Zhang, PRB71, 155115 (2005)

Sign-problem-free fermionic quantum Monte Carlo: Developments and Applications, Z.-X. Li and H. Yao, Annu. Rev. Condens. Matter Phys. 10, 337 (2019)

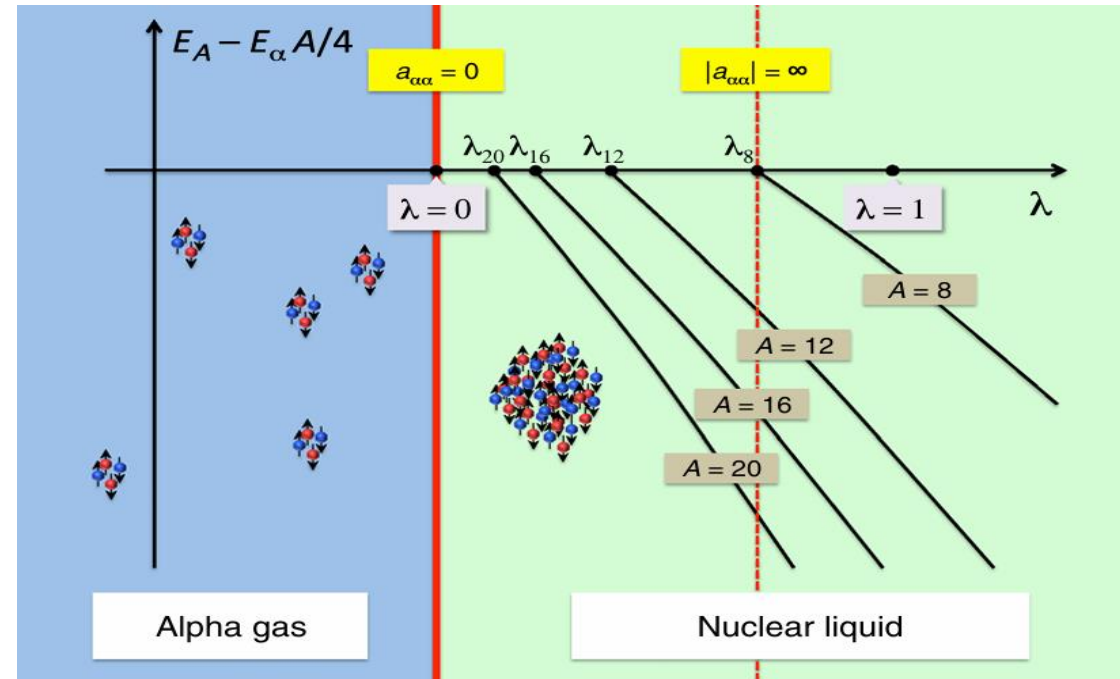
Nuclear binding near a quantum phase transition

$$H_{\text{SU4}} = H_{\text{free}} + \frac{1}{2!} C_2 \sum_{\mathbf{n}} \bar{\rho}(\mathbf{n})^2$$

$$\bar{\rho}(\mathbf{n}) = \rho(\mathbf{n}) + s_{\text{L}} \sum_{|\mathbf{n}' - \mathbf{n}|=1} \rho(\mathbf{n}')$$

$$\rho(\mathbf{n}) = \bar{\Psi}^\dagger(\mathbf{n}) \bar{\Psi}(\mathbf{n})$$

$$\bar{\Psi}(\mathbf{n}) = \Psi(\mathbf{n}) + s_{\text{NL}} \sum_{|\mathbf{n}' - \mathbf{n}|=1} \Psi(\mathbf{n}')$$



Challenge: Minimal nuclear force
That reproduce the binding pattern

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

Simple Wigner-SU(4) central force fails!

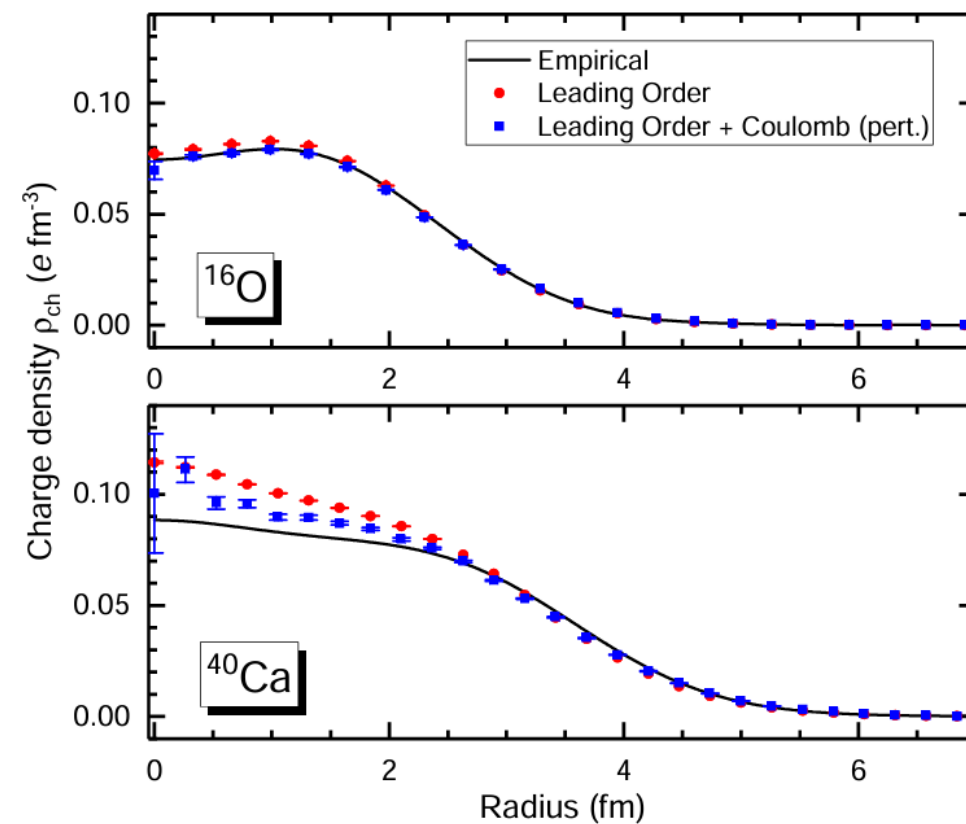
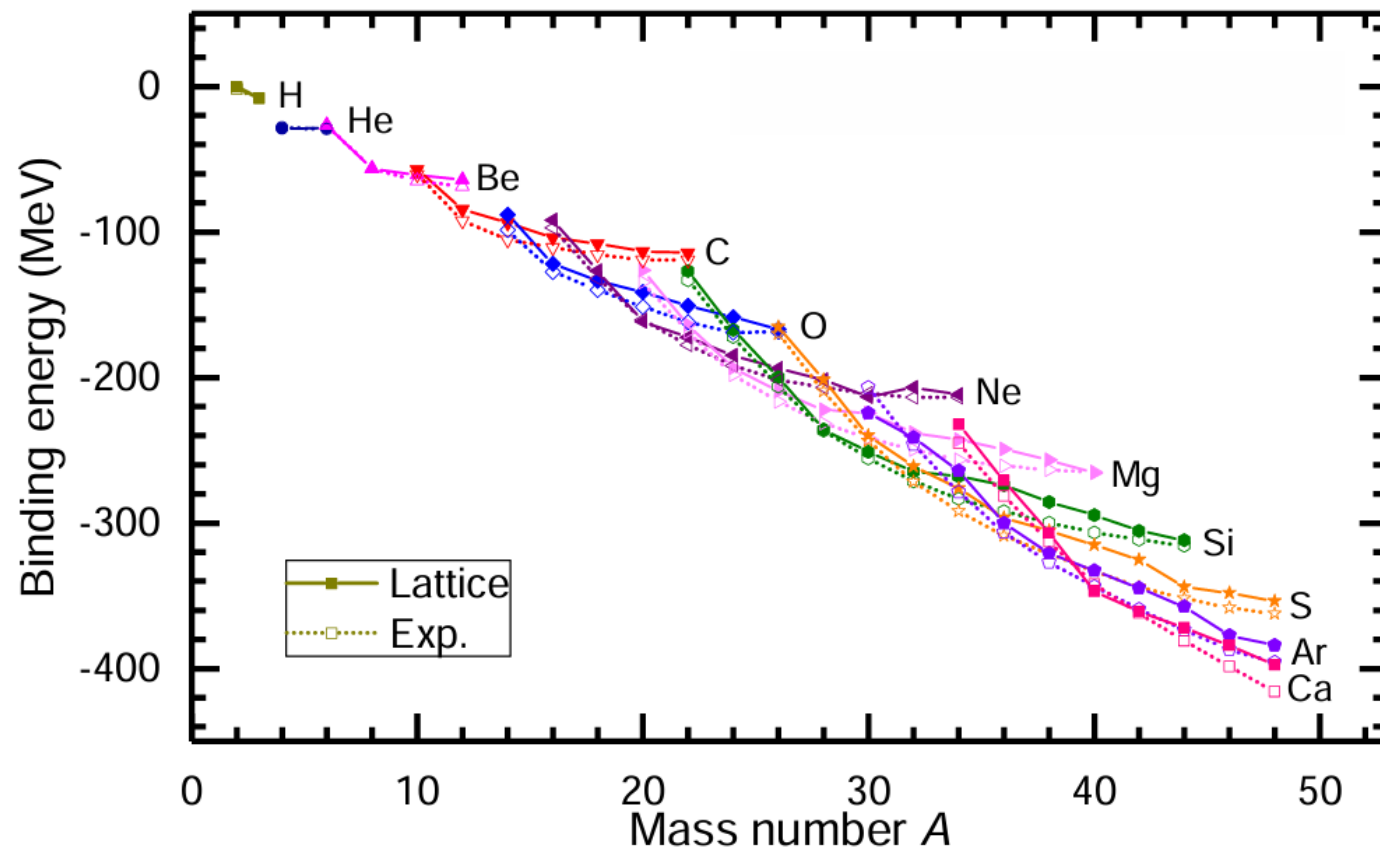
S. Elhatisari et al., PRL 117, 132051 (2016)

Nuclear force with a Wigner-SU(4) symmetry

$$H_{\text{SU}(4)} = H_{\text{free}} + \frac{1}{2!}C_2 \sum_{\mathbf{n}} \tilde{\rho}(\mathbf{n})^2 + \frac{1}{3!}C_3 \sum_{\mathbf{n}} \tilde{\rho}(\mathbf{n})^3$$

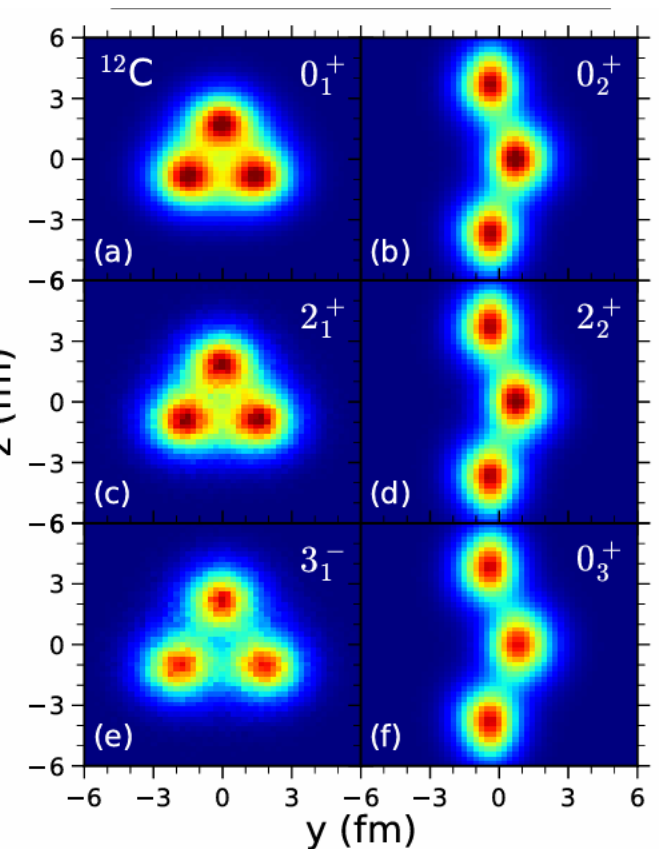
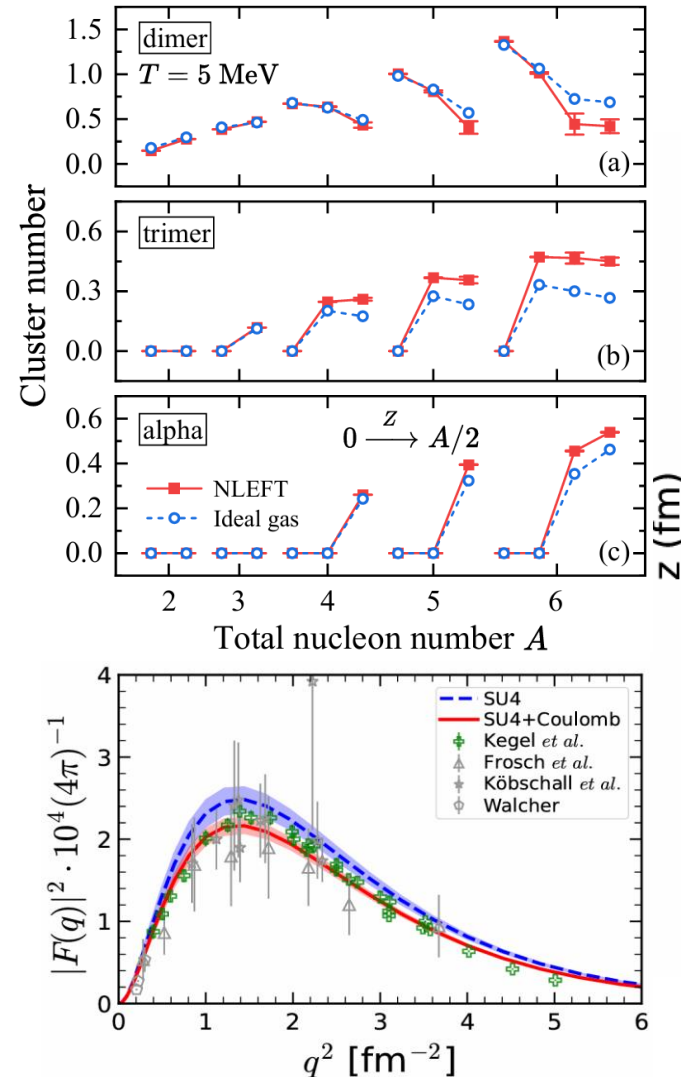
All density operators are smeared

[Lu et al., PLB 797, 134863 \(2019\)](#)



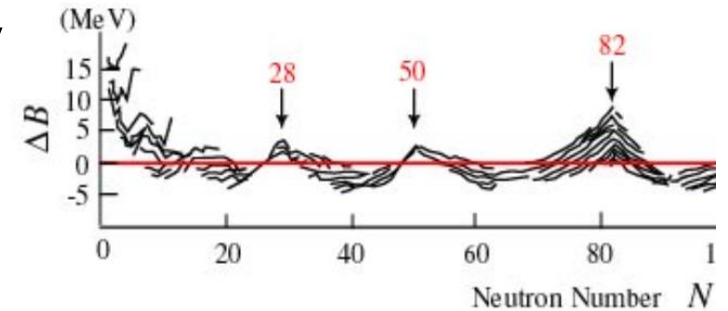
Applications of Wigner-SU(4) interaction

- Ab initio calculations of the isotopic dependence of nuclear clustering, [S. Elhatisari et al., PRL 119, 222505 \(2017\)](#)
- Emergent geometry and duality in the carbon nucleus, [S. Shen et al., EPJA 57, 276 \(2021\)](#); [S. Shen et al., Nat. Comm. 14, 2777 \(2023\)](#);
- Ab initio study of nuclear clustering in hot dilute nuclear matter, [Z. Ren et al., PLB 850, 138463 \(2024\)](#)
- Ab initio calculation of the alpha-particle Monopole transition form factor, [Ulf-G. Meißner et al., PRL 132, 062501 \(2024\)](#)
- Ab initio study of the beryllium isotopes ^7Be to ^{12}Be , [S. Shen et al., PRL 134, 162503 \(2025\)](#)



Improved Wigner-SU(4) interaction

- **Wigner-SU(4) symmetry** is an approximate symmetry
 -Lack correct **shell structure** → Spin-orbit coupling
- We introduce a **spin-orbit coupling**



$$H = \sum_n \left[-\frac{\Psi^\dagger \nabla^2 \Psi}{2M} + \frac{C_2}{2} \bar{\rho}^2 + \frac{C_3}{6} \bar{\rho}^3 + C_s \bar{\rho} \bar{\rho}_s \right]$$

$$\rho = \bar{a}^\dagger \bar{a},$$

$$\rho_s = \sum_{ijk} \epsilon_{ijk} \nabla_i \left[\bar{a}^\dagger (\vec{\nabla}_j - \overleftarrow{\nabla}_j) \sigma_k \bar{a} \right]$$

- **Wigner-SU(4) symmetry** does not mix **spin-up** and **spin-down** particles
 → Fermion determinant factorized into **two identical parts** $\det(Z) = \det(Z_\uparrow)^2 \geq 0$
 → Fermionic **sign problem avoided!**
- **Spin-orbit term** act equivalently for **spin-up** and **spin-down** particles
 → Fermion determinant keeps positive definite

Gradient Descent method

- We fit to binding energies of ${}^4\text{He}$, ${}^{16}\text{O}$, ${}^{24}\text{Mg}$, ${}^{28}\text{Si}$, ${}^{32}\text{S}$, ${}^{40}\text{Ca}$ using a **derivative-based** optimization method

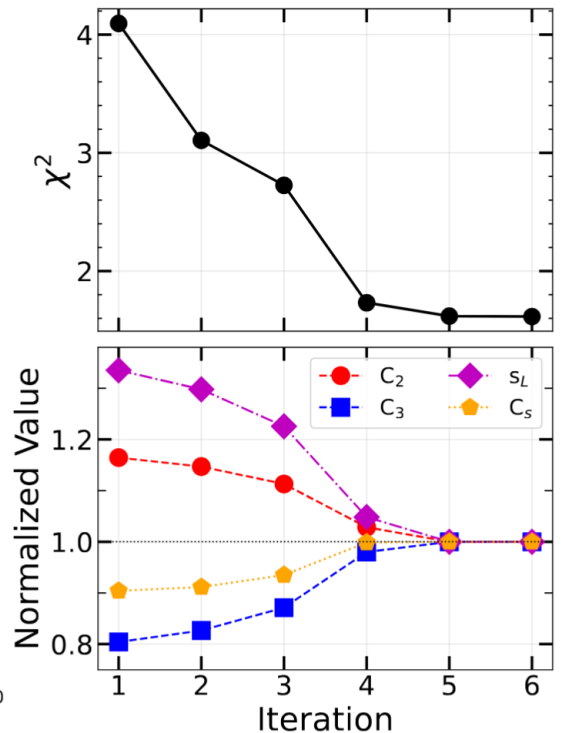
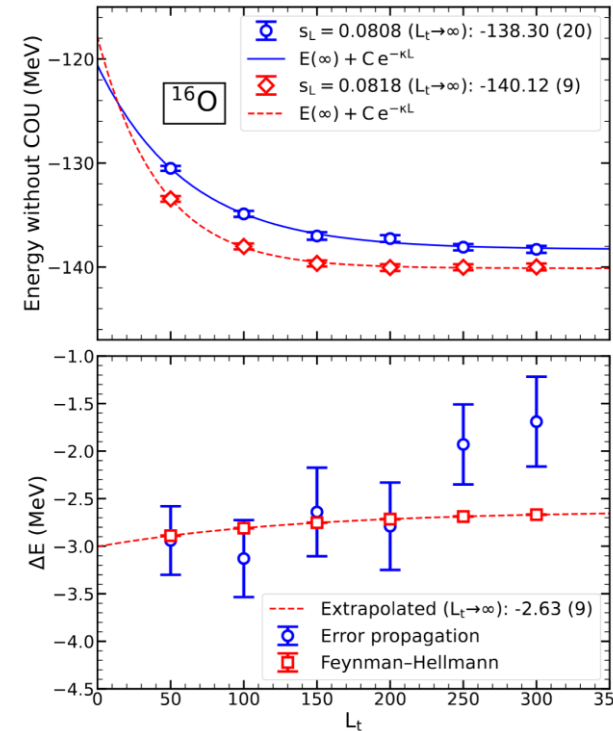
$$\chi^2 = \sum_A \left[\frac{E(A) - E_{\text{exp}}(A)}{\Delta(A)} \right]^2$$

- The derivatives are calculated using the **Feynman-Hellmann theorem**,

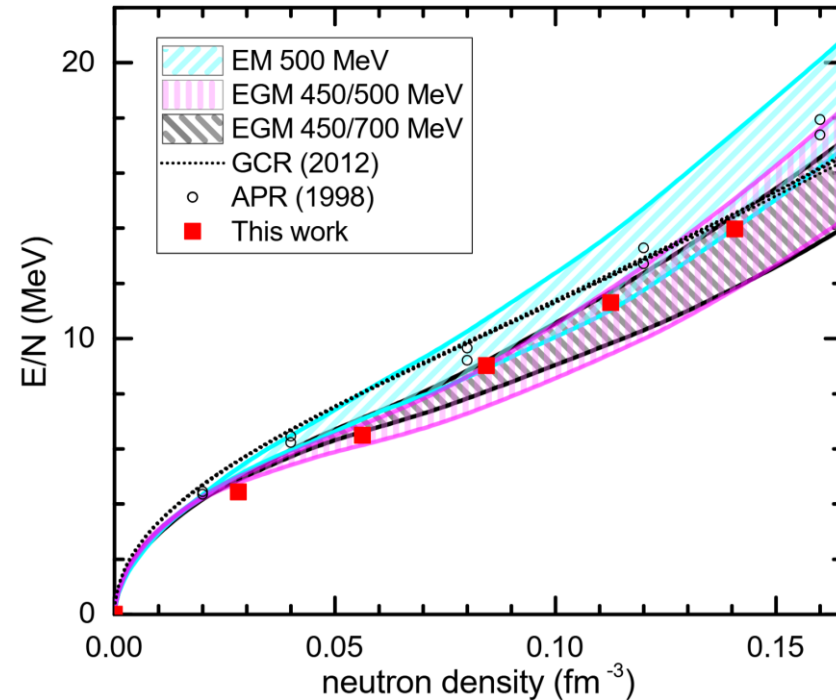
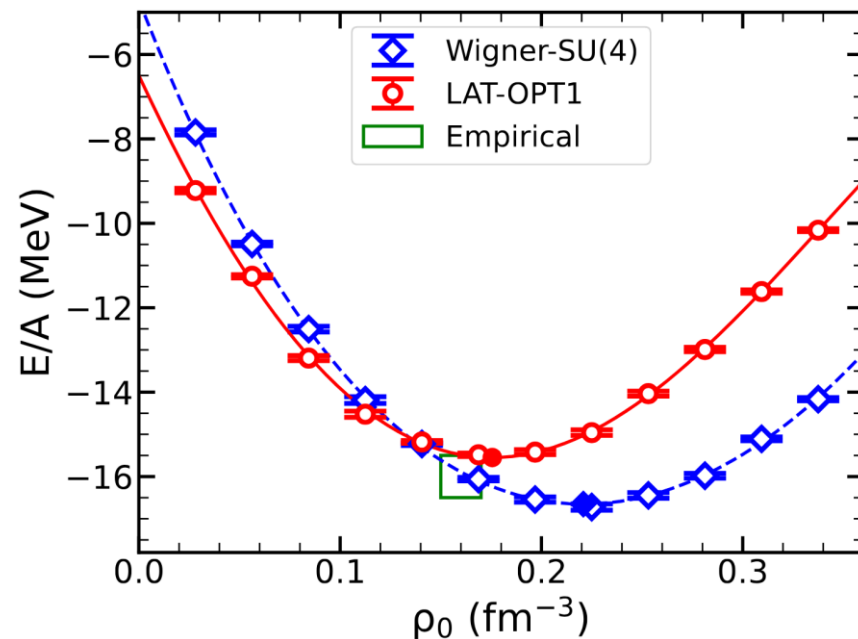
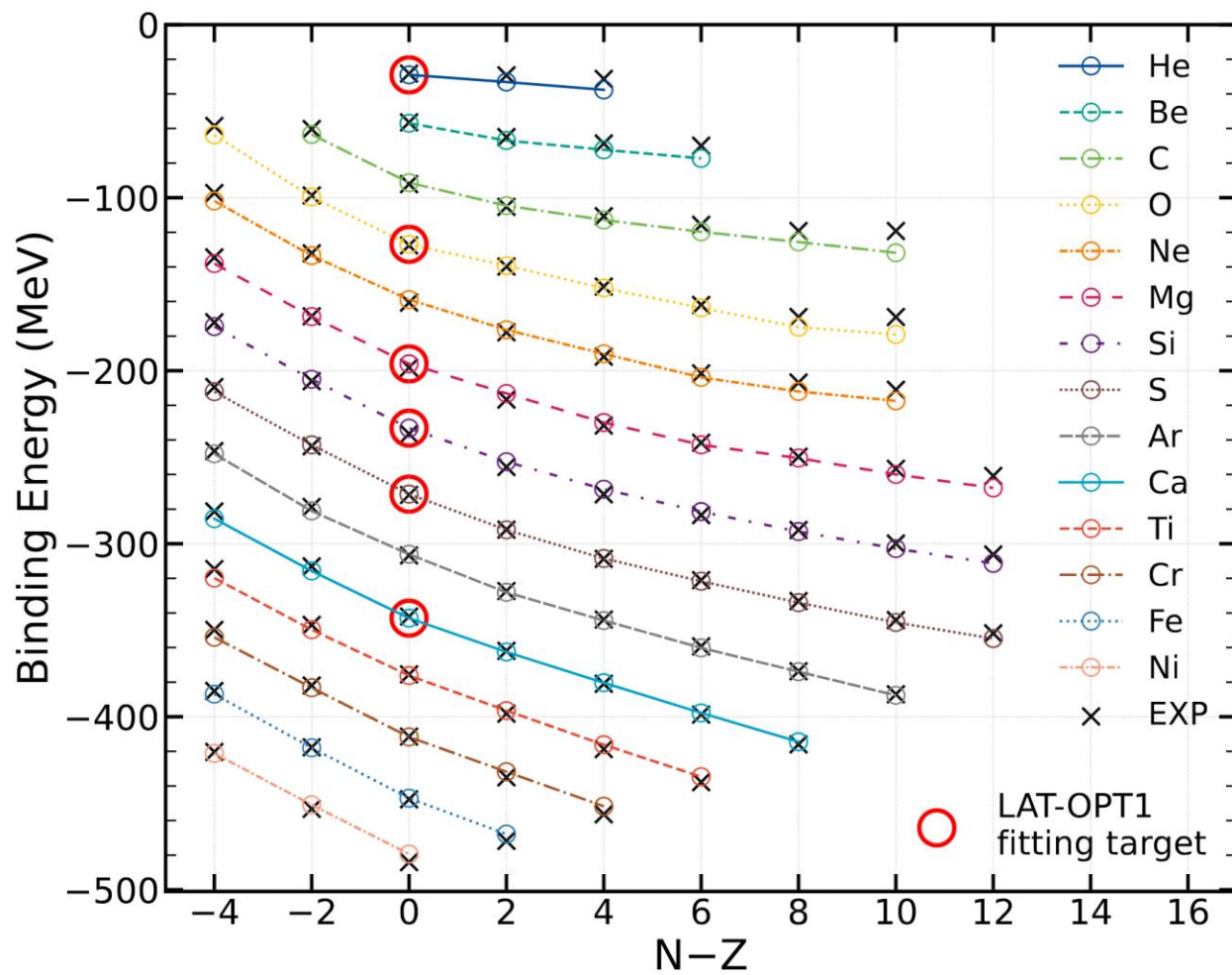
$$\partial E(A)/\partial x = \langle \Phi | H(x + \delta) - H(x) | \Phi \rangle / \delta$$

- Typically converge within 10 iterations
 ← **precise and unbiased**
 derivative computation is essential!

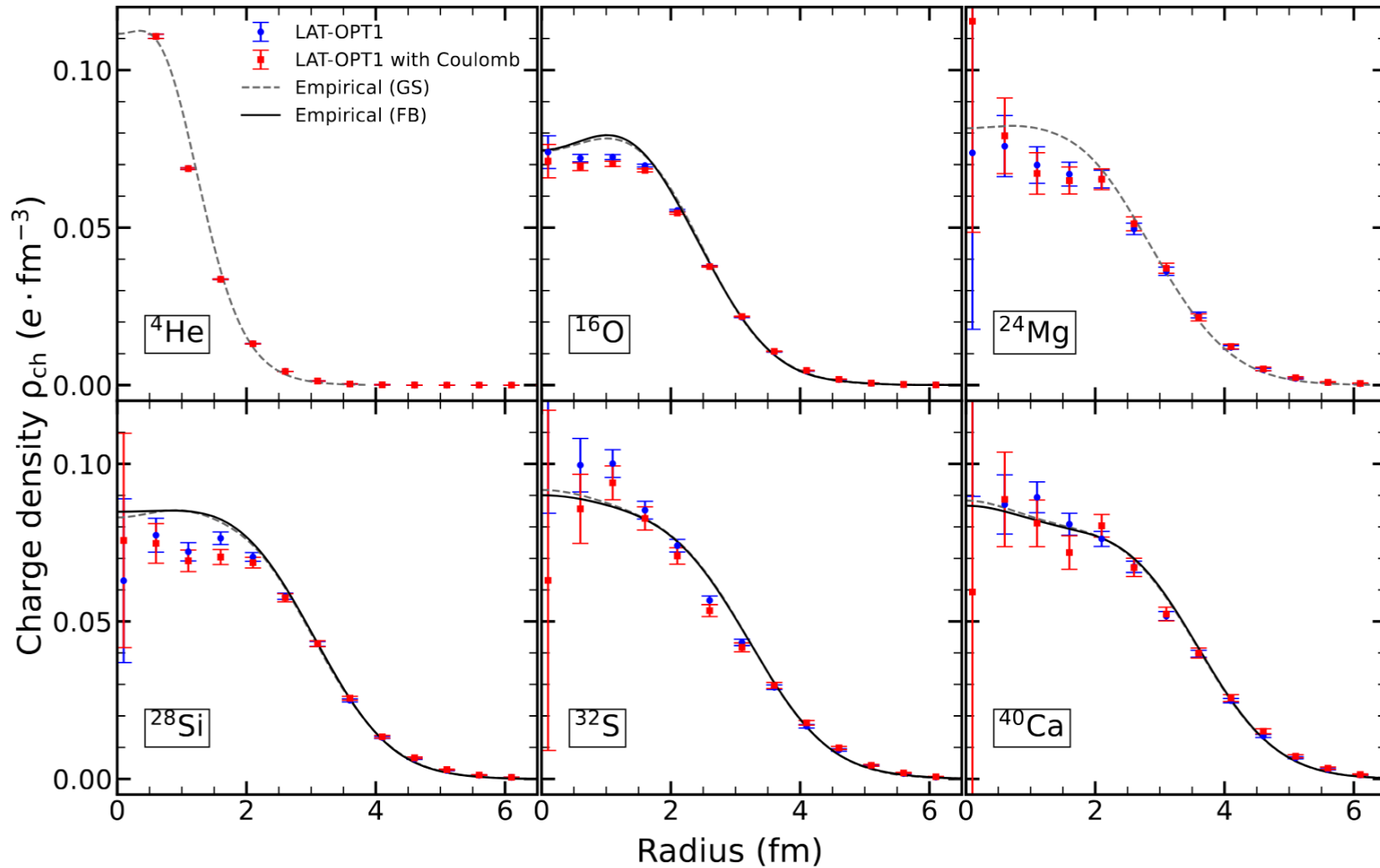
$$C_2 = -4.410 \times 10^{-7} \text{ MeV}^{-2}, C_3 = 1.561 \times 10^{-15} \text{ MeV}^{-5}, C_s = 8.590 \times 10^{-12} \text{ MeV}^{-4}, s_L = 0.081, s_{NL} = 0.45 \quad \text{“LAT-OPT1”}$$



Results from LAT-OPT1



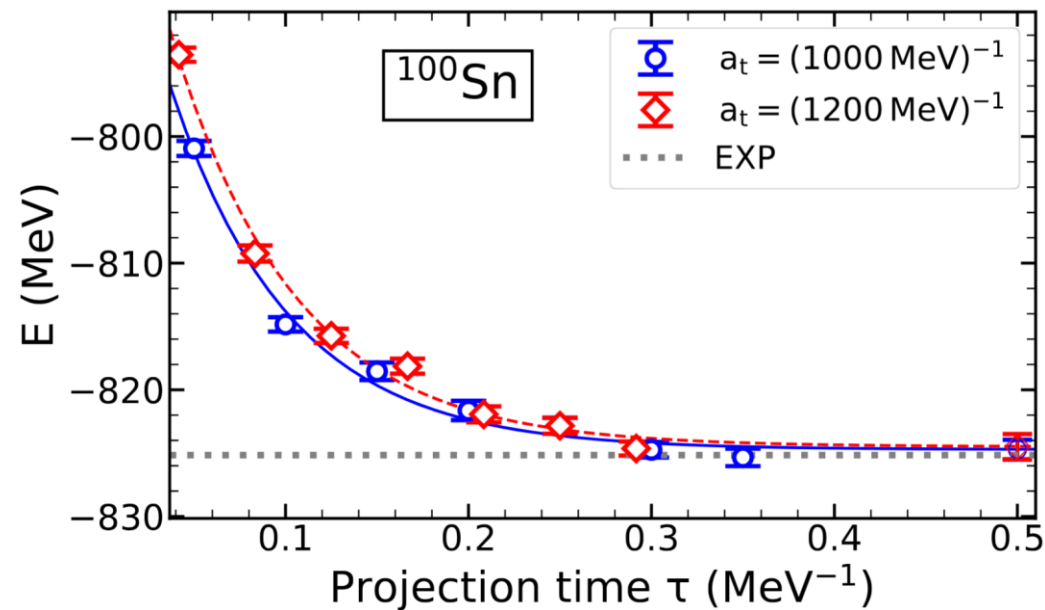
Results from LAT-OPT1: Charge densities



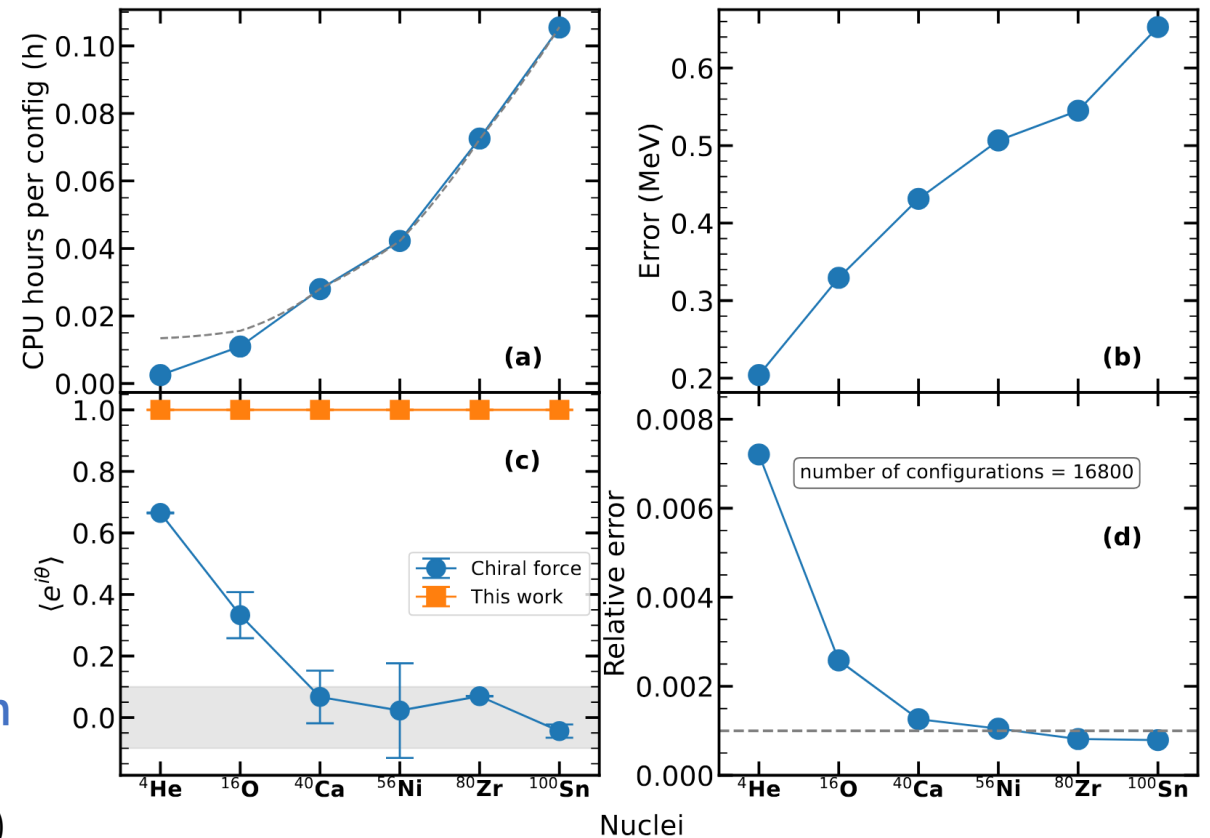
- Charge densities calculated using **pinhole algorithm**
[Elhatisari et al., PRL119, 222505 \(2017\)](#)
- **Pinhole algorithm** induce **mild sign problem**, not available for $A \geq 40$. See **partial pinhole algorithm** for a solution
[Zheng-Xue Ren et al., arXiv:2506.02597](#)

Results from LAT-OPT1: Heavy nuclei

- Sign-problem-free QMC scales polynomially towards heavy nuclei

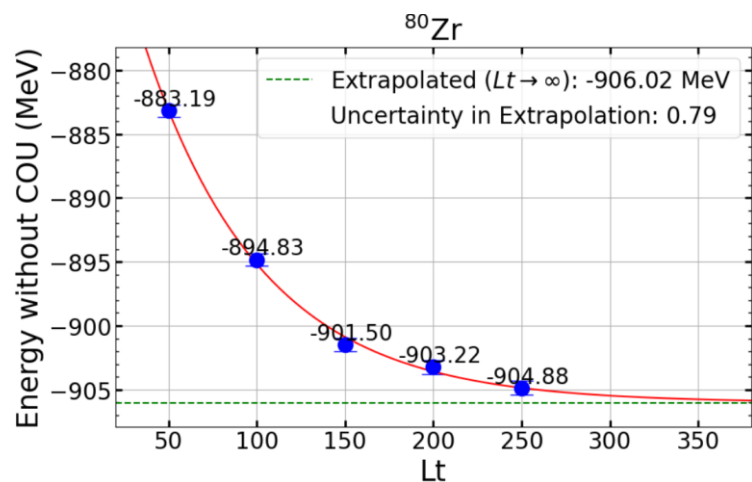


Extract binding energy of ^{100}Sn with **~1 MeV precision**
using **~30000 CPU hours**
(10 days on AMD EPYC [9554@3.1GHz](https://www.amd.com/en/products/processors/epyc), 128 CPU cores)



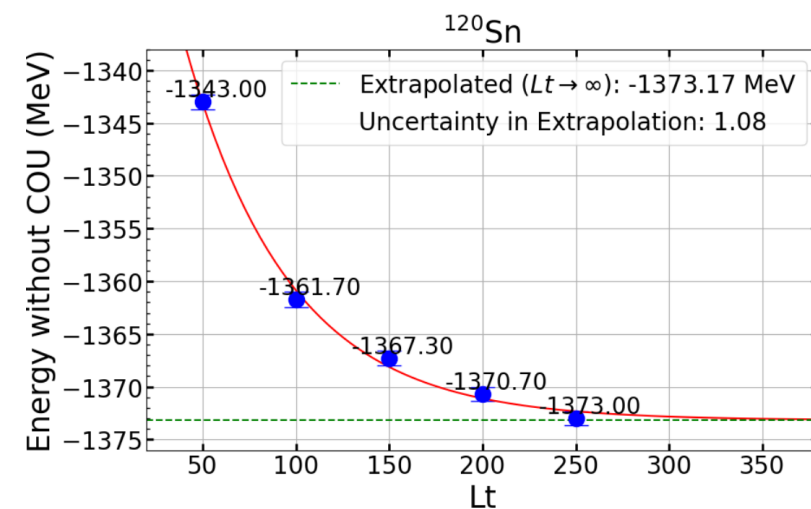
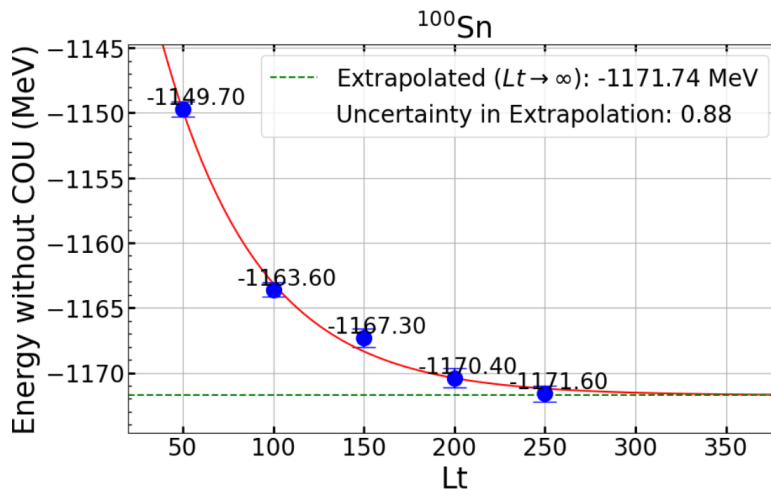
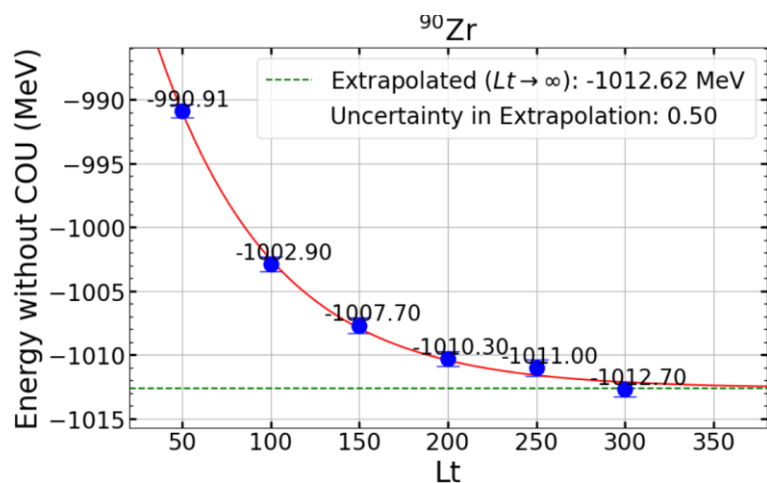
Relative errors <0.1% for heavy nuclei

Results from LAT-OPT1: Heavy nuclei



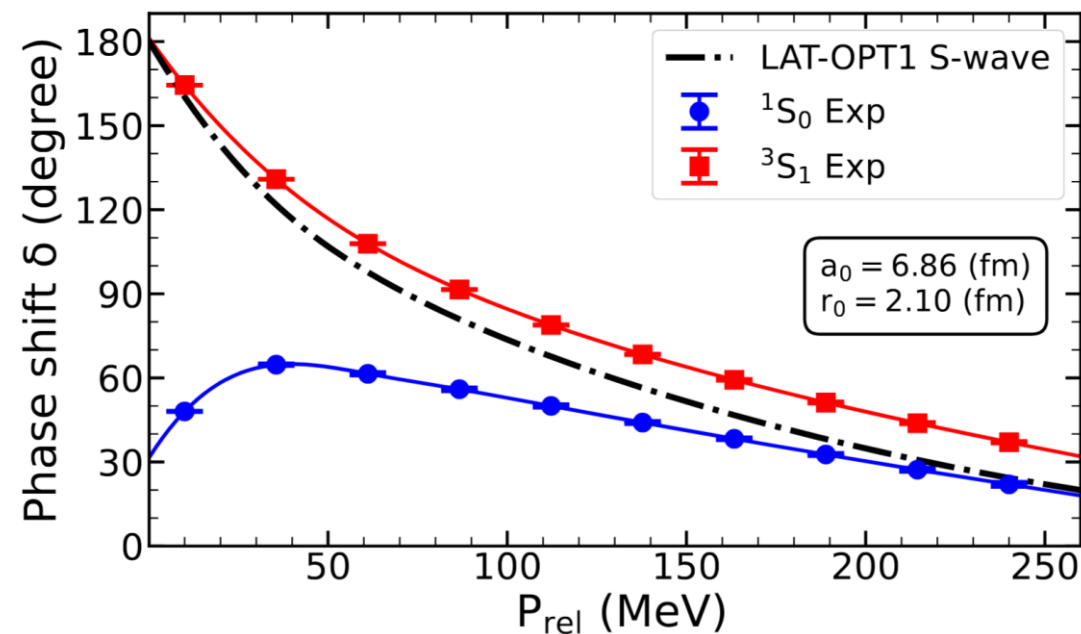
Nucleus	E_{bind} (MeV)	E_{sl} (MeV)	$E_{\text{sl}}/E_{\text{bind}}$	EXP (MeV)
⁴ He	-29.0(2)	-0.3	0.010	-28.3
¹² C	-91.3(1)	-13.3	0.146	-92.2
¹⁴ C	-104.6(1)	-12.7	0.121	-105.3
¹⁶ O	-126.9(2)	-5.6	0.044	-127.6
⁴⁰ Ca	-343.0(2)	-13.6	0.040	-342.1
⁴⁸ Ca	-414.5(3)	-42.3	0.102	-416.0
⁵⁶ Ni	-479.3(6)	-74.6	0.156	-484.0
⁸⁰ Zr	-672.1(8)	-23.3	0.035	-669.2
⁹⁰ Zr	-782.1(5)	-64.8	0.083	-783.9
¹⁰⁰ Sn	-824.7(8)	-103.0	0.125	-825.2
¹³² Sn	-1134.2(27)	-110.9	0.098	-1102.8

- Spin-orbit energy enhanced for **new magic numbers** 28, 50, 82, etc., indicating **shell structure emergence**
- Remarkable **generalization capability** ← all **quantum correlation** included

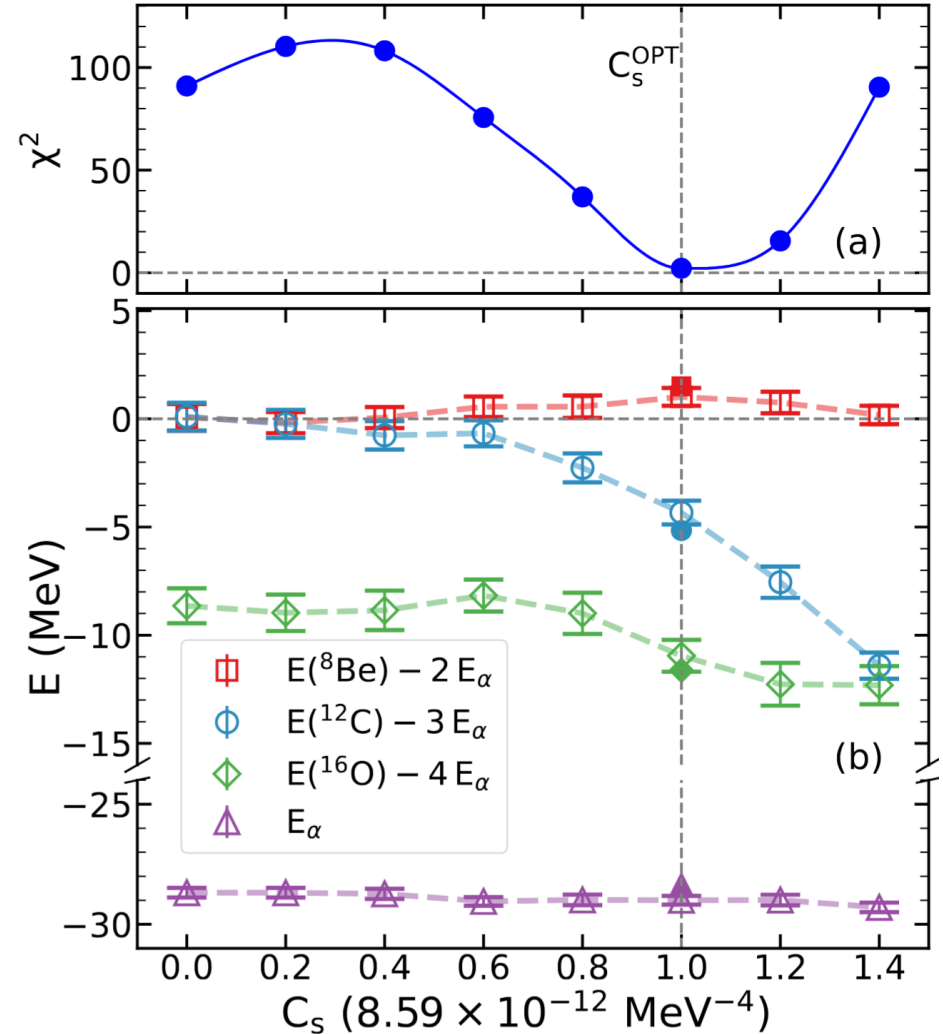
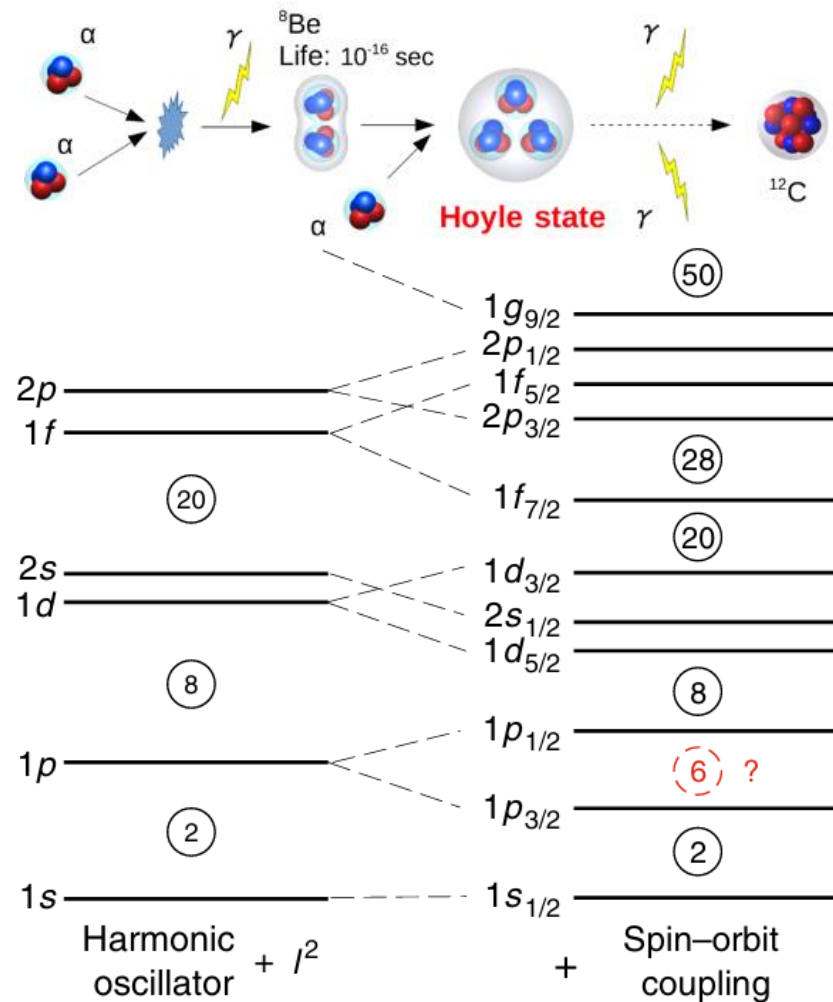


Results from LAT-OPT1: Phase shifts

- *Ab initio* calculations attempt to predict **finite nuclei** from **phase shifts**
- Conversely, we can also predict **phase shifts** from **finite nuclei**
 - ← Binding energies and charge radii can be measured with **extremely high precision**, encoding **complete information** about nuclear forces.
- This requires **high-precision solver** and **efficient optimizer**
- The nuclear force fitted to **binding energies** predict a **S-wave phase shift** falling between $1S_0$ and $3S_1$
- S-wave splitting, S-D mixing, P-wave phase shifts should be reproduced at **higher orders**



Results from LAT-OPT1: Nuclear clustering



Exactly solvable phenomenological nuclear force

- **Ab initio calculations**

- Realistic interactions fitted to few-body data
- Challenging to solve, particularly for heavy nuclei

$$V(1, 2) = t_0(1 + x_0 P^\sigma) \delta(\mathbf{r}_1 - \mathbf{r}_2) \\ + \frac{1}{2} t_1 [\delta(\mathbf{r}_1 - \mathbf{r}_2) \mathbf{k}^2 + \mathbf{k}^2 \delta(\mathbf{r}_1 - \mathbf{r}_2)] + t_2 \mathbf{k} \delta(\mathbf{r}_1 - \mathbf{r}_2) \mathbf{k} \\ + i W_0 (\boldsymbol{\sigma}^{(1)} + \boldsymbol{\sigma}^{(2)}) \mathbf{k} \times \delta(\mathbf{r}_1 - \mathbf{r}_2) \mathbf{k},$$

- **Phenomenological methods**

- Phenomenological interactions fitted to finite nuclei
- Easy to solve, however lack correlations

$$V(1, 2, 3) = t_3 \delta(\mathbf{r}_1 - \mathbf{r}_2) \delta(\mathbf{r}_2 - \mathbf{r}_3).$$

LAT-OPT1 has one-to-one correspondence to Skyrme force with 6 parameters except for x_0

- **Sign-problem-free QMC**

- Phenomenological interactions fitted to finite nuclei
- Scalable and unbiased, full quantum correlations ← **spectrum, reaction, clustering, ...**

Model	Parameterization	Parameters	σ (MeV)	Nuclei	σ_{all} (MeV)
Macroscopic-microscopic	FRDM [9]	> 30	1.15	69	0.56
Relativistic mean field	PC-PK1 [10]	11	2.25	60	1.52
Skyrme DFT	UNEDF1 [11]	12	3.43	75	1.91
Lattice EFT	Wigner-SU(4) [1]	4	10.21	55	—
Lattice EFT	LAT-OPT1	5	2.93	76	—

Summary and perspective

- **Sign-problem-free QMC** represents a group of **quantum many-body problems** that can be solved with **exactly polynomial scaling**. (**Sign problem always induces exponential scaling**)
- The **time-reversal symmetry** protect us from the **sign problem**. However, it also forbids many essential interactions (e.g. tensor force), limiting the calculations to **toy-models**.
- We firstly implement a **sign-problem-free spin-orbit term**, fit parameters to **nuclear binding energies**. The resulting nuclear force is similar to the original Skyrme force, but **exactly solvable**.
- It is promising to apply the methodology from **mean-field** and **density functional theories** to improve the interactions. Our results might also provide hints connecting ***ab initio* calculations** and **established phenomenological models**.

Thank you for your attention!