Sign-problem-free Nuclear Quantum Monte Carlo Simulation

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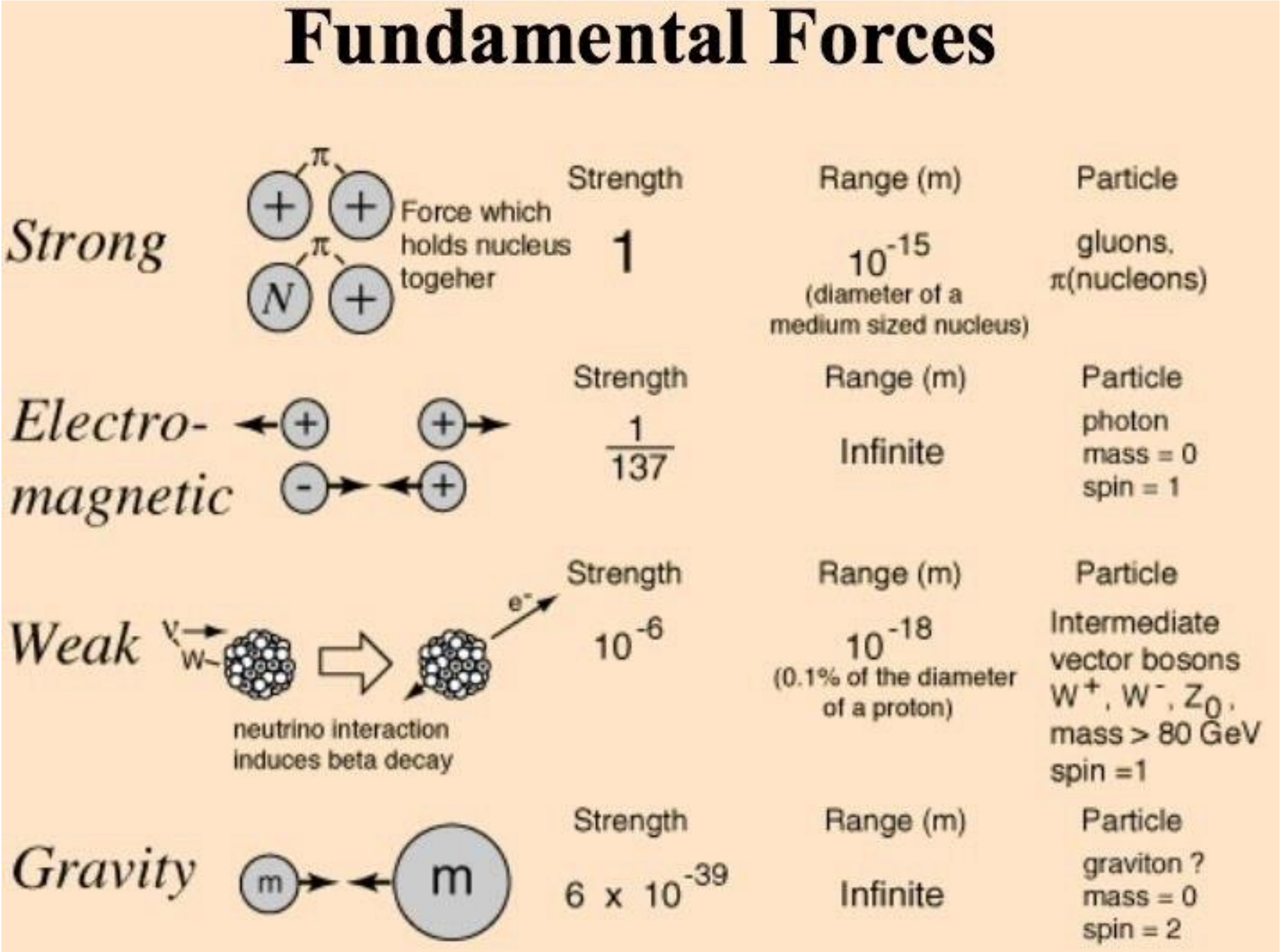
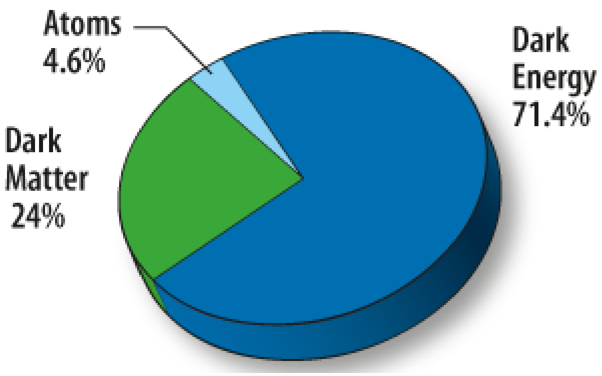
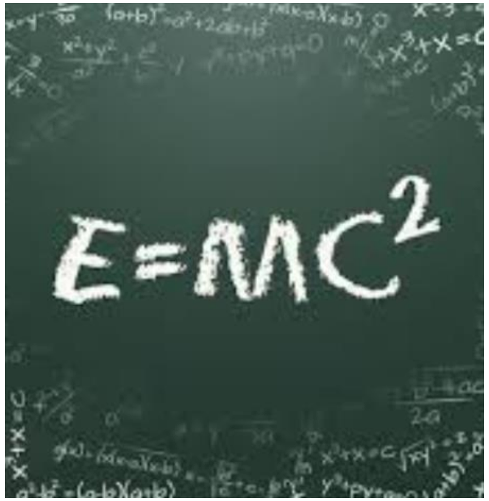
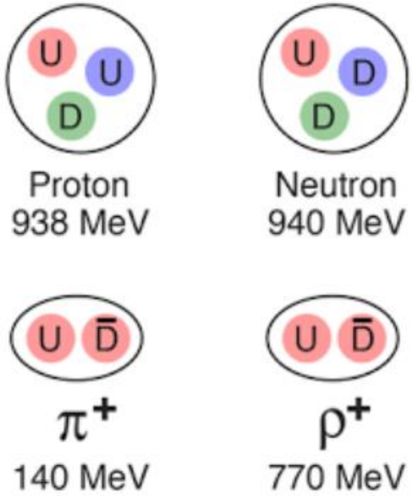
Fundamental forces in the universe



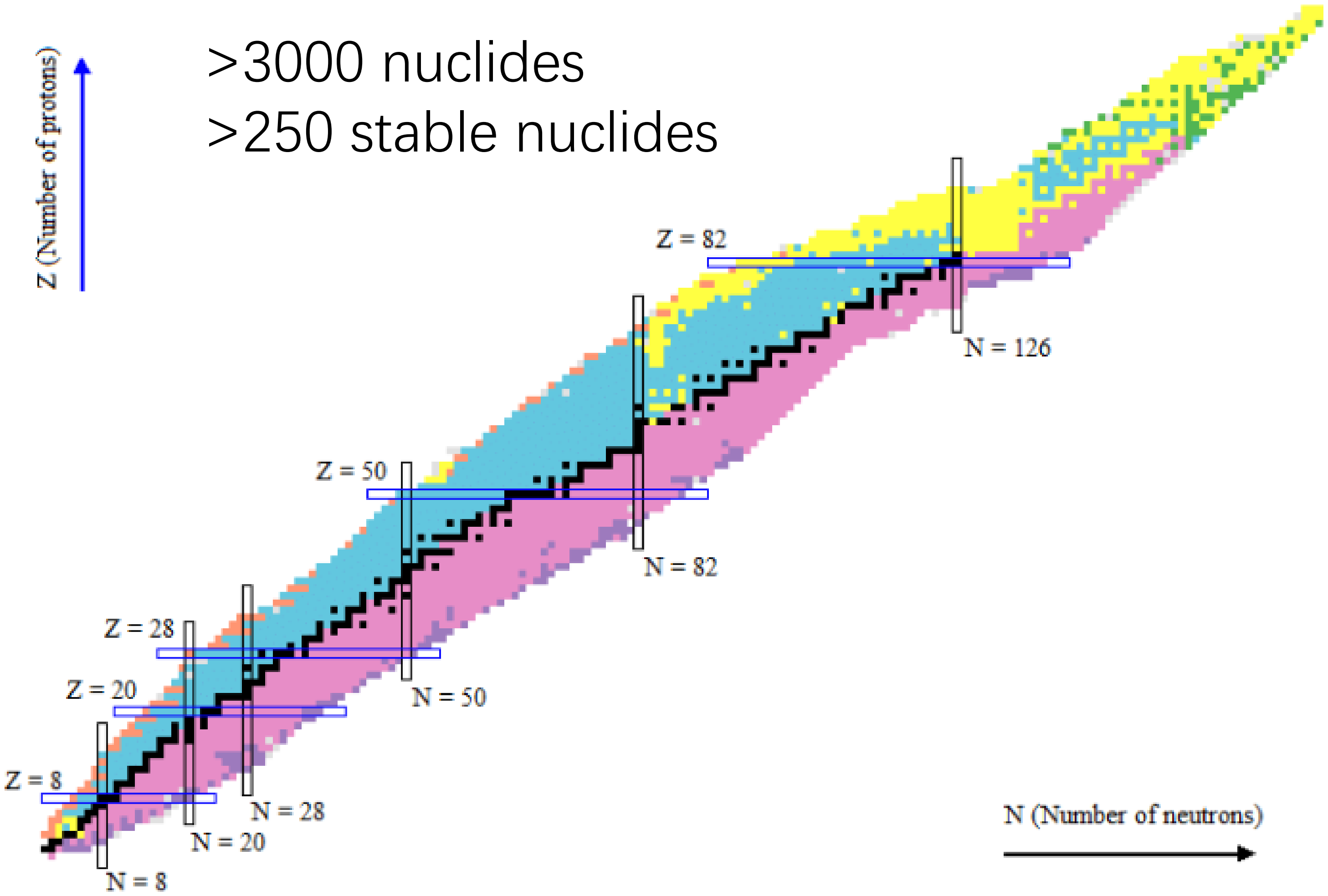






Particle		Mass* (MeV/c^2)
Name	Symbol	
up	u	2.3 ±0.7 ± 0.5
down	d	4.8 ±0.5 ± 0.3

Chart of nuclide



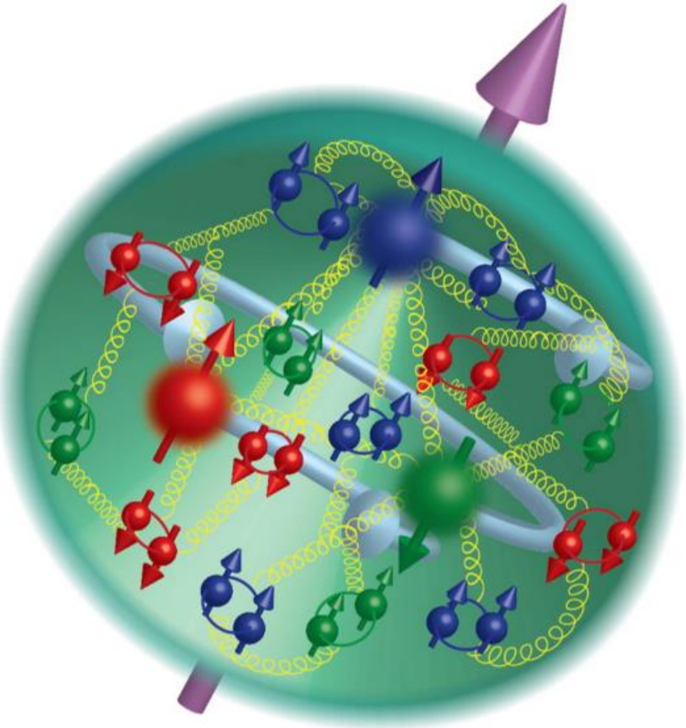
- Mass, Radii
- Magnetic moment
- Reaction rate
- EM transition
- Weak decay
- Strangeness
- Temperature
- …

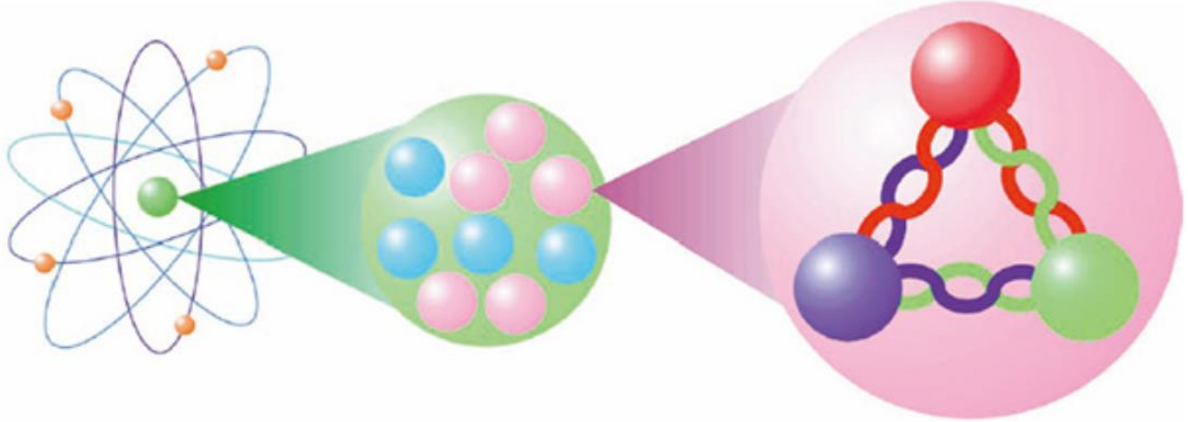
Can **everything** in nuclear physics be derived from **fundamental laws**?

Hierarchy of strongly interacting systems

$$\mathcal{L}_{\mathrm{QCD}} = \bar{\psi}_i \left(i\gamma^\mu (D_\mu)_{ij} - m\,\delta_{ij} \right) \psi_j - \frac{1}{4} G^a_{\mu\nu} G_a^{\mu\nu}$$

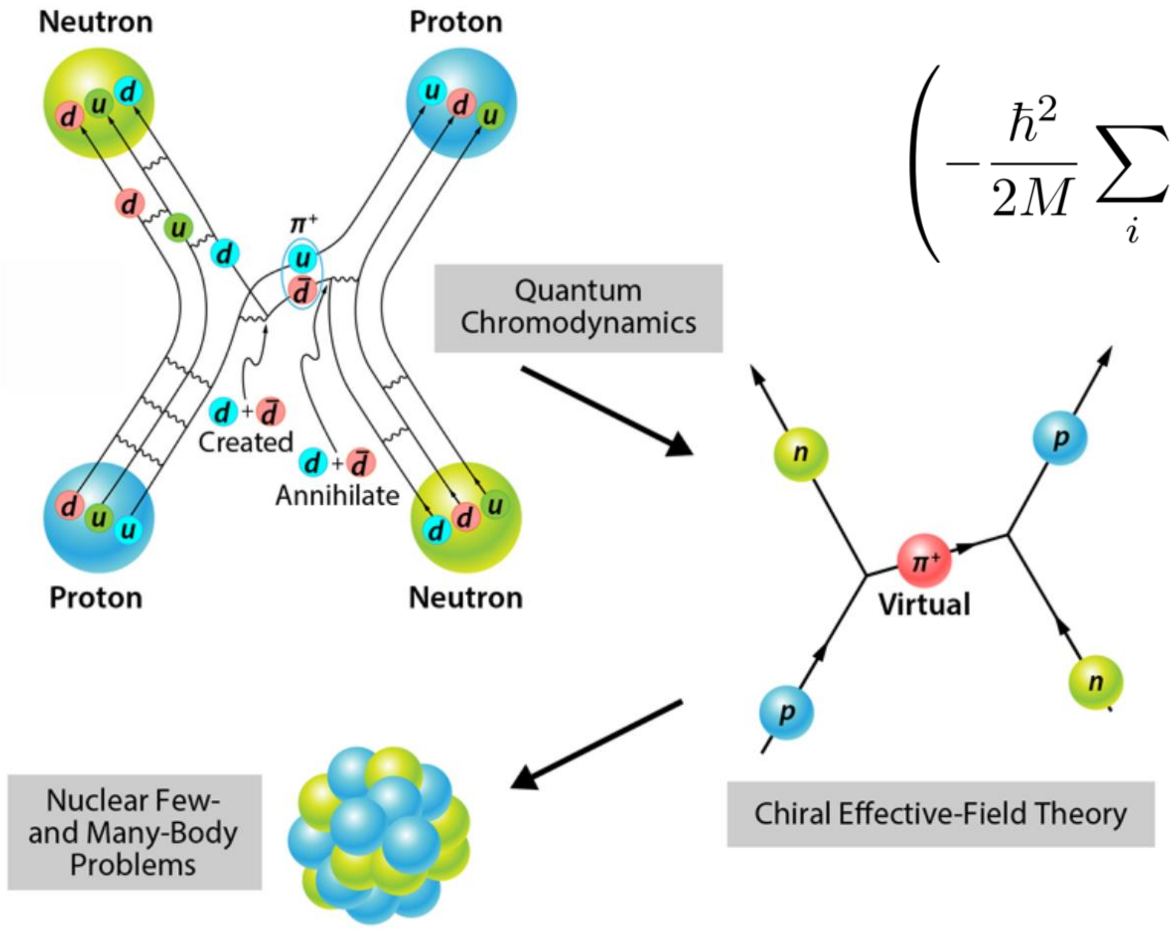
QCD Quark Confinement





- Quarks are confined in nucleons
- Nuclear forces among nucleons are emergent phenomena

What is nuclear *ab initio* calculations?



Nuclear forces

$$\left(-\frac{\hbar^2}{2M}\sum_i \nabla_i^2 + \boxed{\sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \cdots}\right)\Psi = E\Psi$$

Typical nuclear forces

complicated operator structures emerging from QCD

AV18 INTERACTION

$$v_{ij} = \sum_{p=1,18} v_p(r_{ij}) O_{ij}^p$$

$$O_{ij}^{p=1,14} = 1, \tau_i.\tau_j, \sigma_i.\sigma_j, (\sigma_i.\sigma_j)(\tau_i.\tau_j), S_{ij}, S_{ij}(\tau_i.\tau_j), L.S, L.S(\tau_i.\tau_j), L^2, L^2(\tau_i.\tau_j), L^2(\sigma_i.\sigma_j), L^2(\sigma_i.\sigma_j)(\tau_i.\tau_j), (L.S)^2, (L.S)^2(\tau_i.\tau_j),$$

CHARGE DEPENDENT

$$O_{ij}^{p=15,17} = T_{ij}, (\sigma_i.\sigma_j)T_{ij}, S_{ij}T_{ij}$$

CHARGE ASYMMETRIC

$$O_{ij}^{p=18} = (\tau_{zi} + \tau_{zj})$$

R. B. Wiringa, V. G. J. Stoks, and R. Schiavilla, Phys. Rev. C 51, 38, 1995.

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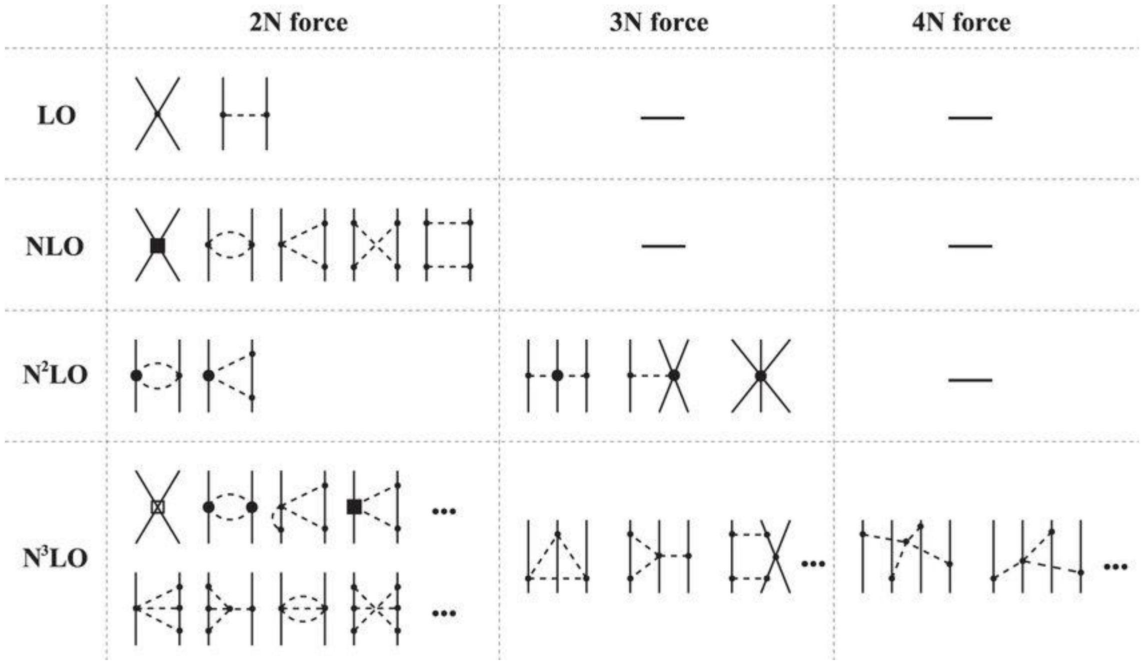
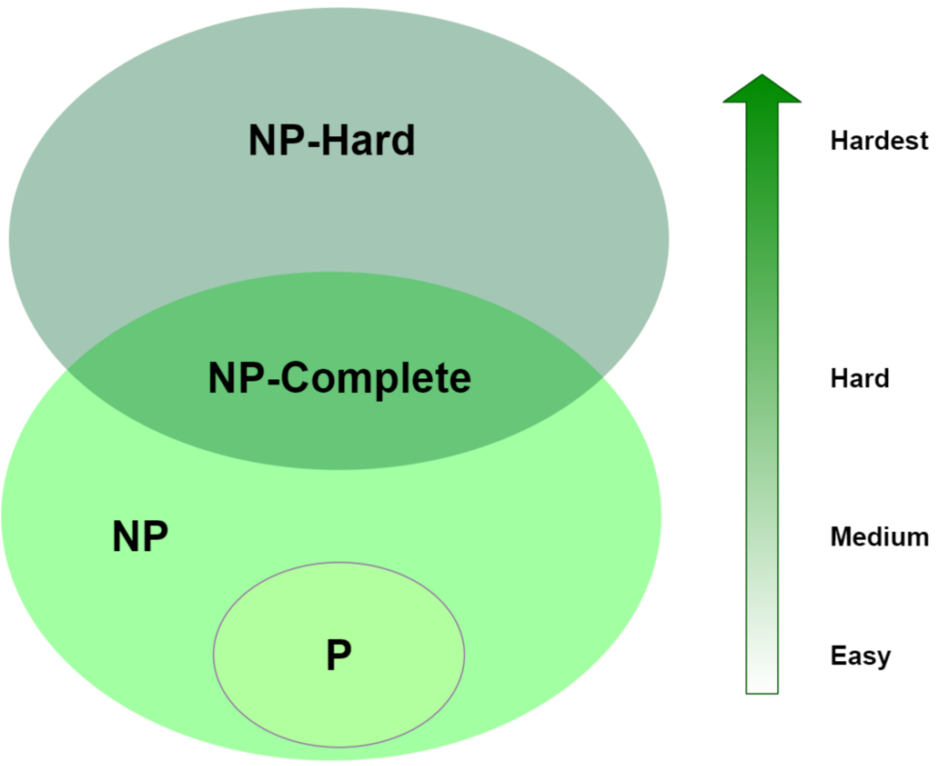
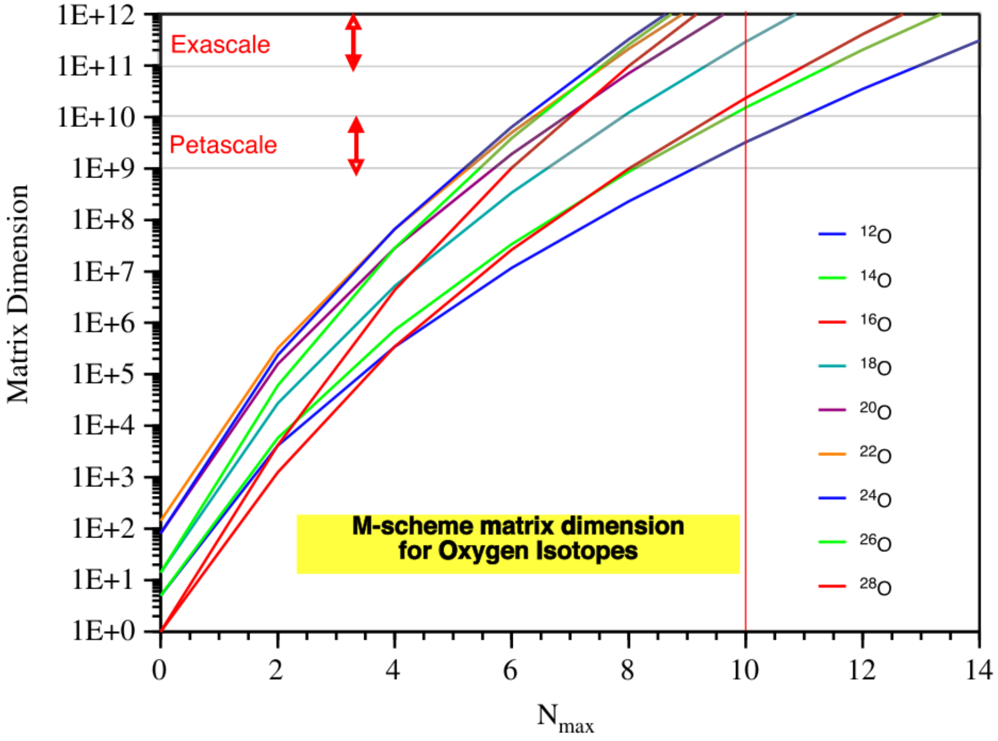
Nuclear chiral EFT



Complexity of nuclear many-body problem





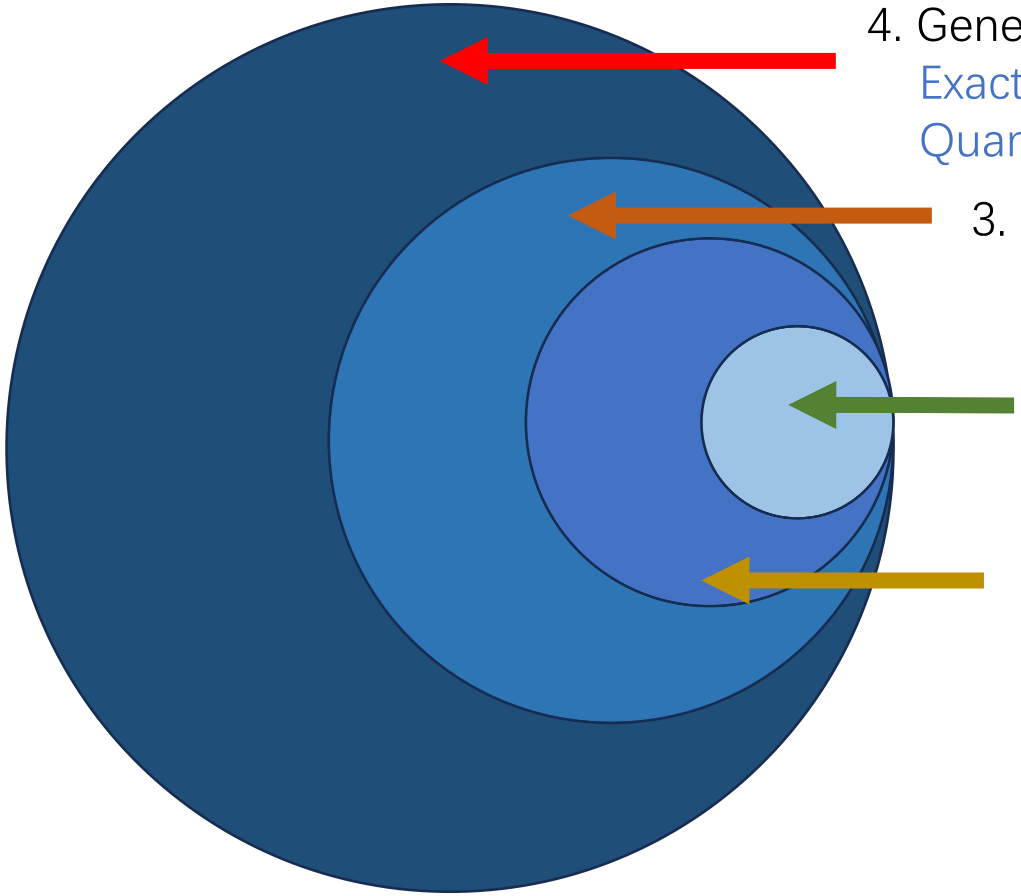
- P: Solvable within polynomial time
- NP: Verifiable within polynomial time

Exponentially increasing Hilbert space

➡ **Find ground state of a general Hamiltonian is NP-Hard**

Quantum many-body problem classification

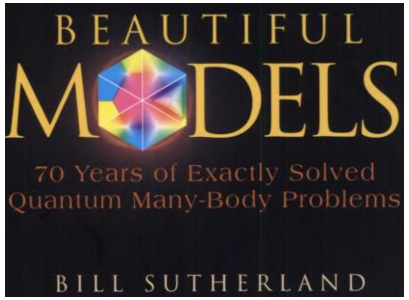
- Models with strong interactions present great challenges



4. General quantum many-body problem (NP-hard)
   Exact diagonalization
   Quantum computing

3. Problems perturbatively solvable
   QMC with sign problem
   (Nuclear *ab initio* calculations)

1. Problems analytically solvable
   only possible in 1-d systems



2. Problems with polynomial algorithms
   QMC without sign problem

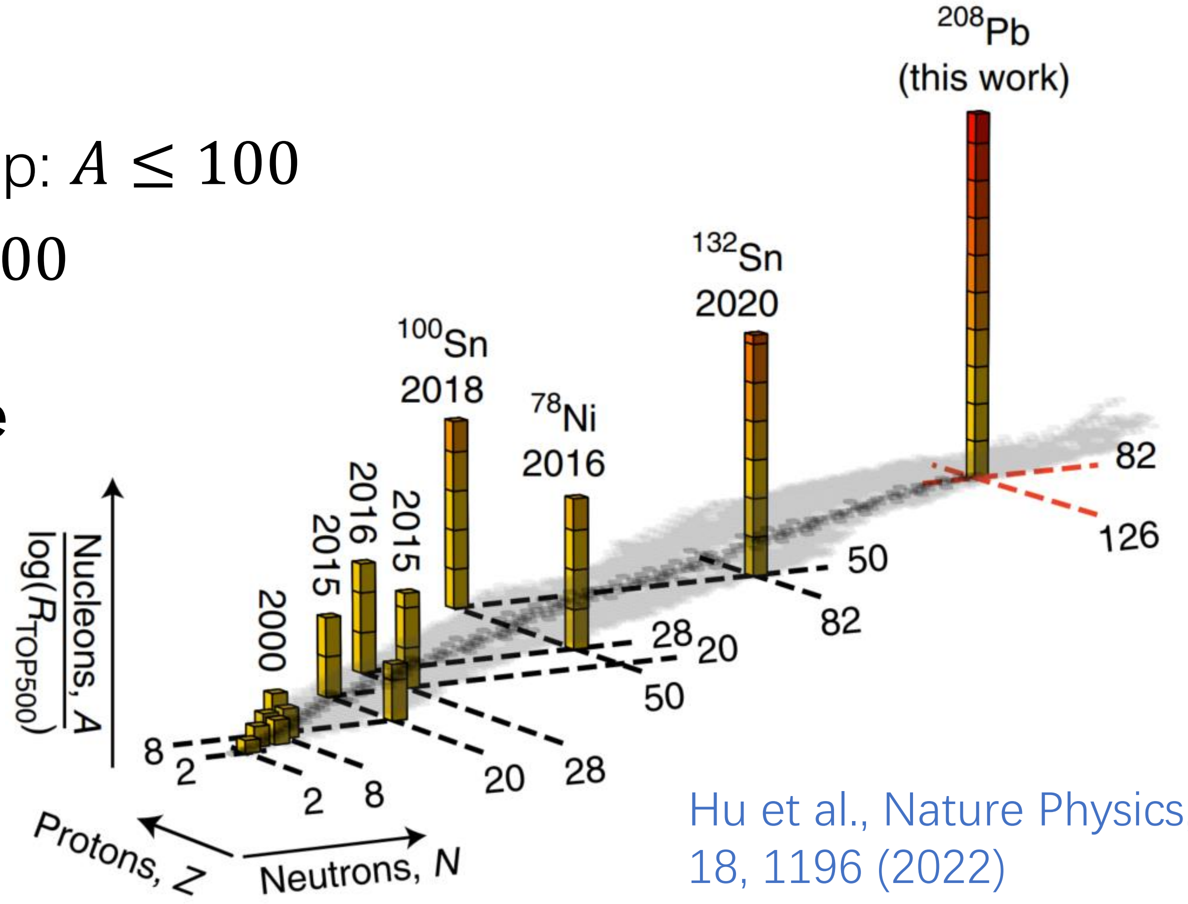
Nuclear *ab initio* algorithms

- No core shell model: $A \leq 20$
- Green's function Monte Carlo: $A \leq 20$
- Coupled cluster: $A \leq 100$
- In-medium similarity renormalization group: $A \leq 100$
- Nuclear lattice effective field theory: $A \leq 100$

Developments of **algorithms** and **hardware** rapidly push the frontiers of **nuclear *ab initio* calculations**

mass / temperature / strangeness /⋯

Rapid growth in last decade



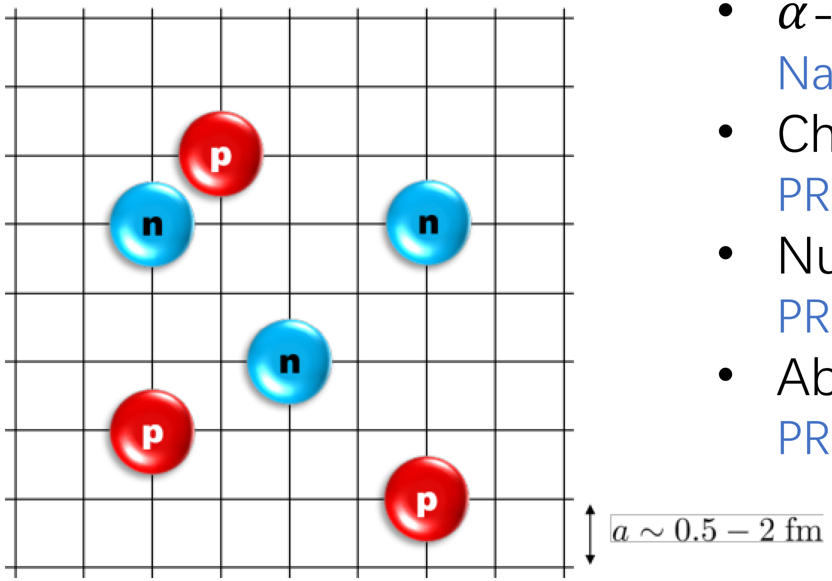
Hu et al., Nature Physics, 18, 1196 (2022)

Nuclear Lattice EFT: An efficient nuclear many-body 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

Nature * 2, PRL > 20

- Hoyle state
  PRL106-192501 (2011)
- α-α scattering
  Nature528-111 (2015)
- Charge distribution
  PRL119-222505 (2017)
- Nuclear thermodynamics
  PRL125-192502 (2020)
- Ab initio ^{100}Sn
  PRL135-222504 (2025)

Lattice EFT: A many-body EFT solver

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

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

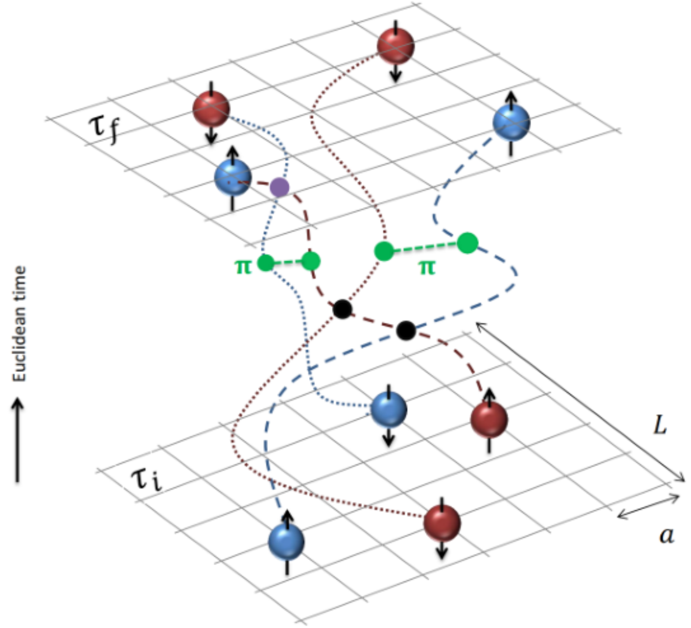
with $|\Psi_A\rangle$ representing A *free* nucleons.

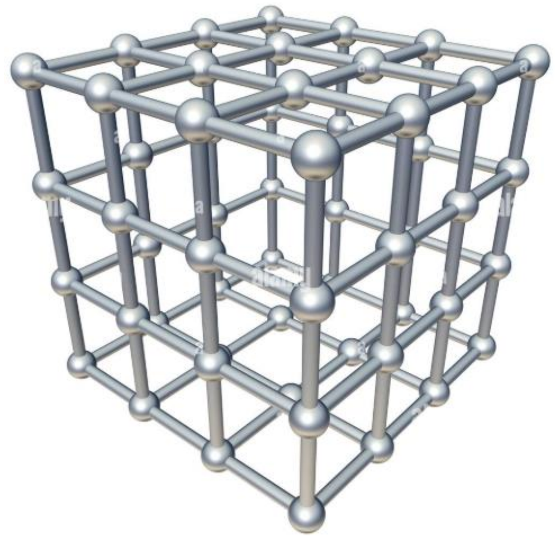
- Expectation value of any operator $\mathscr{O}$:

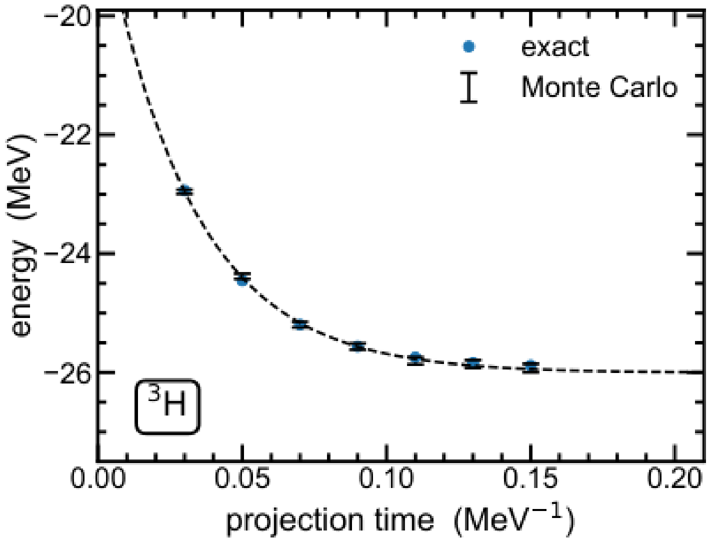
$$\langle O\rangle = \lim_{\tau\to\infty} \frac{\langle\Psi_A|\exp(-\tau H/2)\mathscr{O}\exp(-\tau H/2)|\Psi_A\rangle}{\langle\Psi_A|\exp(-\tau H)|\Psi_A\rangle}$$

- τ is discretized into time slices:

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







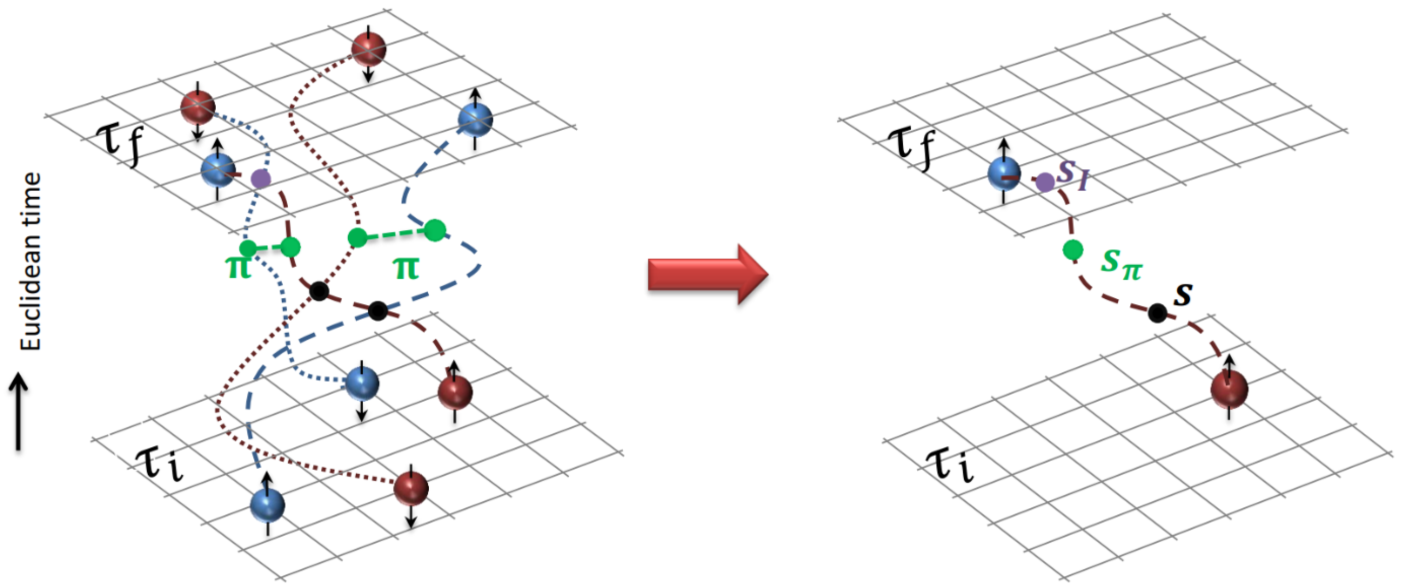
All possible configurations in $\tau \in [\tau_i, \quad \tau_f]$ are sampled.
Complex structures like nucleon clustering emerges naturally.

Lattice EFT: A many-body EFT solver

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

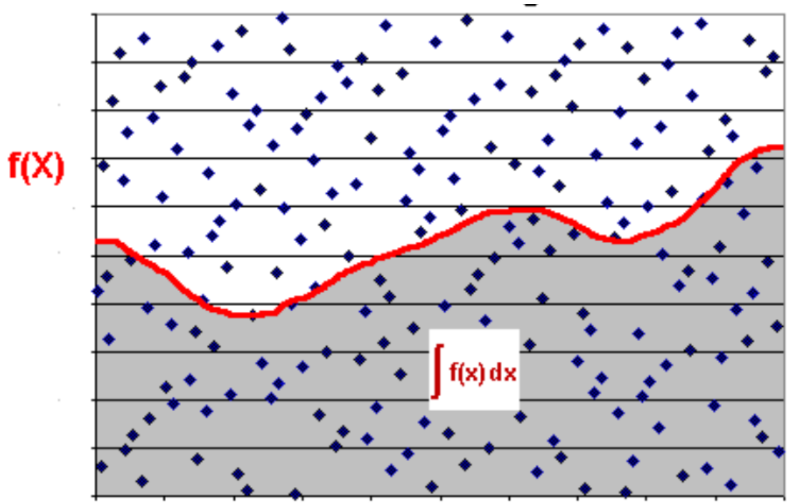
$$: \exp\left[-\frac{a_t C}{2}(\psi^\dagger\psi)^2\right] := \frac{1}{\sqrt{2\pi}}\int ds : \exp\left[-\frac{s^2}{2}+\sqrt{-a_t C}s(\psi^\dagger\psi)\right]:$$

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



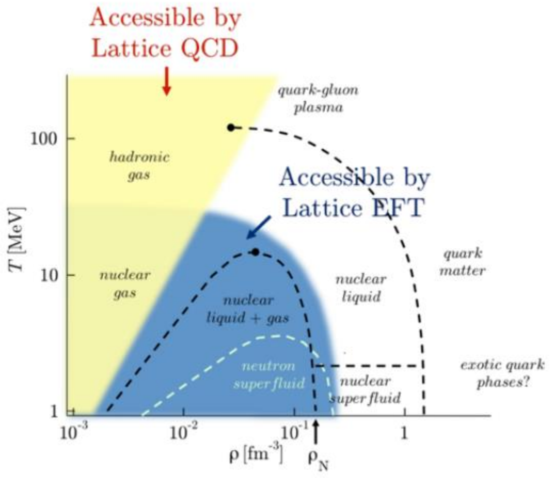
In lattice EFT, solving a general Hamiltonian consists of 5 steps:

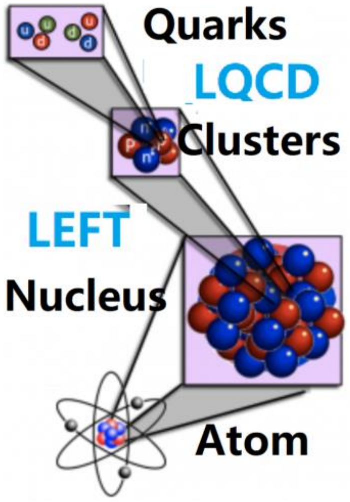
1. Rewrite expectation value as a path integral using auxiliary field transformation.
2. For each field configuration, calculate the amplitude.
3. Integrate over the field variables using Monte Carlo algorithms.
4. Take the limit $\tau \to \infty$ to find the true ground state.
5. Take the limit $L \to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



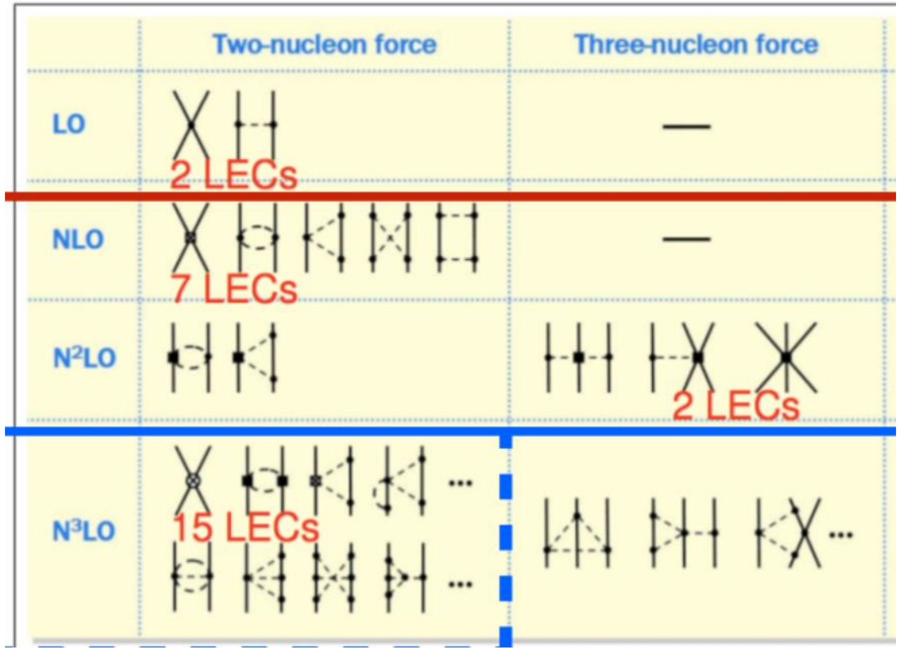
Compare Lattice EFT and Lattice QCD

	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 / ρ_{sat}
sign problem	severe for $\mu > 0$	moderate





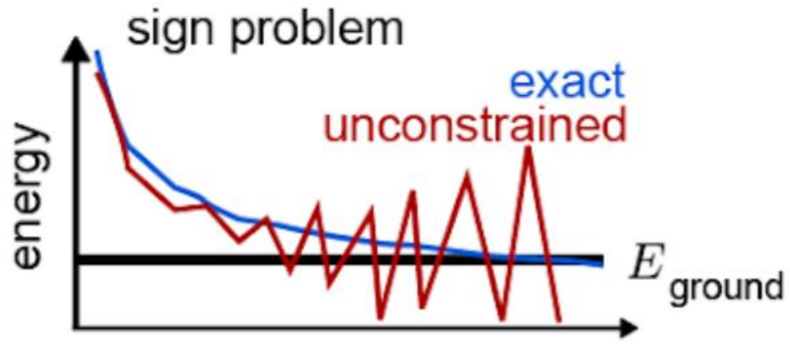
- Lattice EFT share a lot of common features with Lattice QCD. However,
  - Non-rel. → particle number conservation
  - Quadratic dispersion relation
    → no Fermion doubling problem
  - EFT contains non-renormalizable terms
    → no continuum limit



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 ~$O(N^{-1/2})$
- **Sign problem** occurs when the integrand is NOT positive definite ← 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 ← 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 ← **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

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

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

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

- 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)

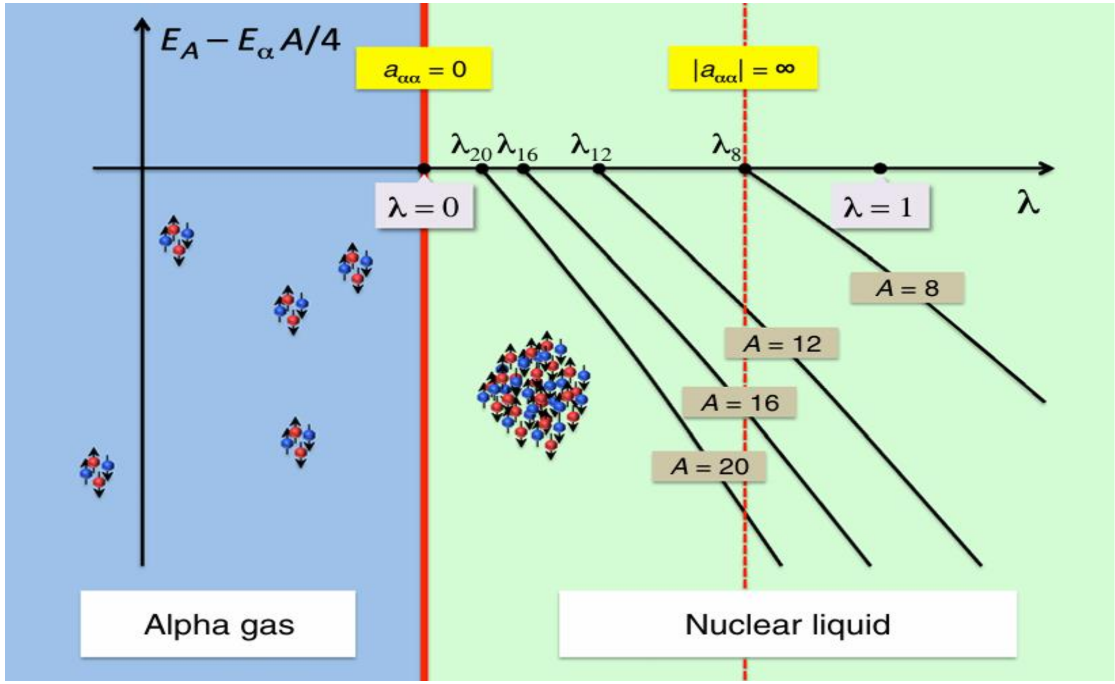
Nuclear binding near a quantum phase transition

$$H_{\mathrm{SU4}} = H_{\mathrm{free}} + \frac{1}{2!} C_2 \sum_{\boldsymbol{n}} \overline{\rho}(\boldsymbol{n})^2$$

$$\overline{\rho}(\boldsymbol{n}) = \rho(\boldsymbol{n}) + s_{\mathrm{L}} \sum_{|\boldsymbol{n}'-\boldsymbol{n}|=1} \rho(\boldsymbol{n}')$$

$$\rho(\boldsymbol{n}) = \overline{\Psi}^{\dagger}(\boldsymbol{n}) \overline{\Psi}(\boldsymbol{n})$$

$$\overline{\Psi}(\boldsymbol{n}) = \Psi(\boldsymbol{n}) + s_{\mathrm{NL}} \sum_{|\boldsymbol{n}'-\boldsymbol{n}|=1} \Psi(\boldsymbol{n}')$$



Challenge: Minimal nuclear force
That reproduce the binding pattern

Simple Wigner-SU(4) central force fails!

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

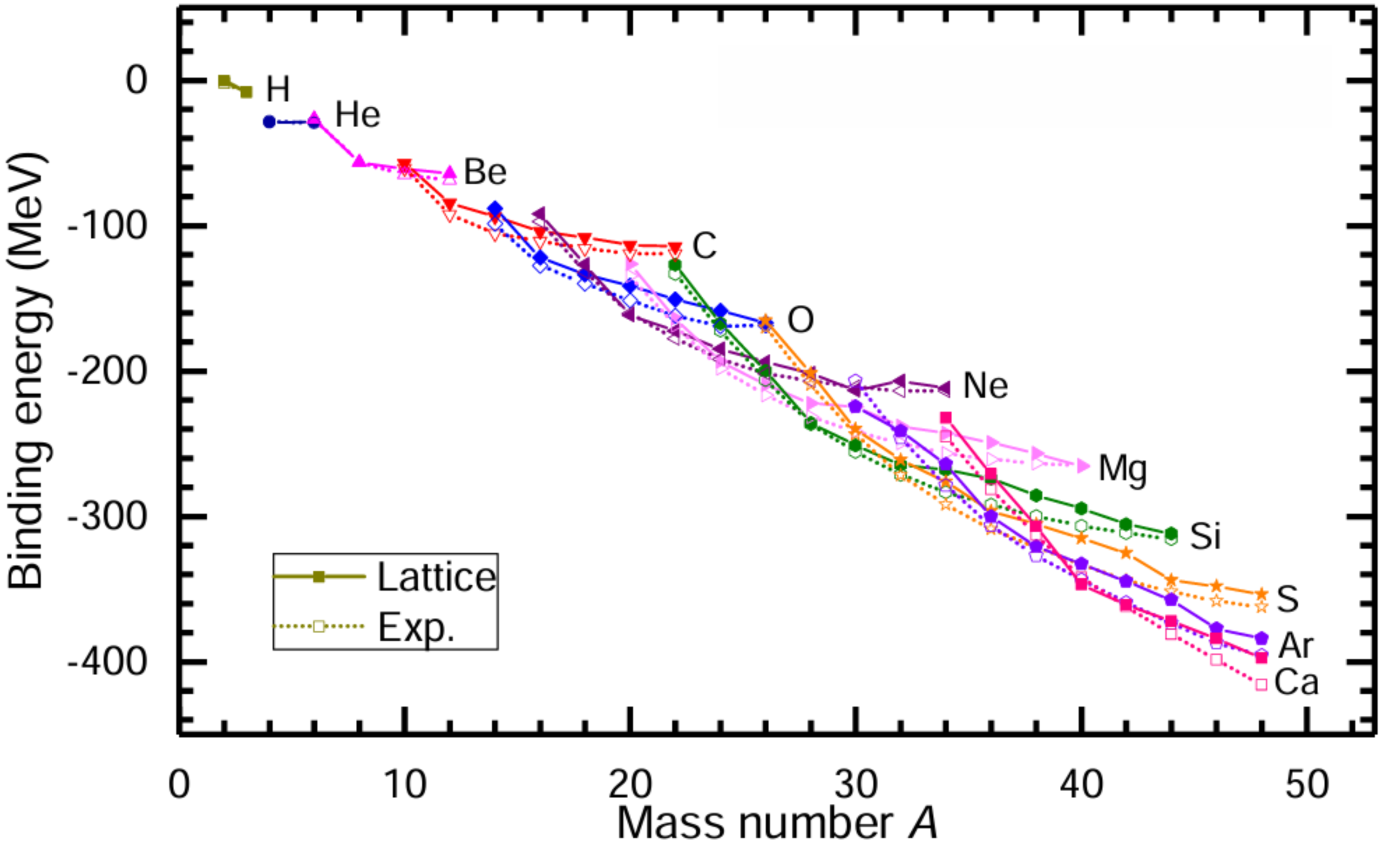
S. Elhatisari et al., PRL 117, 132051 (2016)

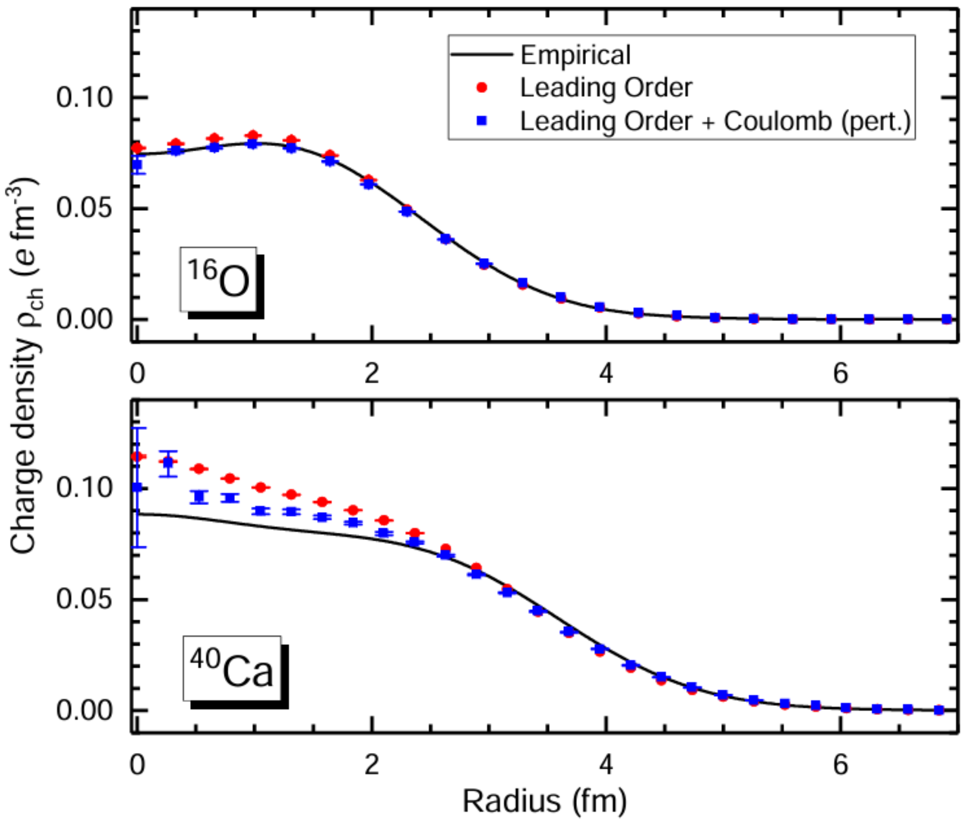
Nuclear force with a Wigner-SU(4) symmetry

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

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 ^{7}Be to ^{12}Be, S. Shen et al., PRL 134, 162503 (2025)
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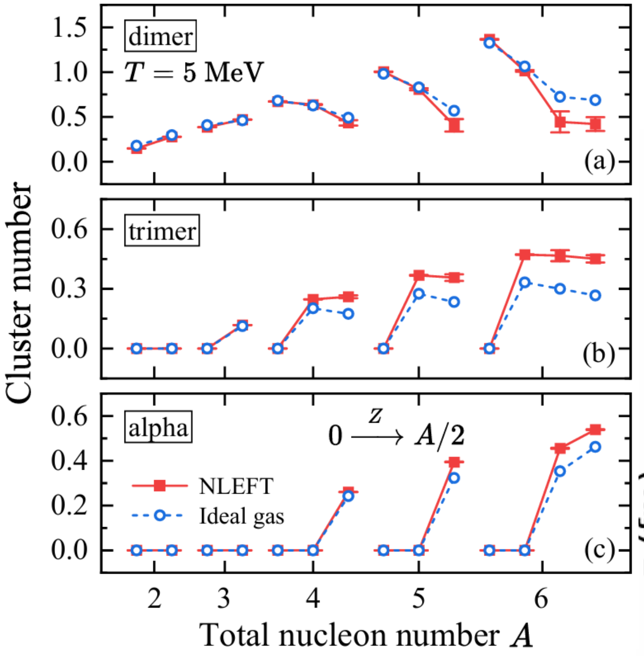
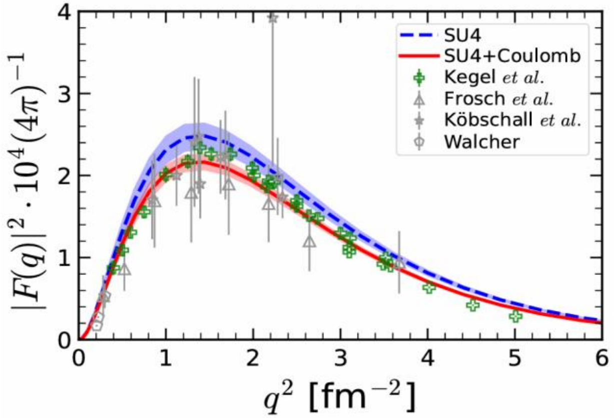
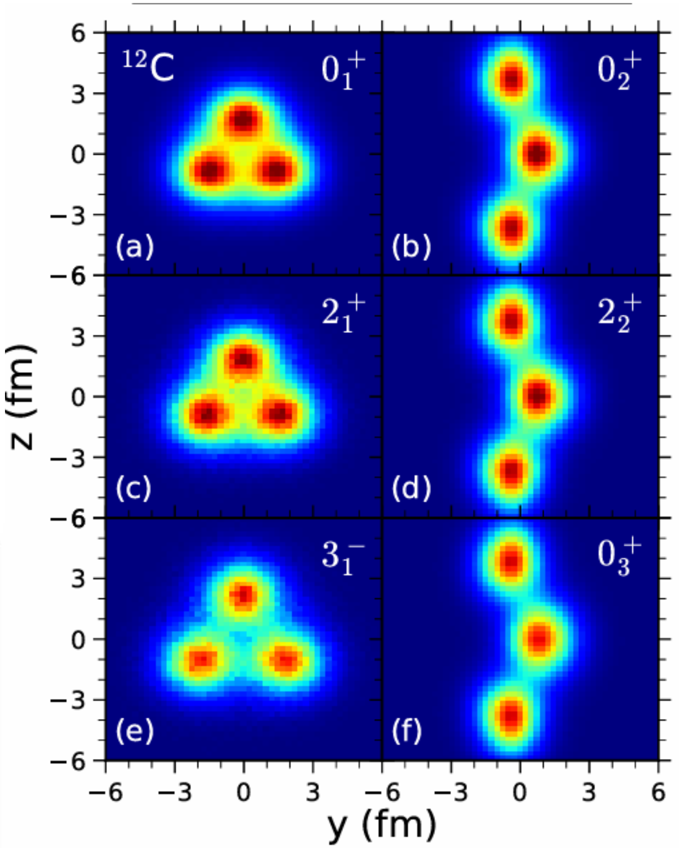
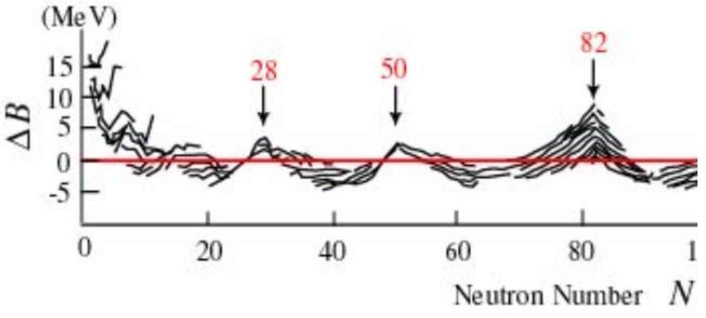






Improved Wigner-SU(4) interaction

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



- We introduce a **spin-orbit coupling**

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

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

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

- **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**

Z.-W. Niu and BL, PRL135-222504 (2025)

Proof for the positivity of the determinant

$$\langle O \rangle = \lim_{\tau\to\infty} \frac{\langle \Phi_T | e^{-\tau H/2} O e^{-\tau H/2} | \Phi_T \rangle}{\langle \Phi_T | e^{-\tau H} | \Phi_T \rangle} = \lim_{L_t\to\infty} \frac{\langle \Phi_T | M^{L_t/2} O M^{L_t/2} | \Phi_T \rangle}{\langle \Phi_T | M^{L_t} | \Phi_T \rangle}$$

$$= \lim_{L_t\to\infty} \frac{\int \mathcal{D}c \exp(-\sum_{i=1}^{L_t} c_i^2/2) \langle \Phi_T | M(c_{L_t}) \cdots M(c_{L_t/2+1}) O M(c_{L_t/2}) \cdots M(c_1) | \Phi_T \rangle}{\int \mathcal{D}c \exp(-\sum_{i=1}^{L_t} c_i^2/2) \langle \Phi_T | M(c_{L_t}) \cdots M(c_1) | \Phi_T \rangle}$$

$$M(c) = \exp\left[\sum_{\boldsymbol{n},\boldsymbol{n}'} a_t \frac{\Psi^\dagger(\boldsymbol{n}) \nabla^2_{\boldsymbol{n}\boldsymbol{n}'} \Psi(\boldsymbol{n}')}{2M} + \sum_{\boldsymbol{n}} \sqrt{-a_t C_2} c(\boldsymbol{n}) \left(\bar{\rho}(\boldsymbol{n}) + \frac{C_s}{2C_2} \bar{\rho}_s(\boldsymbol{n}) \right) \right]$$

$$Z(c) = \left[\langle \phi_i \mid \overline{M}(c) \mid \phi_j \rangle \right]_{i,j=1}^{A} = \begin{pmatrix} \langle \phi_1 \mid \overline{M}(c) \mid \phi_1 \rangle & \langle \phi_1 \mid \overline{M}(c) \mid \phi_2 \rangle & \cdots & \langle \phi_1 \mid \overline{M}(c) \mid \phi_A \rangle \\ \langle \phi_2 \mid \overline{M}(c) \mid \phi_1 \rangle & \langle \phi_2 \mid \overline{M}(c) \mid \phi_2 \rangle & \cdots & \langle \phi_2 \mid \overline{M}(c) \mid \phi_A \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle \phi_A \mid \overline{M}(c) \mid \phi_1 \rangle & \langle \phi_A \mid \overline{M}(c) \mid \phi_2 \rangle & \cdots & \langle \phi_A \mid \overline{M}(c) \mid \phi_A \rangle \end{pmatrix}$$

- The nucleons evolve **independently** under the auxiliary fields.
- Time-reversal pairs are **NOT** broken by the spin-orbit coupling
- Matrix elements of the fermionic correlation matrix respect a **special symmetry**

For even-even nuclei, we prepare the single nucleon wave functions as paired by the time-reversal operation:

$$|\phi_{A/2+k}\rangle = \mathcal{T}|\phi_k\rangle, \qquad k = 1, 2, \ldots, A/2, \qquad ($$

where $\mathcal{T} = i\sigma_y\mathcal{K}$ is the time-reversal operator and $\mathcal{K}$ denotes complex conjugation. The matrix $\overline{M}(c)$ commutes with $\mathcal{T}$ Using the properties of $\mathcal{T}$ and Eq. (22), we obtain the relations:

$$\langle \phi_{A/2+i} | \overline{M}(c) | \phi_{A/2+j} \rangle = \langle \mathcal{T}\phi_i | \overline{M}(c) | \mathcal{T}\phi_j \rangle = \langle \phi_i | \overline{M}(c) | \mathcal{T}^\dagger \mathcal{T} \phi_j \rangle^* = \langle \phi_i | \overline{M}(c) | \phi_j \rangle^*,$$

$$\langle \phi_{A/2+i} | \overline{M}(c) | \phi_j \rangle = \langle \mathcal{T}\phi_i | \overline{M}(c) | \phi_j \rangle = \langle \phi_i | \overline{M}(c) | \mathcal{T}^\dagger \phi_j \rangle^* = -\langle \phi_i | \overline{M}(c) | \phi_{A/2+j} \rangle^*$$

Proof for the positivity of the determinant

The correlation matrix then has the structure:

$$Z = \begin{pmatrix} U & -V^* \\ V & U^* \end{pmatrix}, \tag{24}$$

where U and V are $A/2 \times A/2$ complex matrices.

We define a spin-flipping matrix:

$$\Sigma = i\sigma_y \otimes I_{A/2} = \begin{pmatrix} 0 & I_{A/2} \\ -I_{A/2} & 0 \end{pmatrix}, \tag{25}$$

where $I_{A/2}$ is the $A/2 \times A/2$ identity matrix. Direct verification shows that

$$Z\,\Sigma = \Sigma\,Z^*. \tag{26}$$

For any eigenvalue $\lambda \in \mathbb{C}$ with corresponding eigenvector v satisfying $Z\,v = \lambda\,v$, we have

$$Z\,(\Sigma\,v^*) = \Sigma\,Z^*\,v^* = \Sigma\,(\lambda^*\,v^*) = \lambda^*\,(\Sigma\,v^*), \tag{27}$$

implying that λ^* is also an eigenvalue with eigenvector $w = \Sigma v^*$. Thus, complex eigenvalues of Z always appear in conjugate pairs. If λ is real, we find

$$\langle v \mid w \rangle = v^\dagger\,\Sigma\,v^* = (v^T\,\Sigma\,v)^* = 0, \tag{28}$$

indicating that v and w are orthogonal eigenvectors corresponding to the same real eigenvalue. In this case, the real eigenvalue appears twice in the diagonalized form of Z. Consequently, the determinant $\det(Z)$, being the product of all eigenvalues, is always nonnegative.

Gradient Descent method

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

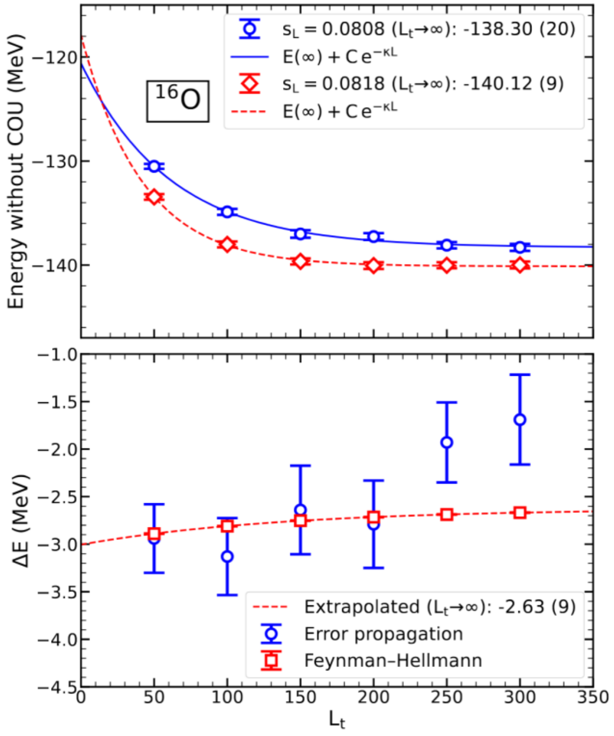
$$\chi^2 = \sum_A \left[\frac{E(A) - E_{\rm exp}(A)}{\Delta(A)} \right]^2$$

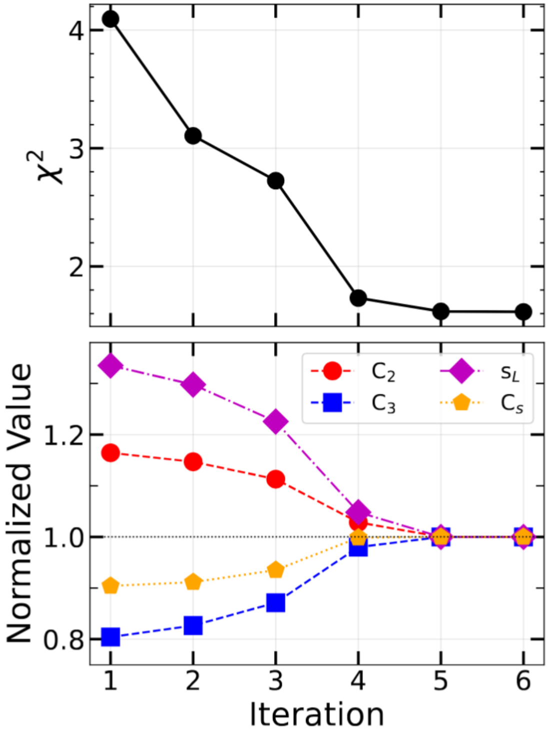
- The derivatives are calculated using the **Feynman-Hellmann theorem,**

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

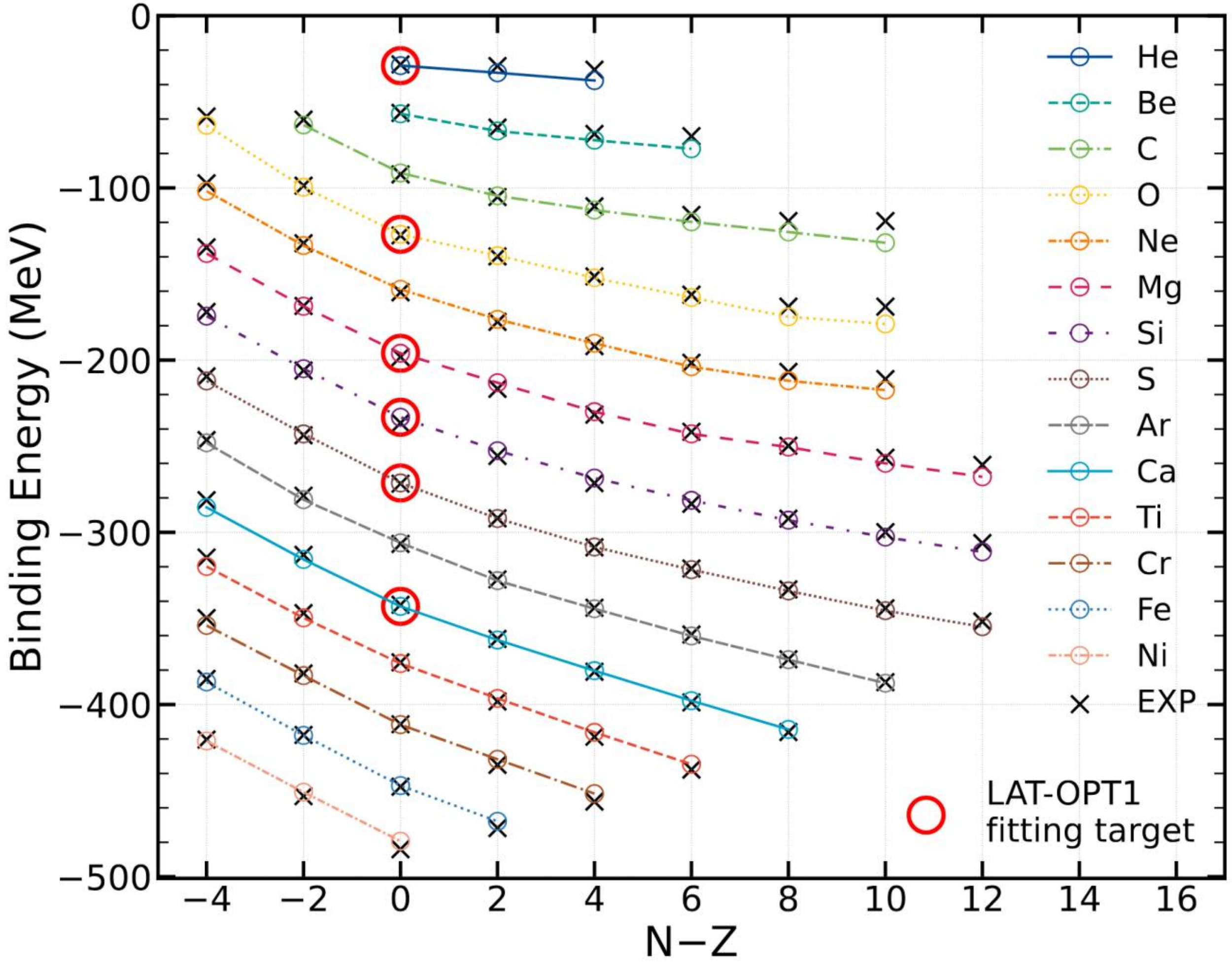
- Typically converge within 10 iterations ← **precise and unbiased** derivative computation is essential!

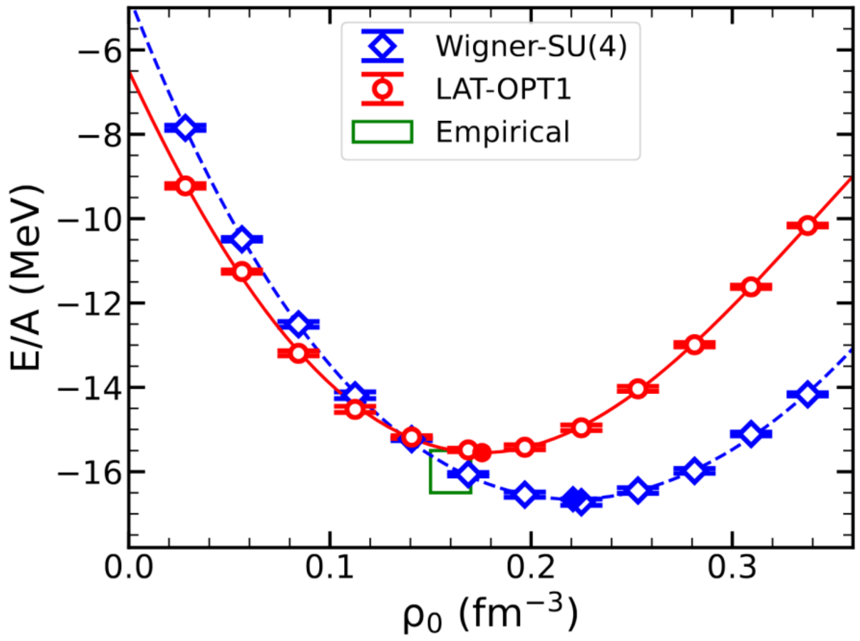
$C_2 = -4.410 \times 10^{-7}$ MeV^{-2}, $C_3 = 1.561 \times 10^{-15}$ MeV^{-5}, $C_s = 8.590 \times 10^{-12}$ MeV^{-4}, $s_{\rm L} = 0.081$, $s_{\rm NL} = 0.45$ "LAT-OPT1"

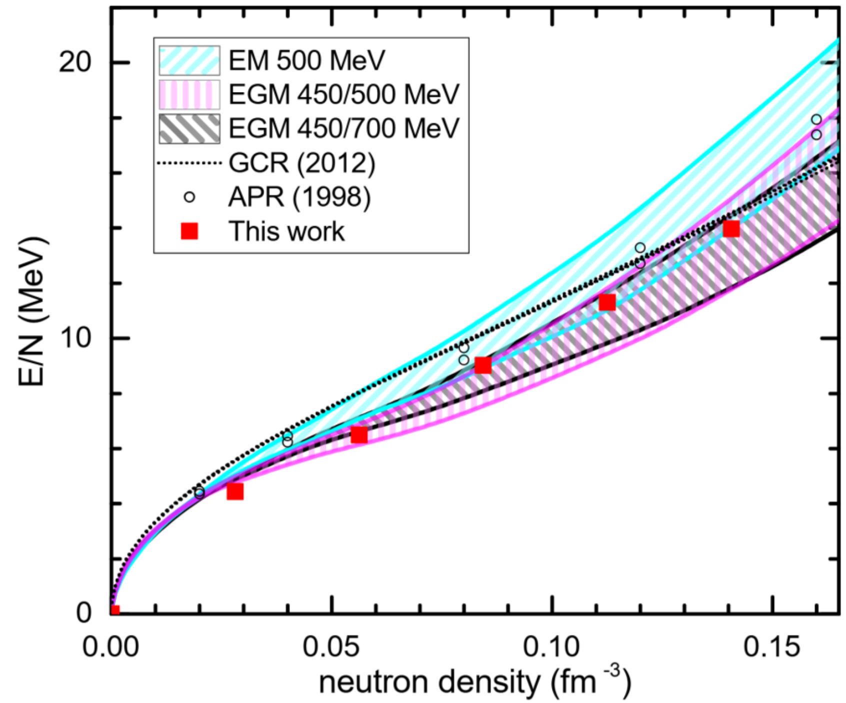




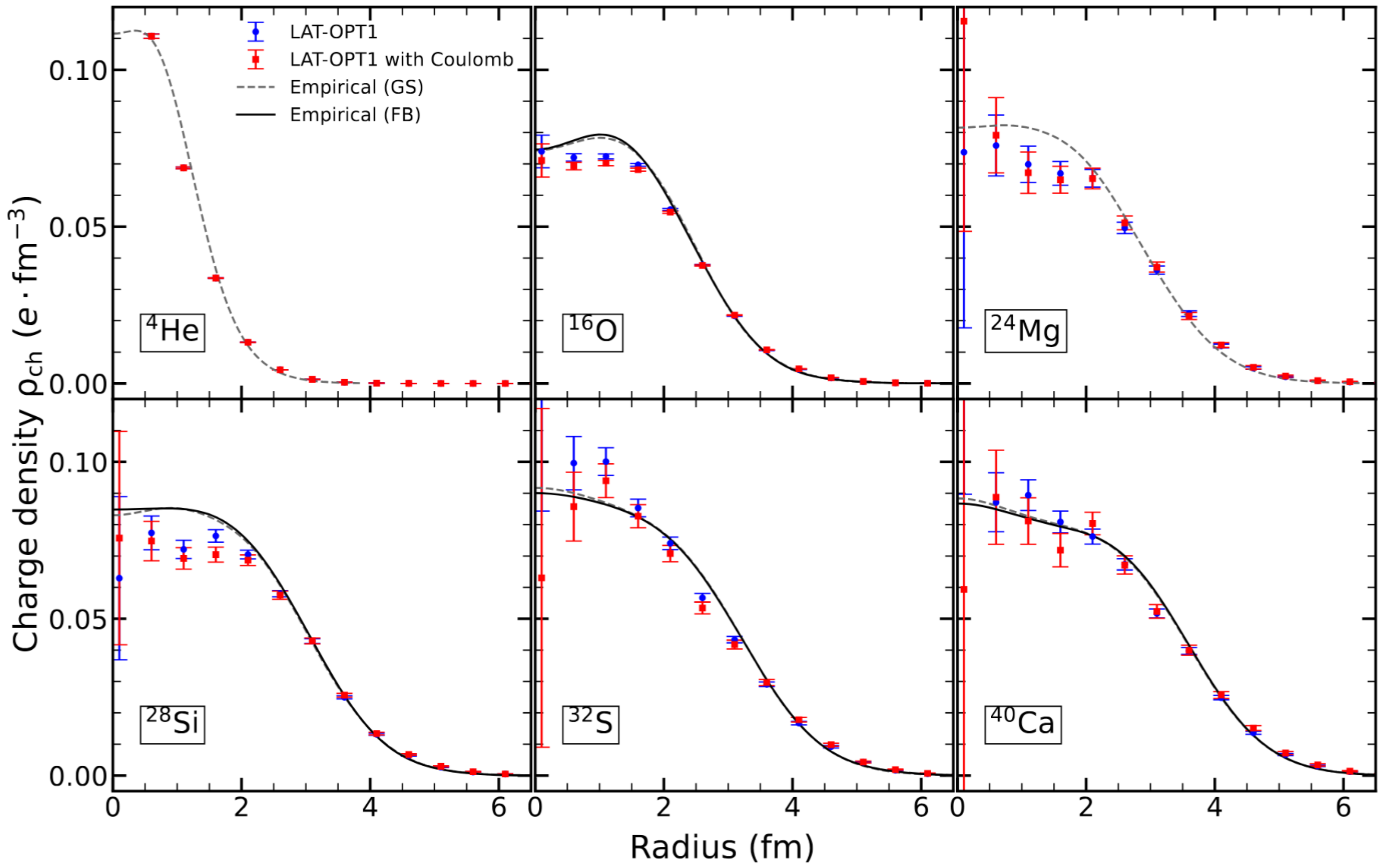
Results from LAT-OPT1







Results from LAT-OPT1: Charge densities

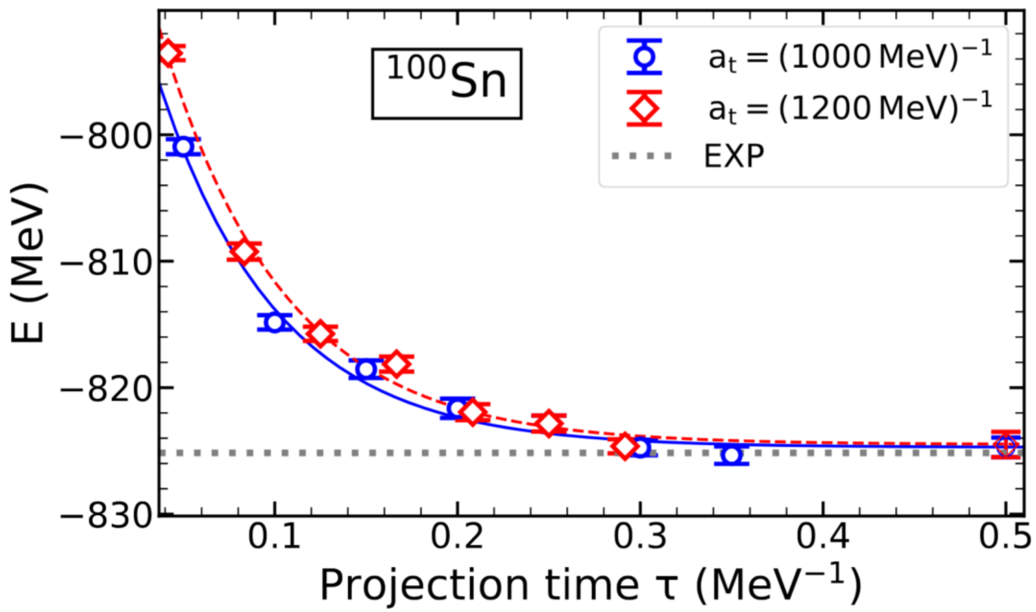


- Charge densities calculated using **pinhole algorithm**
  Elhatisari et al., PRL119, 222505 (2017)

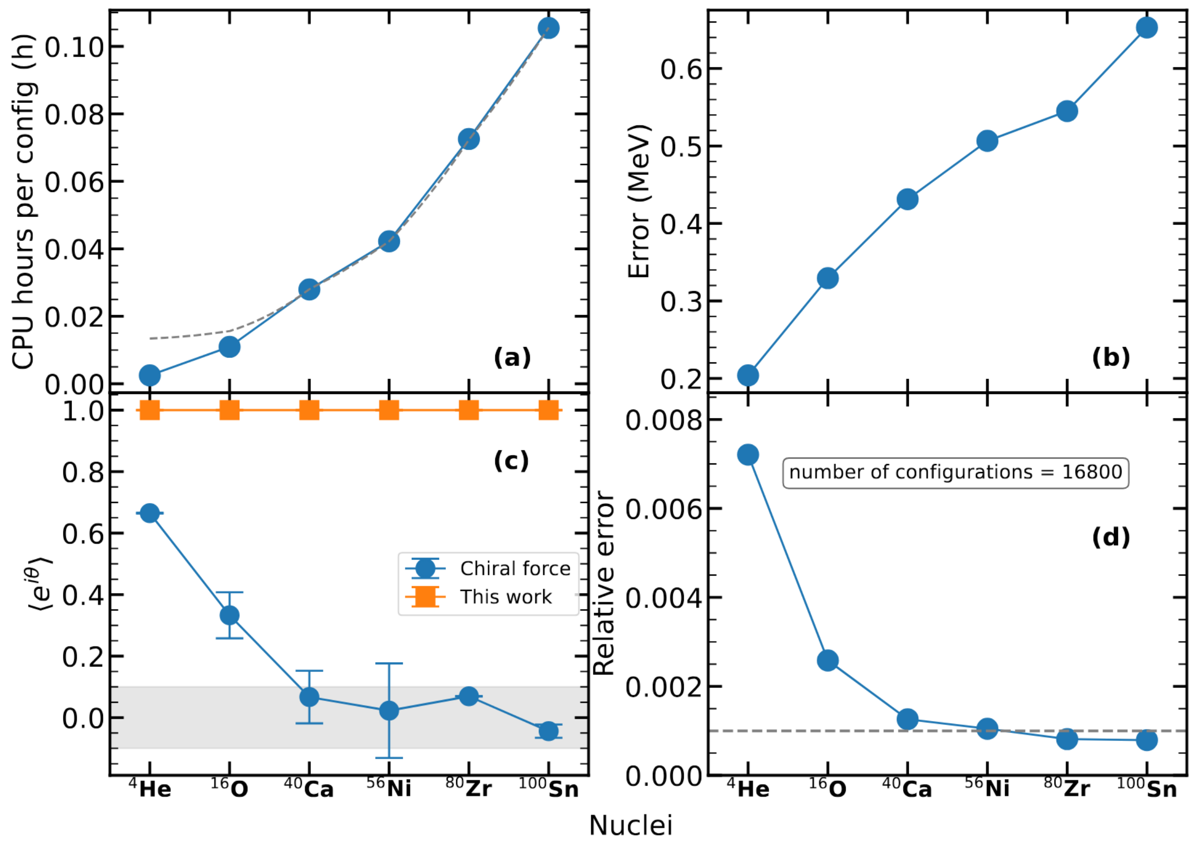
- **Pinhole algorithm** induce **mild sign problem**, not available for A>=40. See **partial pinhole algorithm** for a solution
  Zheng-Xue Ren et al., PRL135-152502 (2025)

Results from LAT-OPT1: Heavy nuclei

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

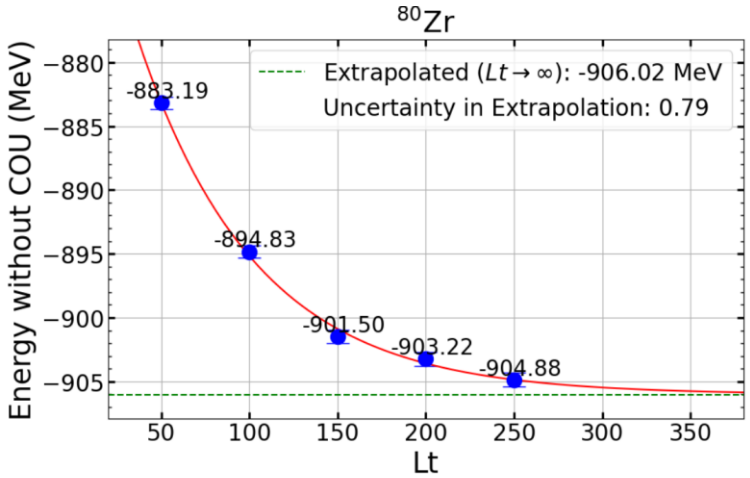


Extract binding energy of ^{100}Sn with **~1 MeV precision** using **~30000 CPU hours**
(10 days on AMD EPYC 9554@3.1GHz, 128 CPU cores)



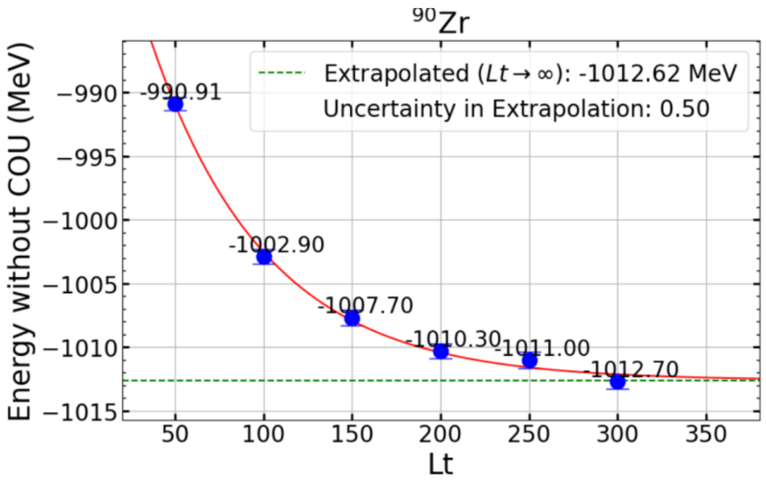
Relative errors <0.1% for heavy nuclei

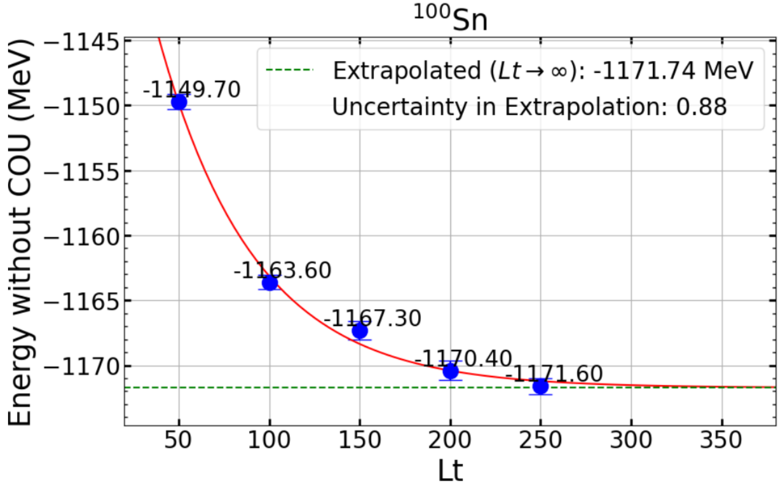
Results from LAT-OPT1: Heavy nuclei

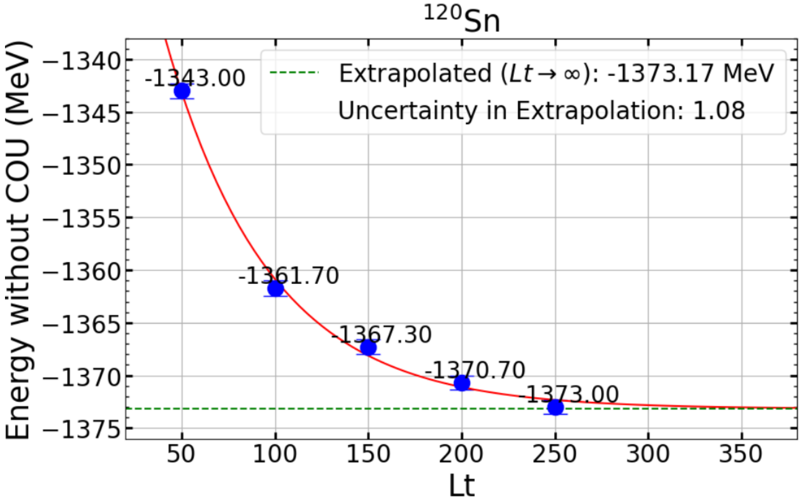


Nucleus	E_{bind} (MeV)	E_{sl} (MeV)	$E_{\text{sl}}/E_{\text{bind}}$	EXP (MeV)
^{4}He	$-29.0(2)$	-0.3	0.010	-28.3
^{12}C	$-91.3(1)$	-13.3	0.146	-92.2
^{14}C	$-104.6(1)$	-12.7	0.121	-105.3
^{16}O	$-126.9(2)$	-5.6	0.044	-127.6
^{40}Ca	$-343.0(2)$	-13.6	0.040	-342.1
^{48}Ca	$-414.5(3)$	-42.3	0.102	-416.0
^{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





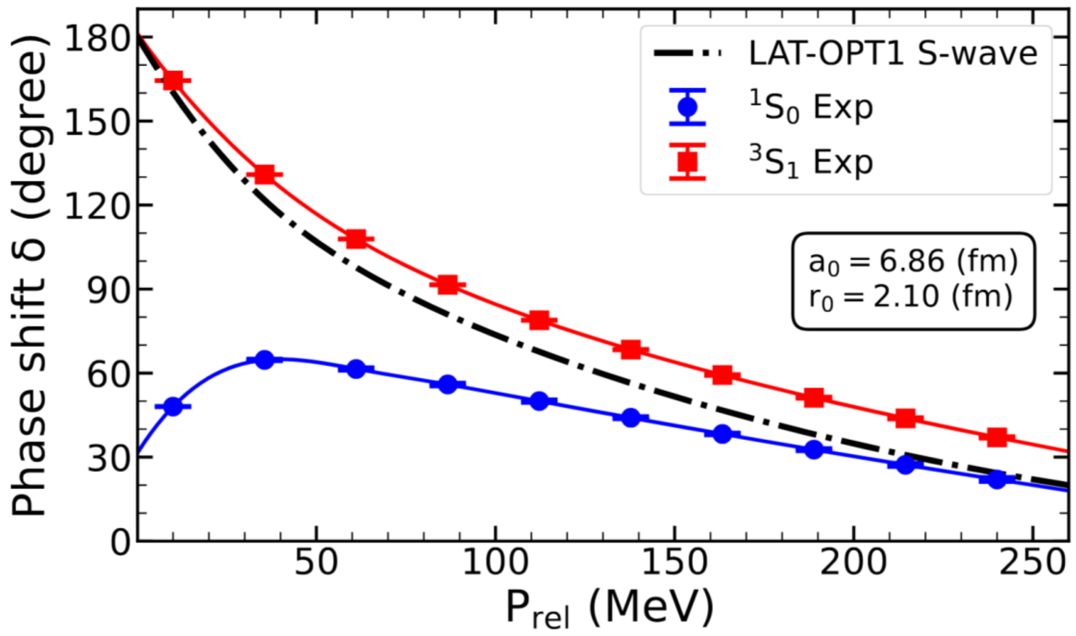


Results from LAT-OPT1: Phase shifts

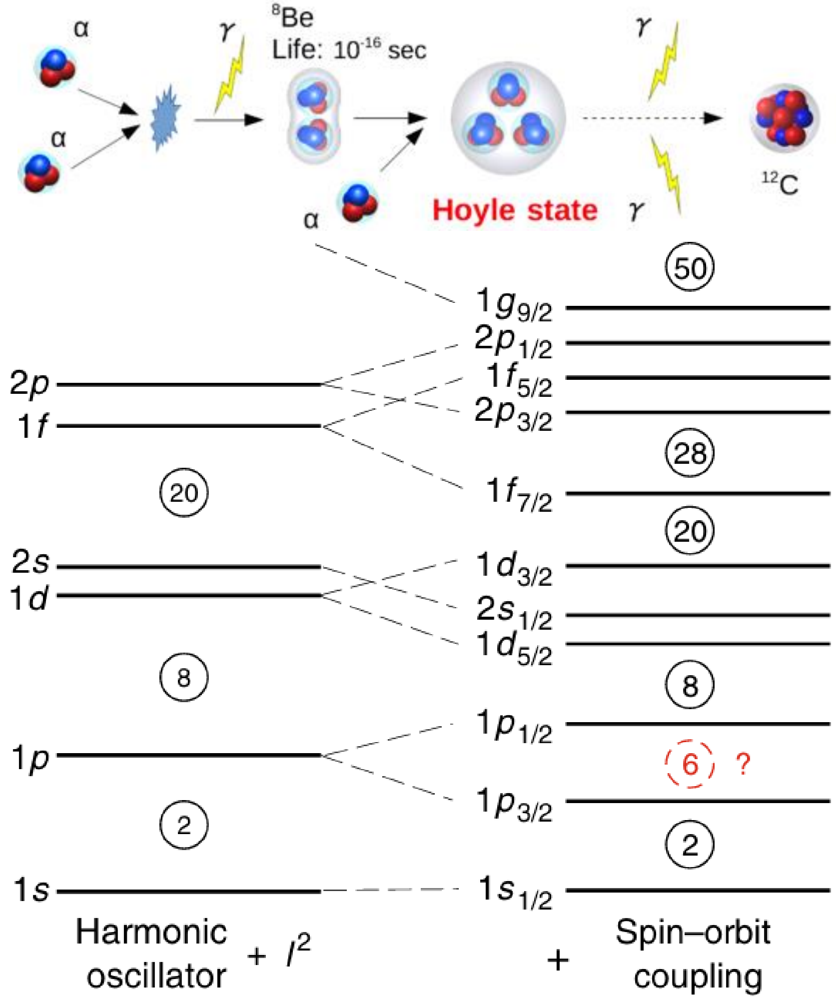
- ***Ab initio* calculations** attempt to predict **finite nuclei** from **phase shifts**
- Conversely, we can also predict phase shifts from **finite nuclei**
  ← Binding energies and charge radii can be measured with **extremely high precision**, encoding complete information about nuclear forces.

- The nuclear force fitted to **binding energies** predict a **S-wave phase shift** falling between 1S0 and 3S1

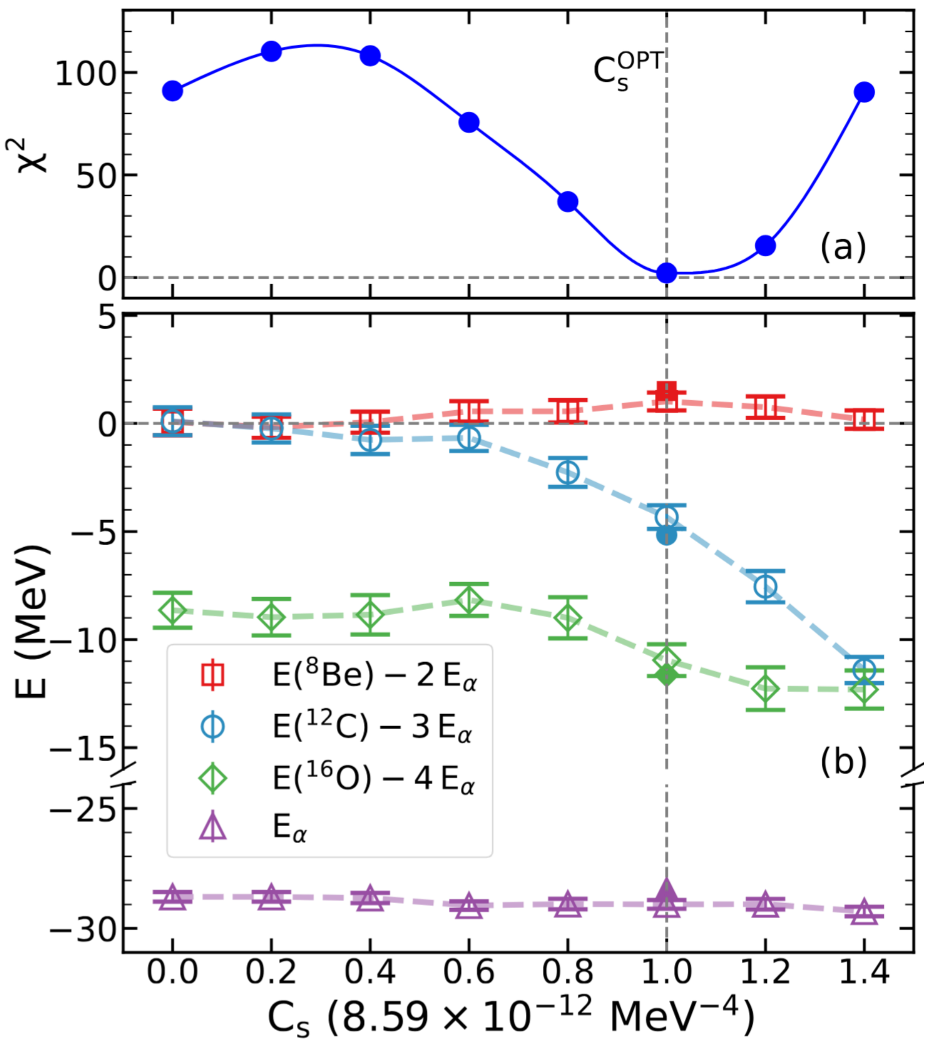
- S-wave splitting, S-D mixing, P-wave phase shifts should be reproduced at higher orders



Results from LAT-OPT1: Nuclear clustering



D. T. Tran et al., Nat. Comm. 9, 1594 (2018)



Exactly solvable phenomenological nuclear force

- ***Ab initio* calculations**
  - Realistic interactions fitted to few-body data
  - Challenging to solve, particularly for heavy nuclei
- **Phenomenological methods**
  - Phenomenological interactions fitted to finite nuclei
  - Easy to solve, however lack correlations
- **Sign-problem-free QMC**
  - Phenomenological interactions fitted to finite nuclei
  - Scalable and unbiased, full quantum correlations ← **spectrum, reaction, clustering, ⋯**

$$V(1,2) = t_0(1 + x_0 P^\sigma)\delta(\mathbf{r}_1 - \mathbf{r}_2) + \tfrac{1}{2}t_1\left[\delta(\mathbf{r}_1 - \mathbf{r}_2)\mathbf{k}^2 + \mathbf{k}'^2\delta(\mathbf{r}_1 - \mathbf{r}_2)\right] + t_2\mathbf{k}'\delta(\mathbf{r}_1 - \mathbf{r}_2)\mathbf{k} + iW_0(\boldsymbol{\sigma}^{(1)} + \boldsymbol{\sigma}^{(2)})\mathbf{k}' \times \delta(\mathbf{r}_1 - \mathbf{r}_2)\mathbf{k},$$

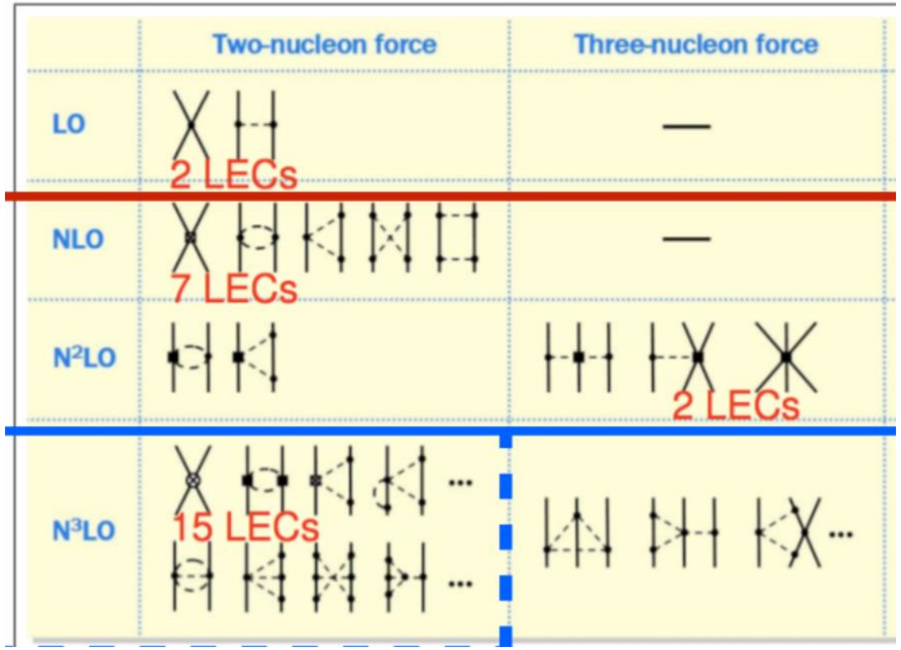
$$V(1,2,3) = t_3\delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(\mathbf{r}_2 - \mathbf{r}_3)$$

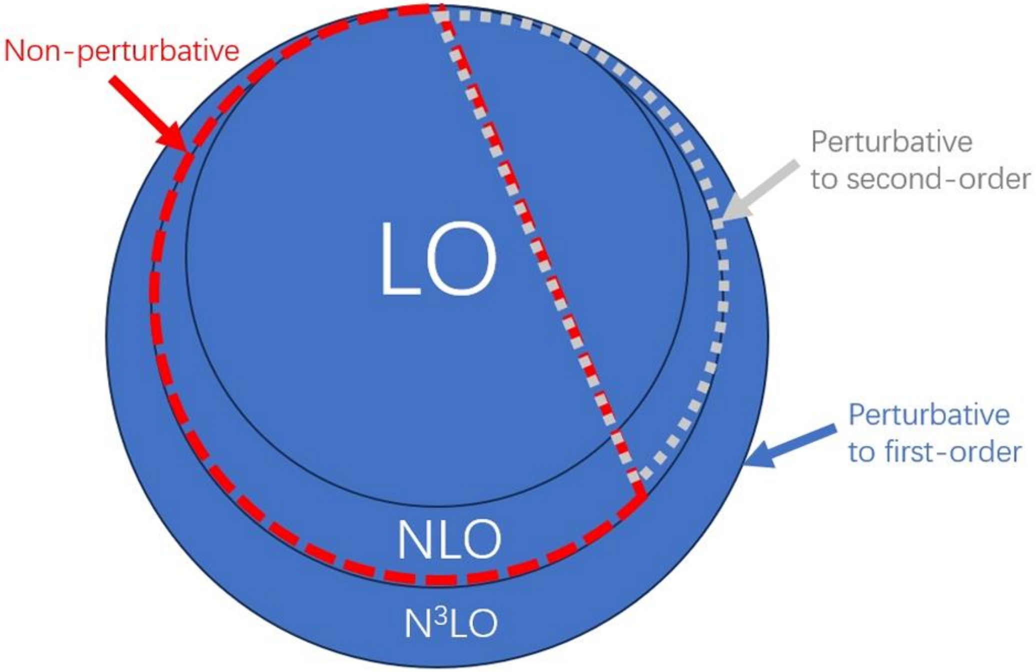
LAT-OPT1 has one-to-one correspondence to Skyme force with 6 parameters except for x_0

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	—

Go beyond leading order

- Complicated structures of the nuclear forces can be included using perturbation theory



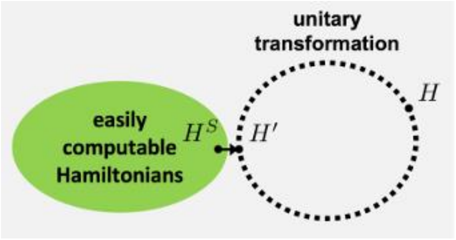


$$H_{\mathrm{N3LO}} = H_{\mathrm{SU4}} + \lambda\,(H_{\mathrm{NLO}} - H_{\mathrm{SU4}})$$

Advanced perturbative techniques

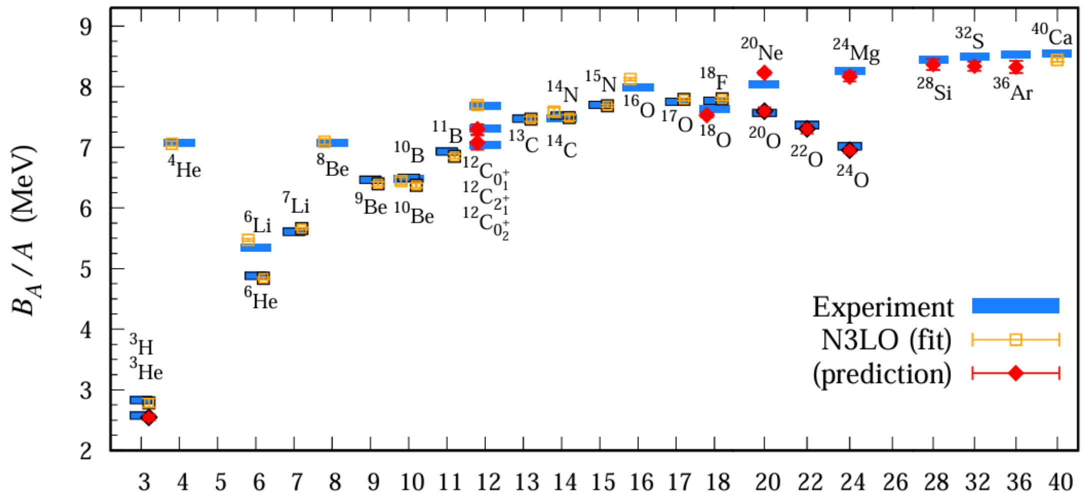
Perturbation theory can be improved with advanced algorithms

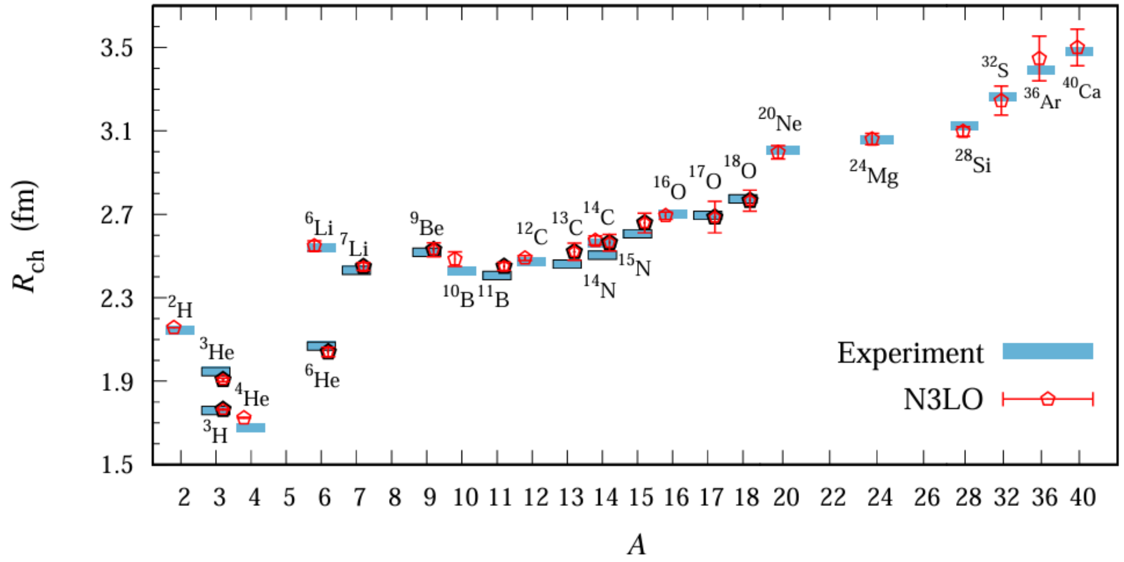
- **Perturbative quantum Monte Carlo method**, BL. et al.. PRL 128. 242501 (2022); J. Liu et al., EPJA 61, 85 (2025)
  Calculate second order corrections directly
  $$E_{\lambda^2} = \sum_{n>0} \frac{|\langle \Psi_0 | V_C | \Psi_n \rangle|^2}{E_0 - E_n}$$
- **Wavefunction matching method**, S. Elhatisari et al., Nature 630, 59 (2024); PRL 134, 162503 (2025); 2502.18722
  Improved first order correction

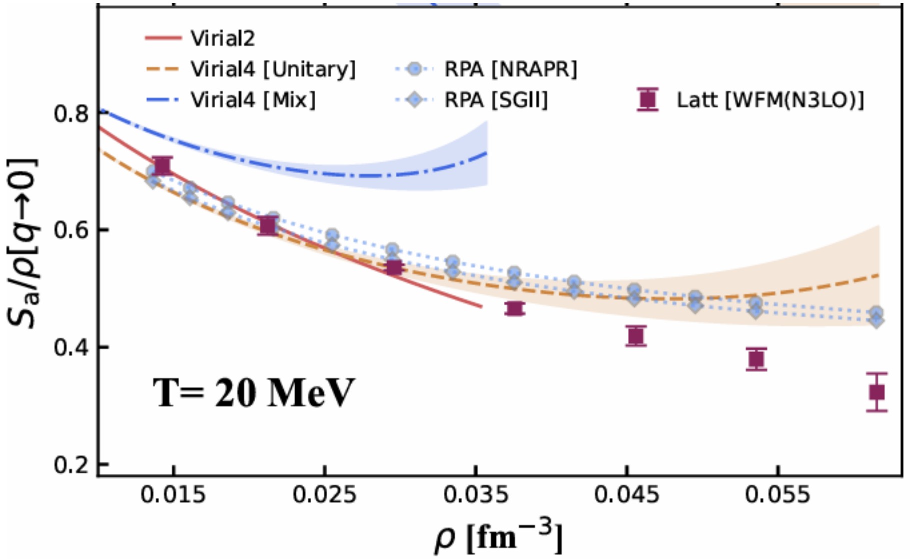


- **Rank-one operator method**, Y. Ma et al., PRL 132, 232502 (2024)
  Perturbatively calculate structure factors
- **Multi-channel perturbative calculations**, T. Wang et al., 2503.23840 (2025)
  Perturbatively calculate beta-decay in light nuclei

Calculations with high-fidelity nuclear forces



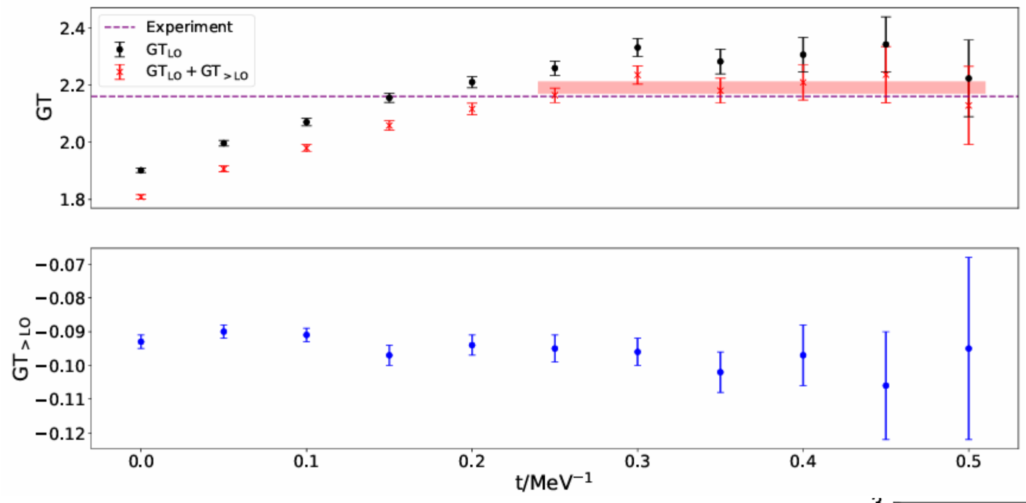


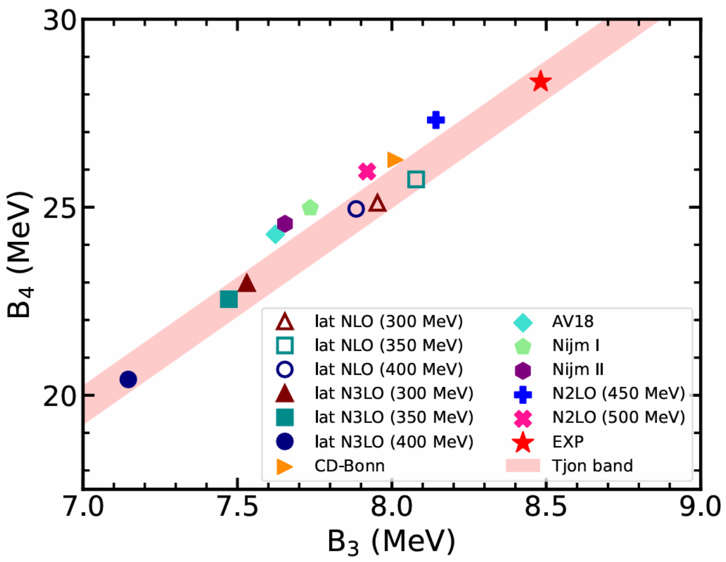


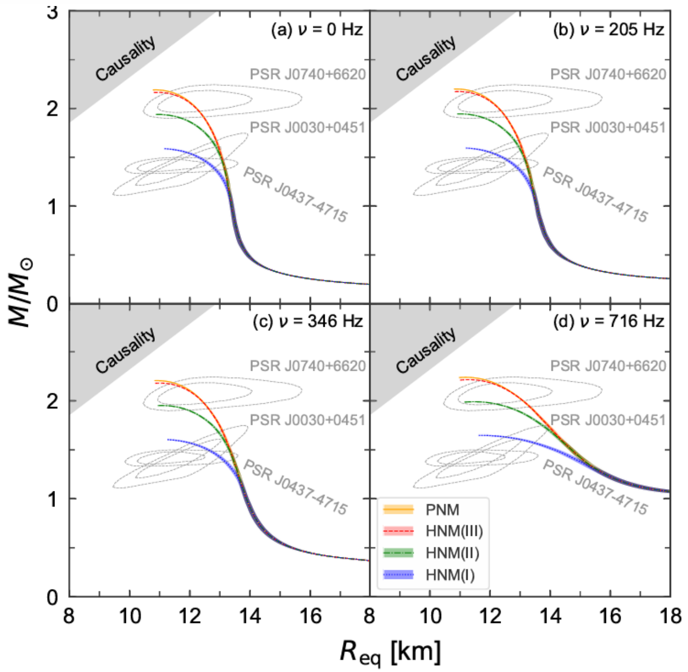
Calculations with N^{3}LO chiral forces:

- Binding energies and radii
  S. Elhatisari et al., Nature 630, 59 (2024)
- Structure factors at finite temperature
  Y. Ma et al., PRL 132, 232502 (2024)
- Structures of beryllium isotopes
  S. Shen et al., PRL 134, 162503 (2025)
- Structures of carbon and oxygen isotopes
  Y. Song et al., 2502.18722 (2025)

Calculations with high-fidelity nuclear forces







Calculations with N^3LO chiral forces (continued):

- Hypernuclei
  F. Hildenbrand et al., EPJA 60,215 (2024)
- Triton beta-decay
  S. Elhatisari et al., PLB 859, 139086 (2024)
- Structure of silicon isotopes
  S. Zhang et al., 2411.17462 (2024)
- Hyper-neutron matter
  H. Tong et al., Sci. Bull. 70, 825 (2025)
- DD^*K three-hadron system
  Z. Zhang et al., PRD 111, 036002 (2025)
- Correlation in light nuclei
  J. Liu et al., EPJA 61, 85 (2025)
- Beta-decay of ^6He
  T. Wang et al., 2503.23840 (2025)

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 Skyme 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!