Lattice simulation for *ab initio* nuclear many-body problems

Bing-Nan Lu
吕炳楠

Graduate School of China Academy of Engineering Physics
中国工程物理研究院研究生院



中国科学院高能物理所

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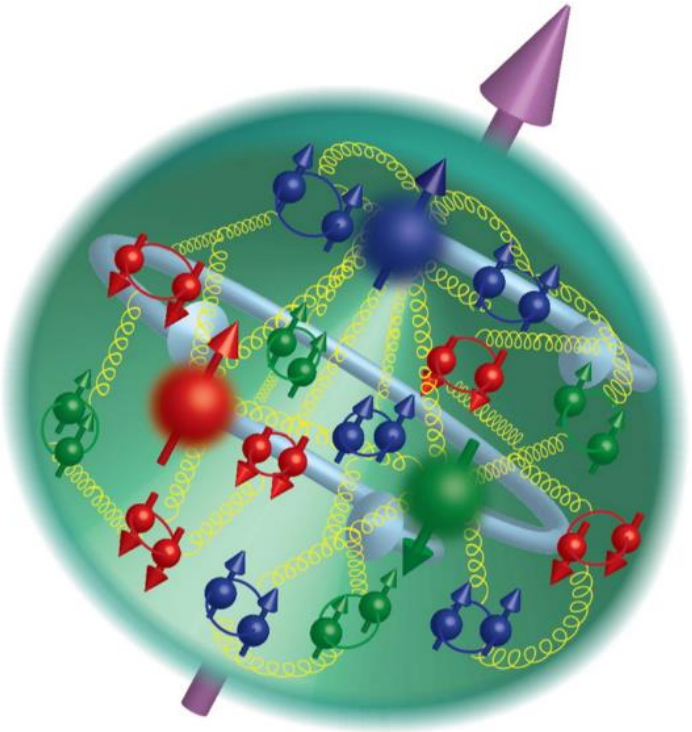
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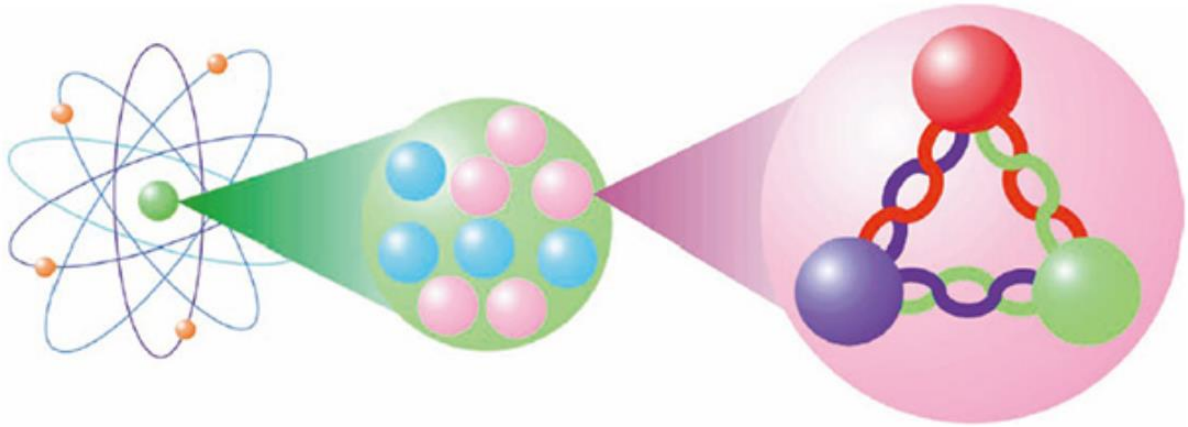
- **Introduction to Nuclear Lattice Effective Field Theory**
- Non-perturbative QMC and sign problem
- Perturbative QMC
- Renormalization of NLEFT
- Ab initio nuclear thermodynamics
- Summary and perspective

Hierarchy of strongly interacting systems

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

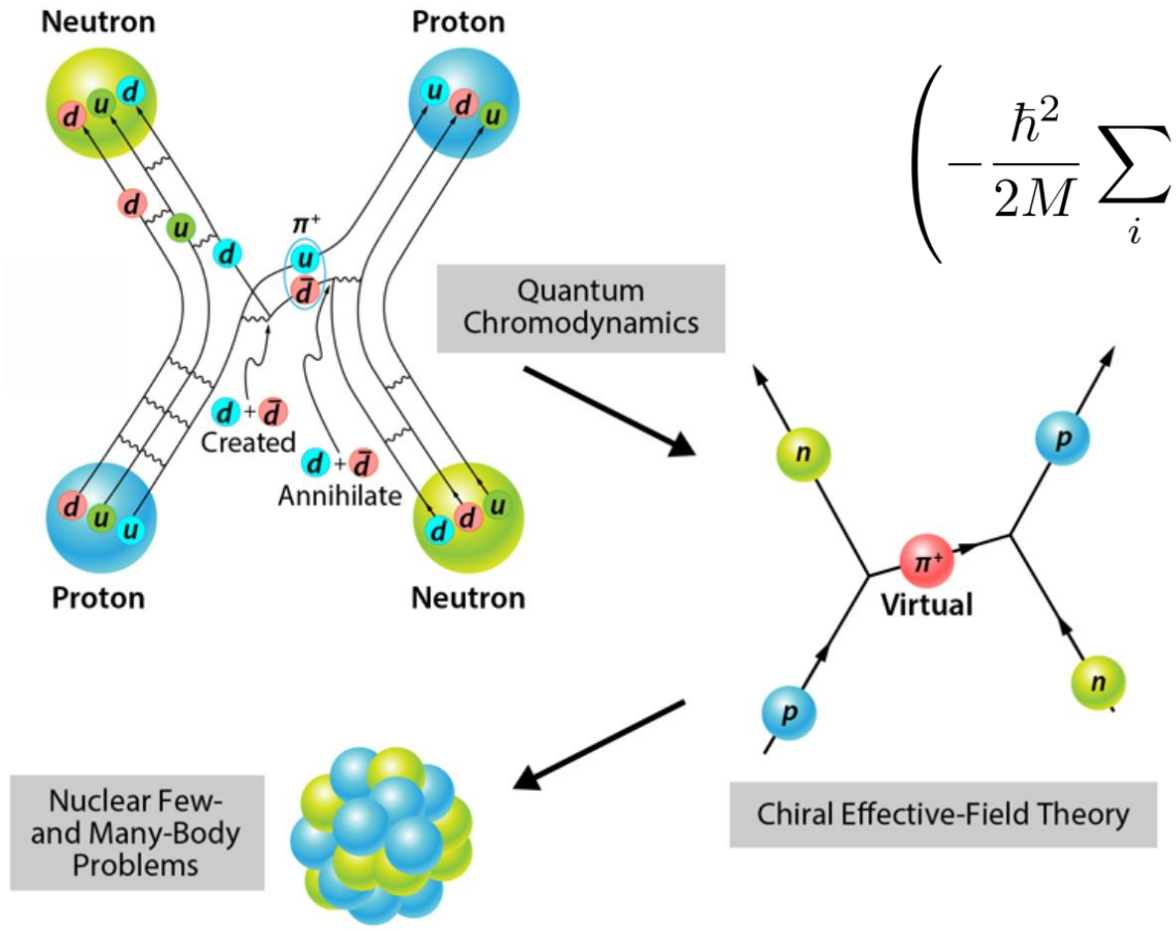
QCD Quark Confinement





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

Nuclear *ab initio* calculations

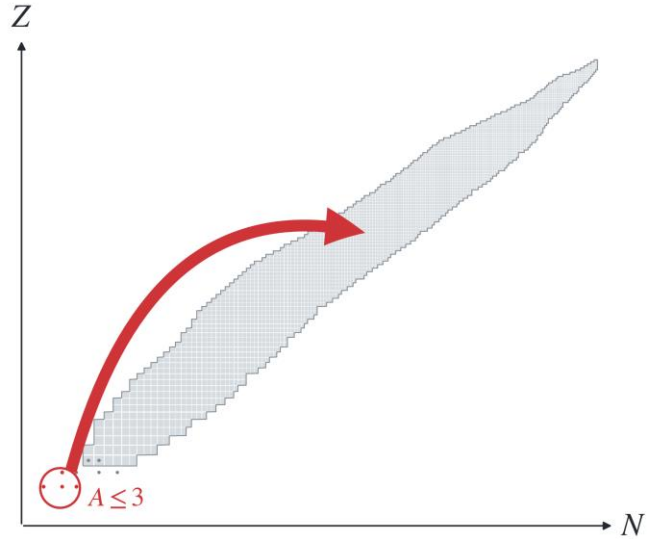


Nuclear forces

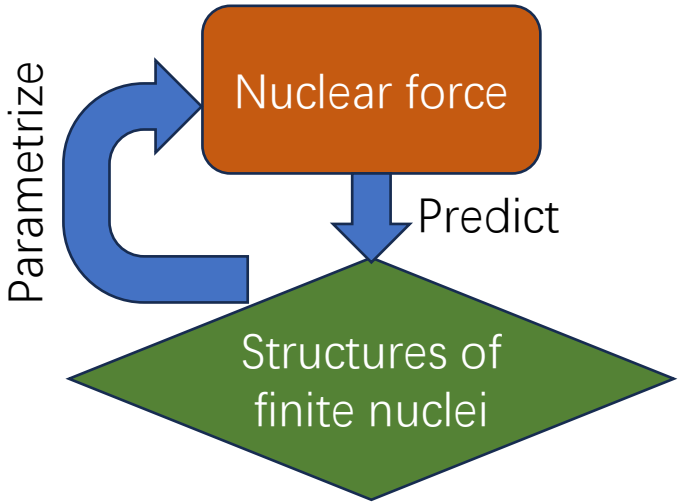
$$\left(-\frac{\hbar^2}{2M}\sum_i \nabla_i^2 + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \cdots\right)\Psi = E\Psi$$



Nuclear Force Problem

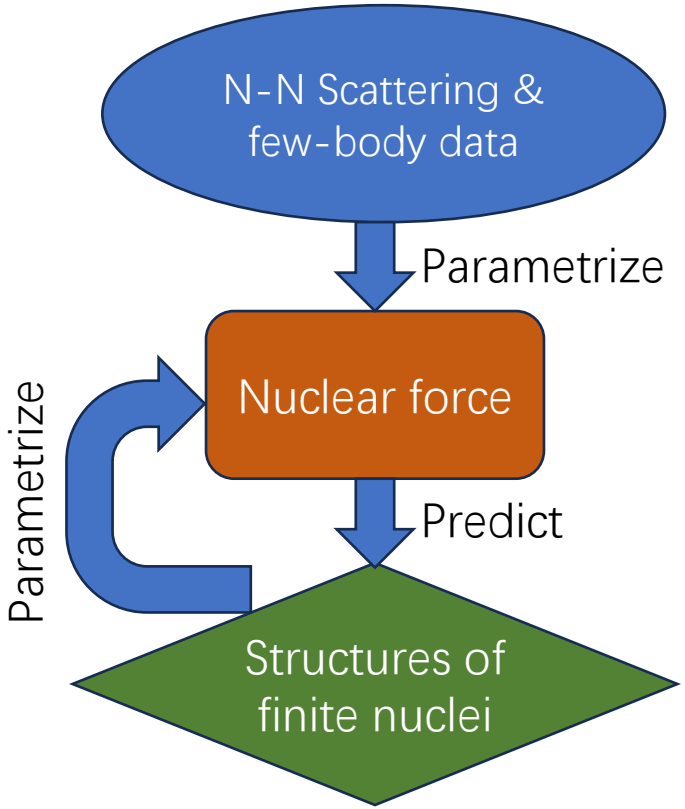


Effective nuclear forces
(Skyrme, RMF, shell model, etc.)

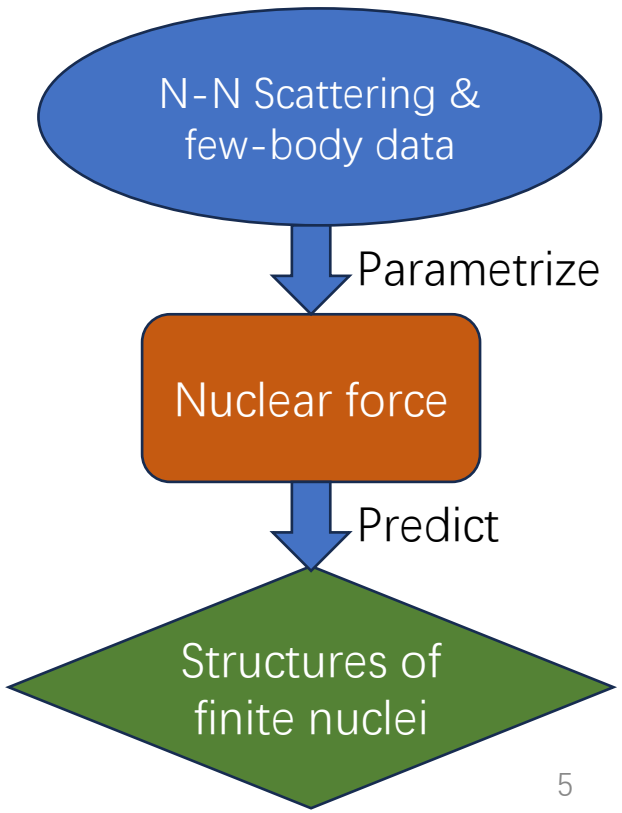


Nuclear Force Problem: Can the nuclear force calibrated with the **N-N scattering and few-body data** uniquely and correctly predict the **structures of finite nuclei**?

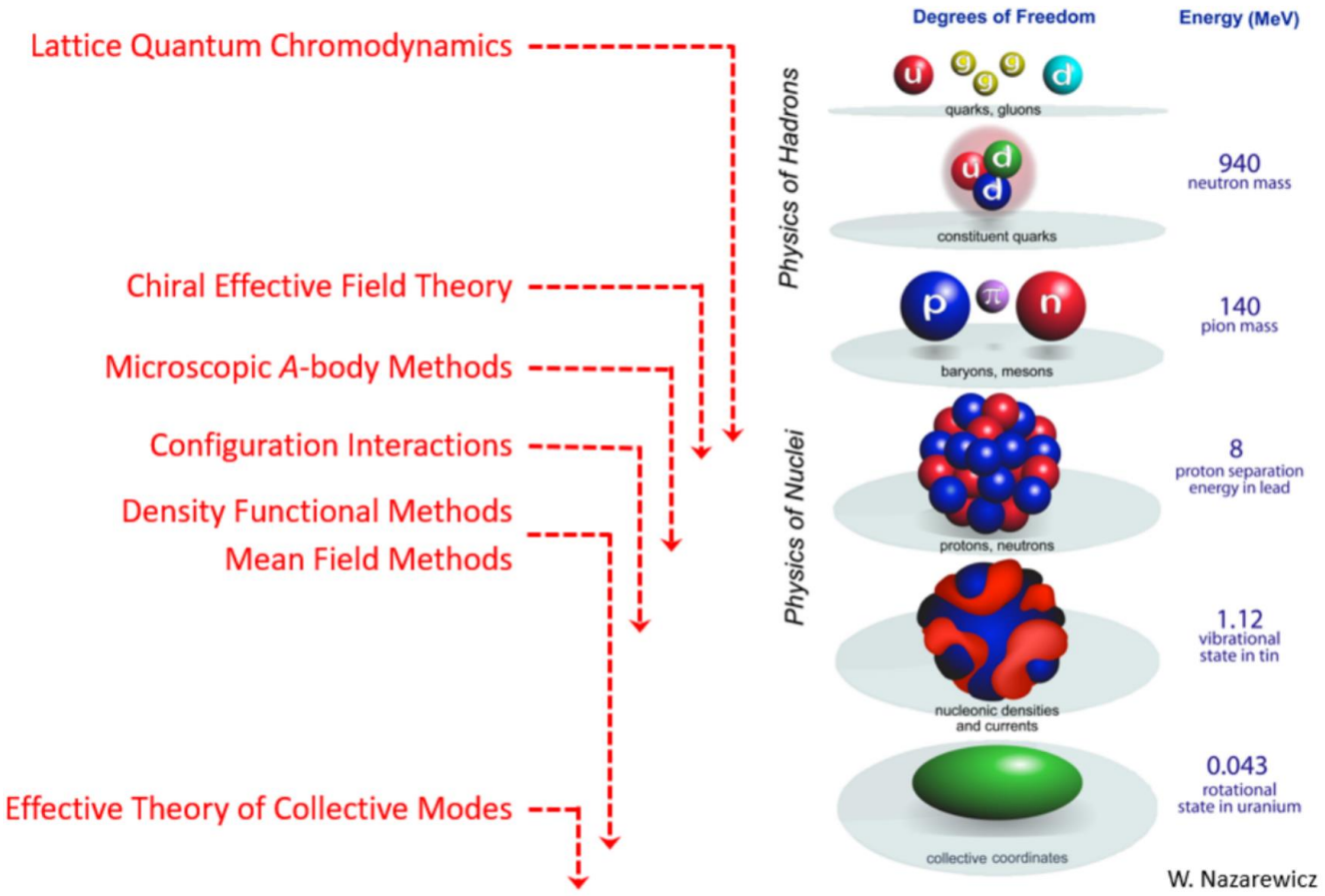
Ab initio (Weak form)



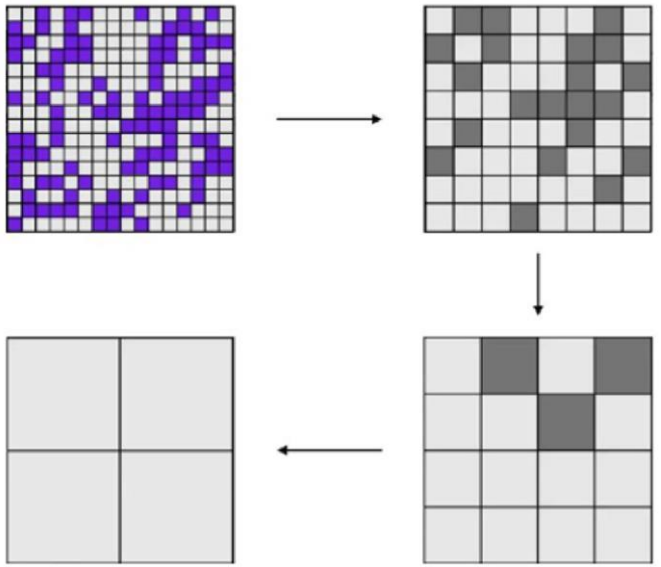
Ab initio (Strong form)



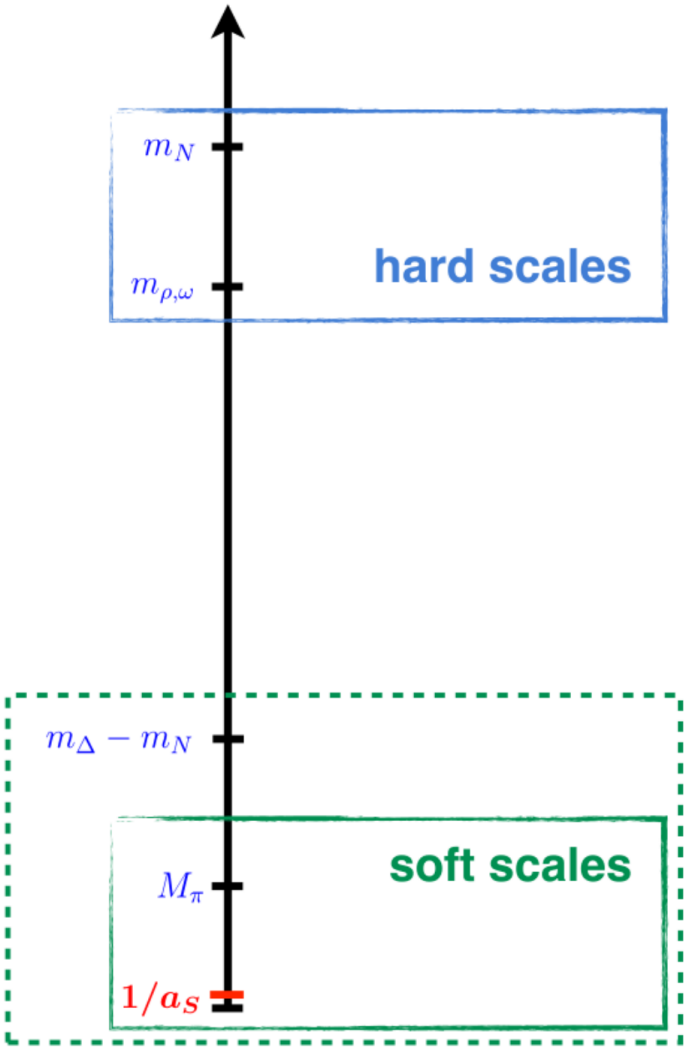
What is a nuclear EFT?

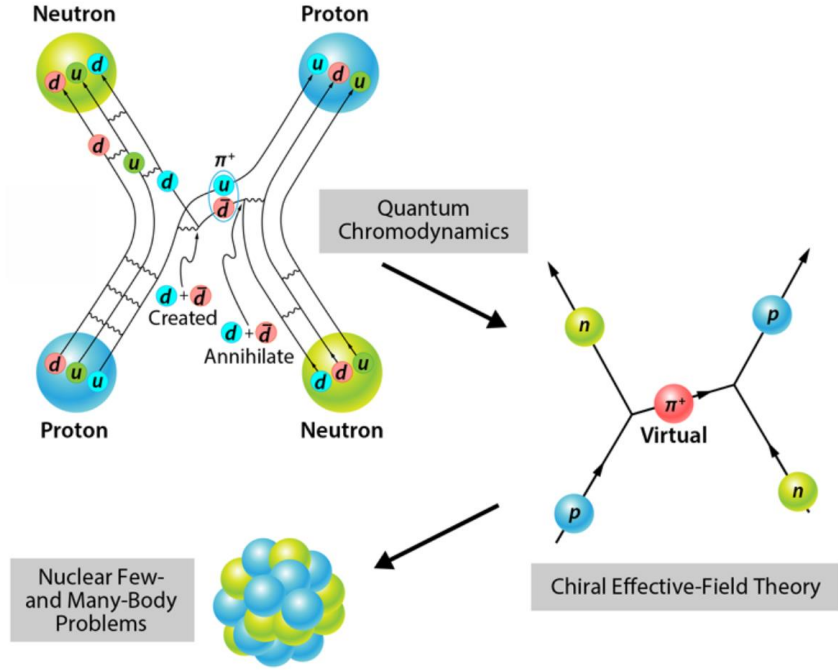


- **Modern nuclear force constructions are based on the Effective Field Theory**
- **Theoretical foundation of EFT is the Wilsonian renormalization group**:
  - **High-momentum** details can be integrated out & hidden in LECs
  - **Low-momentum** physics kept invariant under RG transformations



Scales in nuclear physics





- Chiral EFT: Perturbative expansion of the N-N and π-N potentials in powers of **pion mass m_π** and **nucleon momenta Q**
- QCD has an approximate chiral symmetry
  - Explicitly broken by non-zero quark mass ($m_q \approx 3$ MeV)
  - Spontaneously broken SU(2)×SU(2)→SU(2)
  - Sp. broken **exact** symmetry → massless Goldstone boson
  - Sp. Broken **approximate** symmetry → very light bosons ($m_\pi \approx 140$ MeV)

  → **Long-range part of the nuclear force**
- In nucleus, Fermi momentum p_F~200 MeV

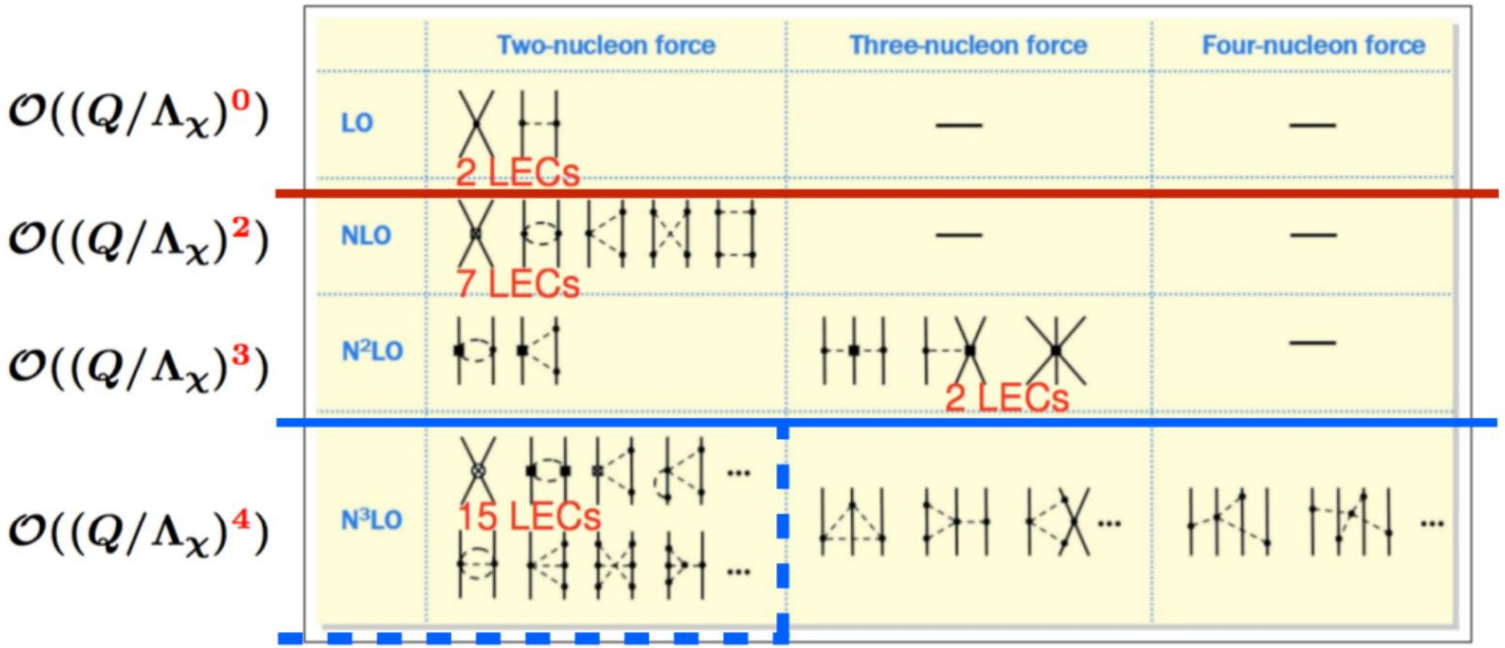
  → **Short-range part of the nuclear force**

Hard scale: Λ_χ~ 1 GeV: Chiral EFT works for Q ≪ Λ_χ

N-N interaction in nuclear chiral EFT

$$\langle \boldsymbol{p}_1', \boldsymbol{p}_2' | V_{N-N} | \boldsymbol{p}_1, \boldsymbol{p}_2 \rangle = \Big\{ B_1 + B_2(\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) + C_1 q^2 + C_2 q^2 (\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) + C_3 q^2 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) + C_4 q^2 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2)$$
$$+ C_5 \frac{i}{2} (\boldsymbol{q} \times \boldsymbol{k}) \cdot (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) + C_6 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{q})(\boldsymbol{\sigma}_2 \cdot \boldsymbol{q}) + C_7 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{q})(\boldsymbol{\sigma}_2 \cdot \boldsymbol{q})(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2)$$
$$- \frac{g_A^2}{4F_\pi^2} \left[\frac{(\boldsymbol{\sigma}_1 \cdot \boldsymbol{q})(\boldsymbol{\sigma}_2 \cdot \boldsymbol{q})}{q^2 + M_\pi^2} + C_\pi \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \right] (\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) + \cdots \Big\} \delta(\boldsymbol{p}_1 + \boldsymbol{p}_2 - \boldsymbol{p}_1' - \boldsymbol{p}_2'),$$

$\boldsymbol{q} = \boldsymbol{p}_1' - \boldsymbol{p}_1, \boldsymbol{k} = \boldsymbol{p}_1' - \boldsymbol{p}_2, \boldsymbol{\sigma}_{1,2}$ for spins, $\boldsymbol{\tau}_{1,2}$ for isospins, C_{1-7}, g_A, etc. are Low Energy Constants fitted to N-N scattering data



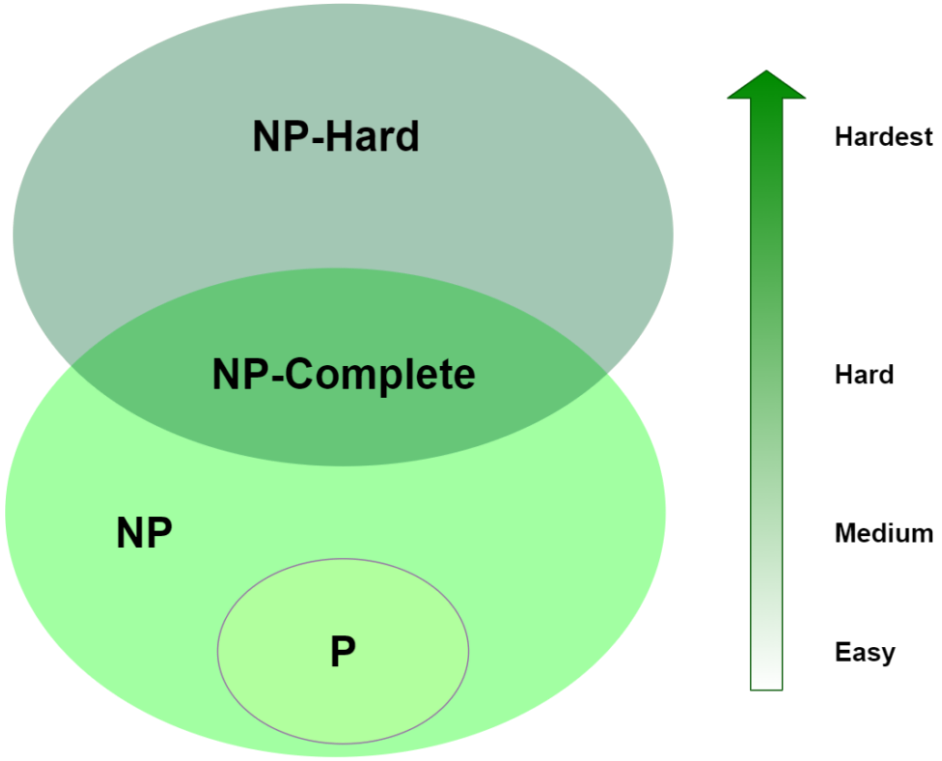
- **Long-range part**: pion-exchange Feymann diagrams
- **Short-range part**: δ functions and their derivatives

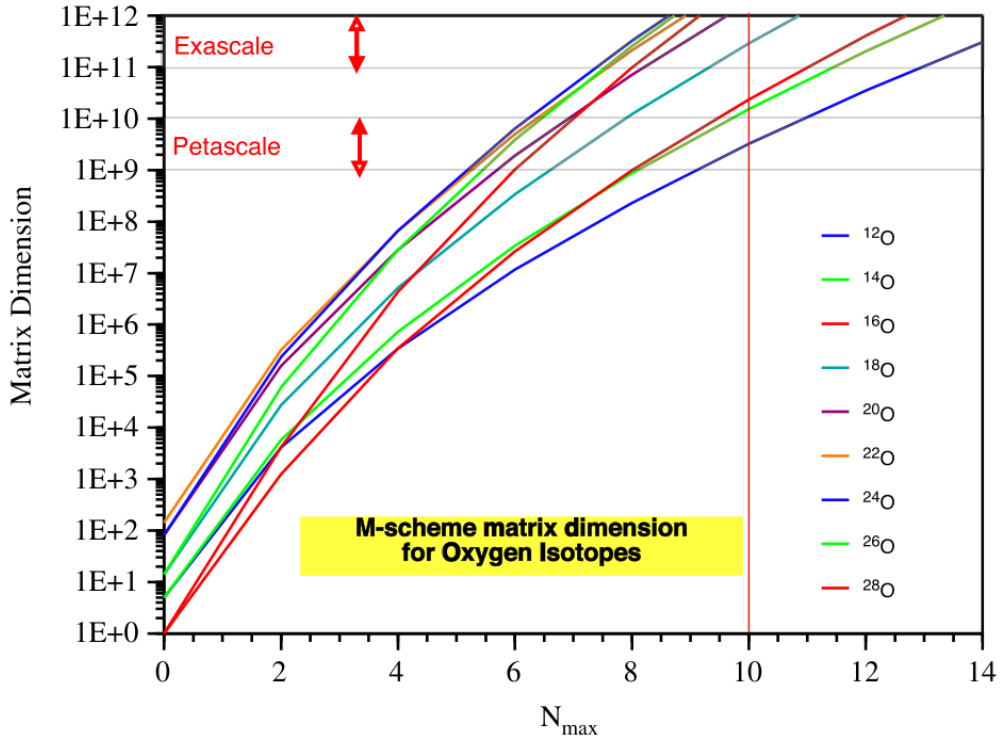
Both interactions need regularization

- **Pion-exchange**:
  - Dimensional regularization
  - Spectral function regulator
  - Local momentum regulator
- **Contact terms**:
  - Local regulator
  - Non-local regulator
  - Single-particle regulator

All chiral EFTs are defined with certain cutoffs Λ, Λ_π etc. Are they equivalent?

Complexity of nuclear many-body problem





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

Exponentially increasing Hilbert space

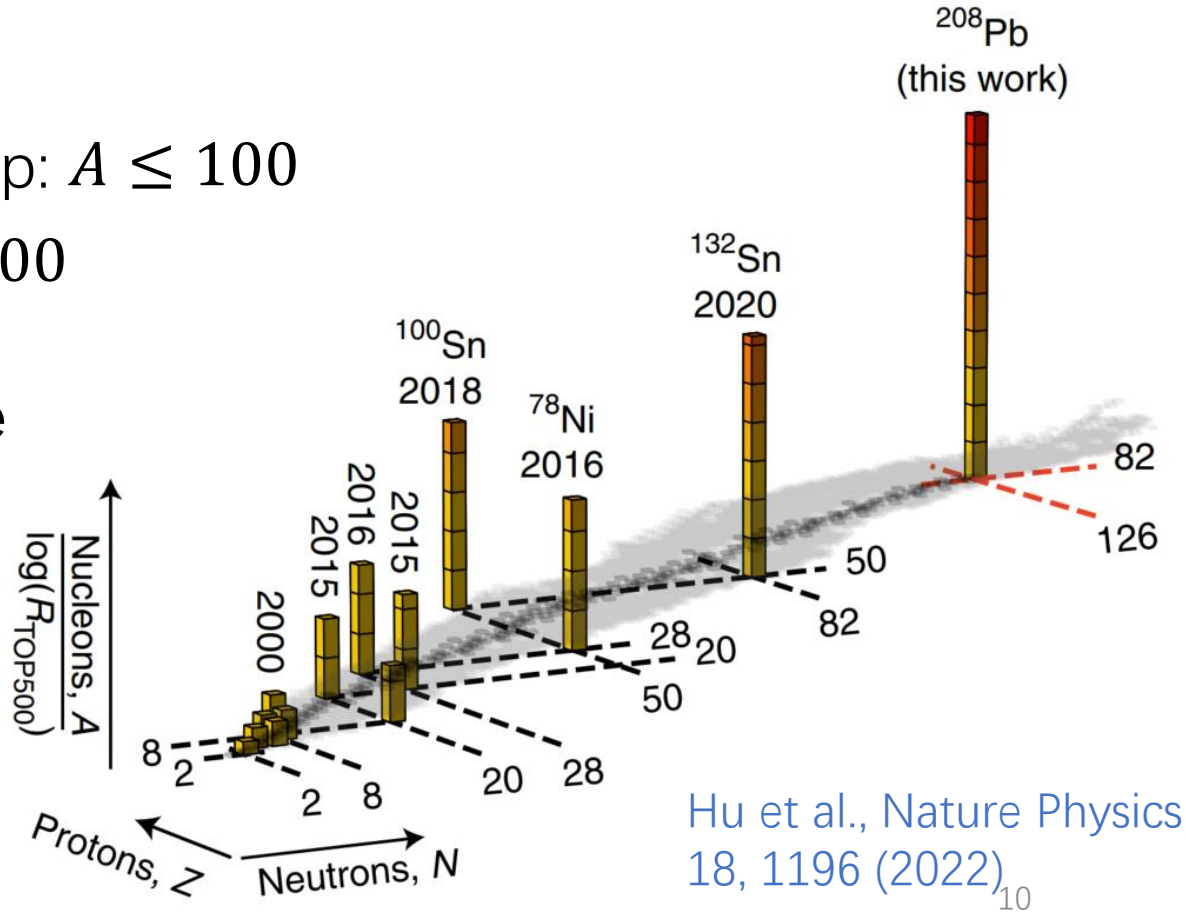
➡ **Find ground state of a general Hamiltonian is NP-Hard**

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



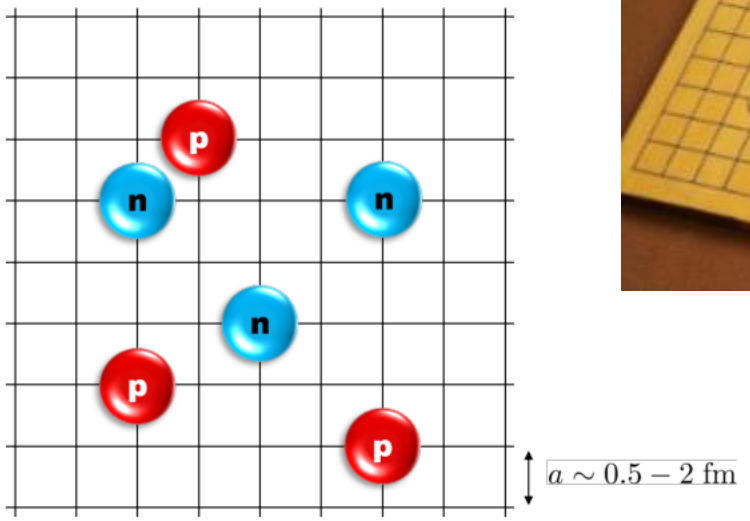
Hu et al., Nature Physics, 18, 1196 (2022)

Lattice EFT: A many-body EFT solver

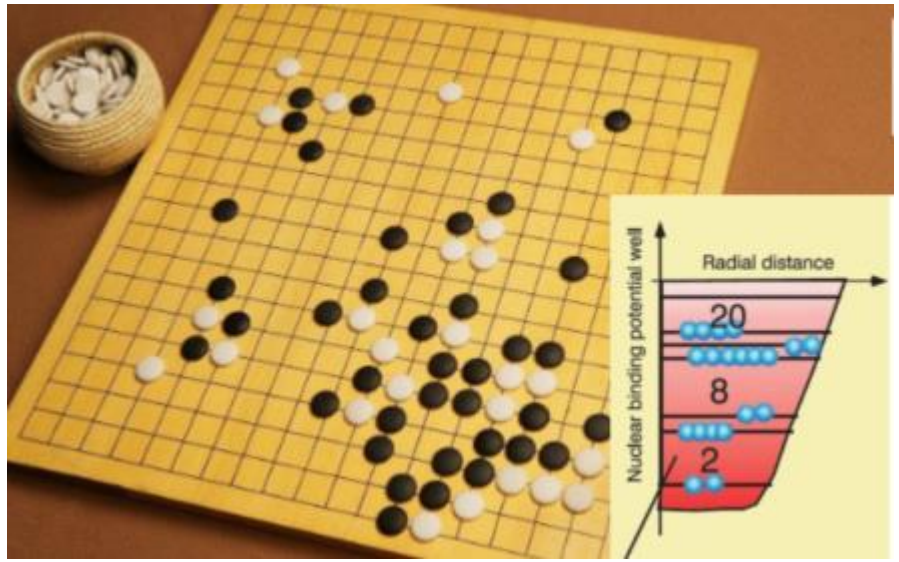
Lattice EFT = Chiral EFT + Lattice + Monte Carlo

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



- Solve the non-perturbative nuclear many-body problem by sampling all configurations

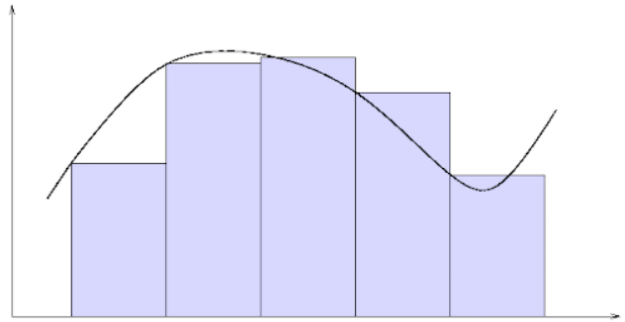
Many-body correlations emerge naturally without a reference mean-field solution

Naïve discretization of chiral Hamiltonian

$$\begin{aligned}\langle \boldsymbol{p}_1', \boldsymbol{p}_2' | V_{N-N} | \boldsymbol{p}_1, \boldsymbol{p}_2 \rangle = & \Big\{ B_1 + B_2(\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) + C_1 q^2 + C_2 q^2 (\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) + C_3 q^2 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) + C_4 q^2 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) \\ & + C_5 \frac{i}{2} (\boldsymbol{q} \times \boldsymbol{k}) \cdot (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) + C_6 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{q})(\boldsymbol{\sigma}_2 \cdot \boldsymbol{q}) + C_7 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{q})(\boldsymbol{\sigma}_2 \cdot \boldsymbol{q})(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) \\ & - \frac{g_A^2}{4F_\pi^2} \left[\frac{(\boldsymbol{\sigma}_1 \cdot \boldsymbol{q})(\boldsymbol{\sigma}_2 \cdot \boldsymbol{q})}{q^2 + M_\pi^2} + C_\pi \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \right] (\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) + \cdots \Big\} \delta(\boldsymbol{p}_1 + \boldsymbol{p}_2 - \boldsymbol{p}_1' - \boldsymbol{p}_2'),\end{aligned}$$

$$f''(x) + O(a^{2N}) = c_0^{(N)} f(x) + a^{-2} \sum_{k=1}^{N} \frac{2(N!)^2 (-1)^{k+1}}{k^2 (N+k)!(N-k)!} [f(x+ka) + f(x-ka)]$$

$$\int_a^b f(x)\, dx \approx \frac{1}{3} h \sum_{i=1}^{n/2} [f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i})]$$



- Derivative → **Finite difference / FFT**
- Integration → **Summation**

Discretization error $O(a^N)$ → Systematically improvable

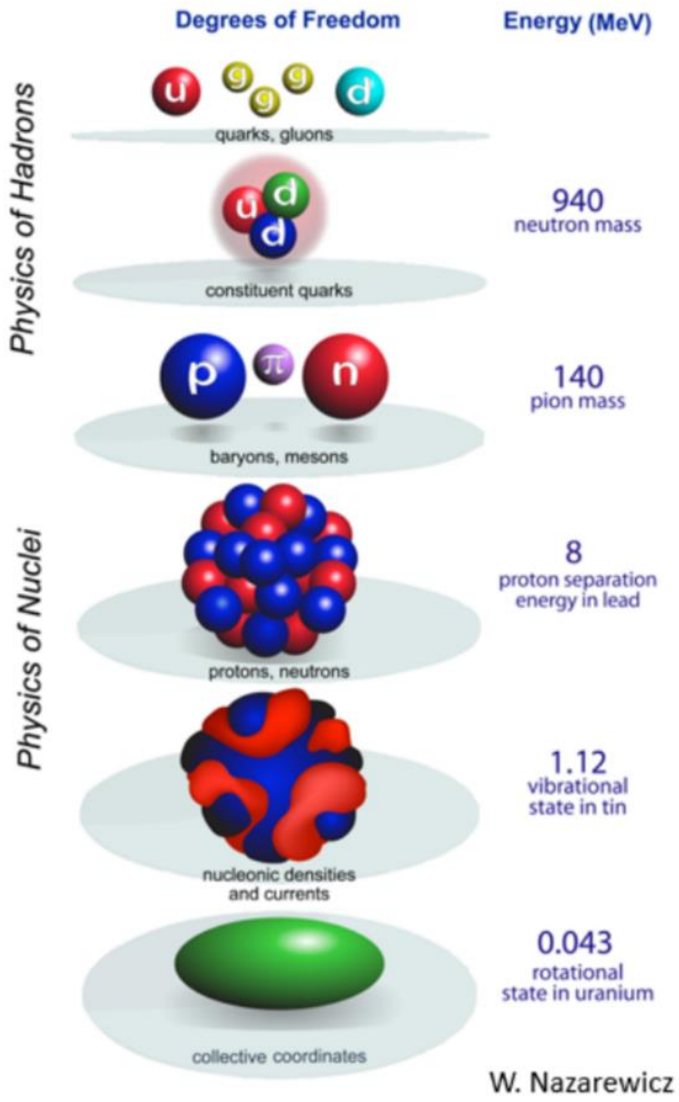
Dual role of the lattice

- Lattice is used to **discretize the action** and **regulate the delta-functions**

- QCD coupling is dimensionless
  → QCD is **renormalizable**
  → Safe to take the continuum limit $a \to 0$

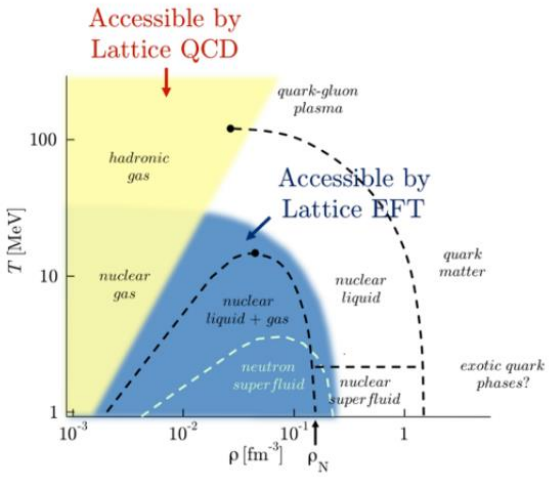
- EFT couplings has negative mass dimensions
  →EFT is **non-renormalizable**
  →Break down at a small lattice spacing

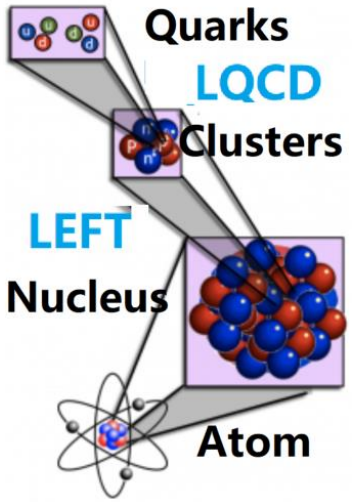
Example: Wigner bound Wigner, PR98, 145 (1955)
For $\Lambda \to \infty$, effective range $r_{\text{eff}} \leq 0$
However, experimental n-p scattering $r_{\text{eff}} \approx 1$ fm



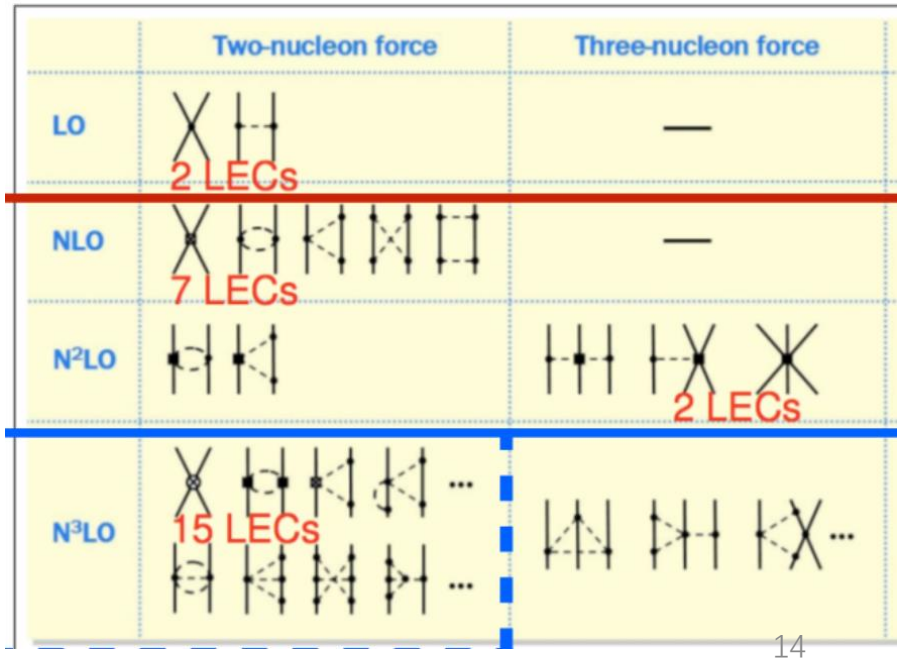
Compare Lattice EFT and Lattice QCD

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

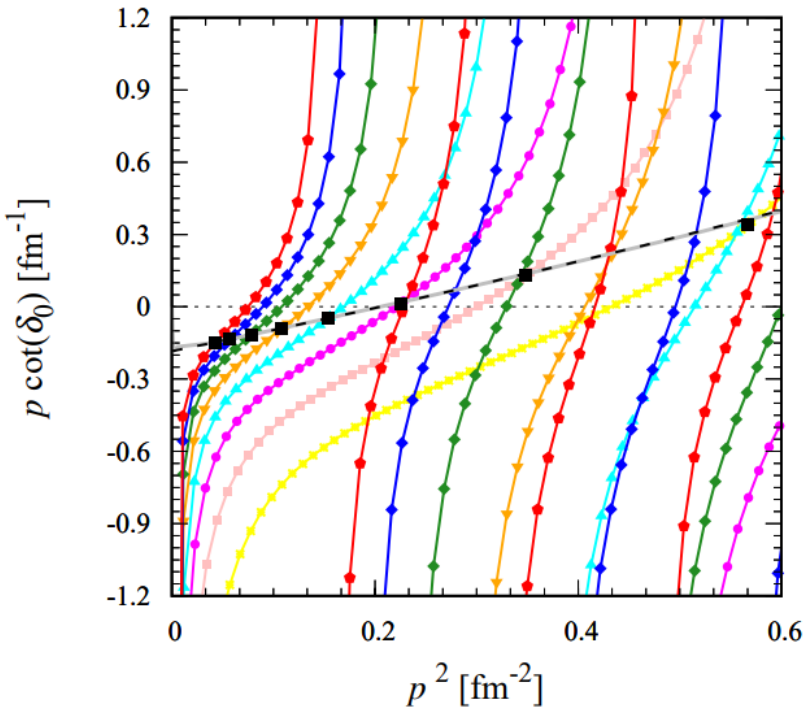


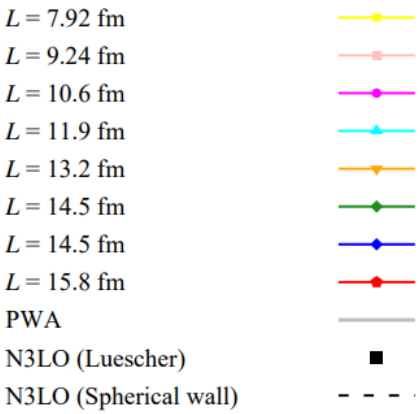


- Lattice EFT share a lot of common features with Lattice QCD. However,
  - Non-rel. → particle number conservation
  - Quadratic dispersion relation
    → no Fermion doubling problem
  - EFT contains non-renormalizable terms
    → no continuum limit



Scattering on the lattice





$$p\cot\delta_0(p) = \frac{1}{\pi L}\left[\sum_{\vec{n}}^{\Lambda}\frac{\theta(\Lambda^2-\vec{n}^2)}{\vec{n}^2-(Lp/2\pi)^2} - 4\pi\Lambda\right]$$

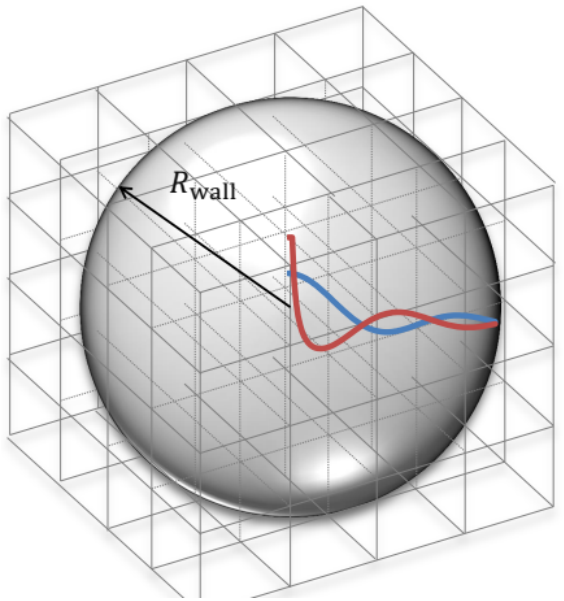
Lüscher's finite volume method:

Lüscher, Comm. Math. Phys. 105 (1986) 153; NPB 354 (1991) 531

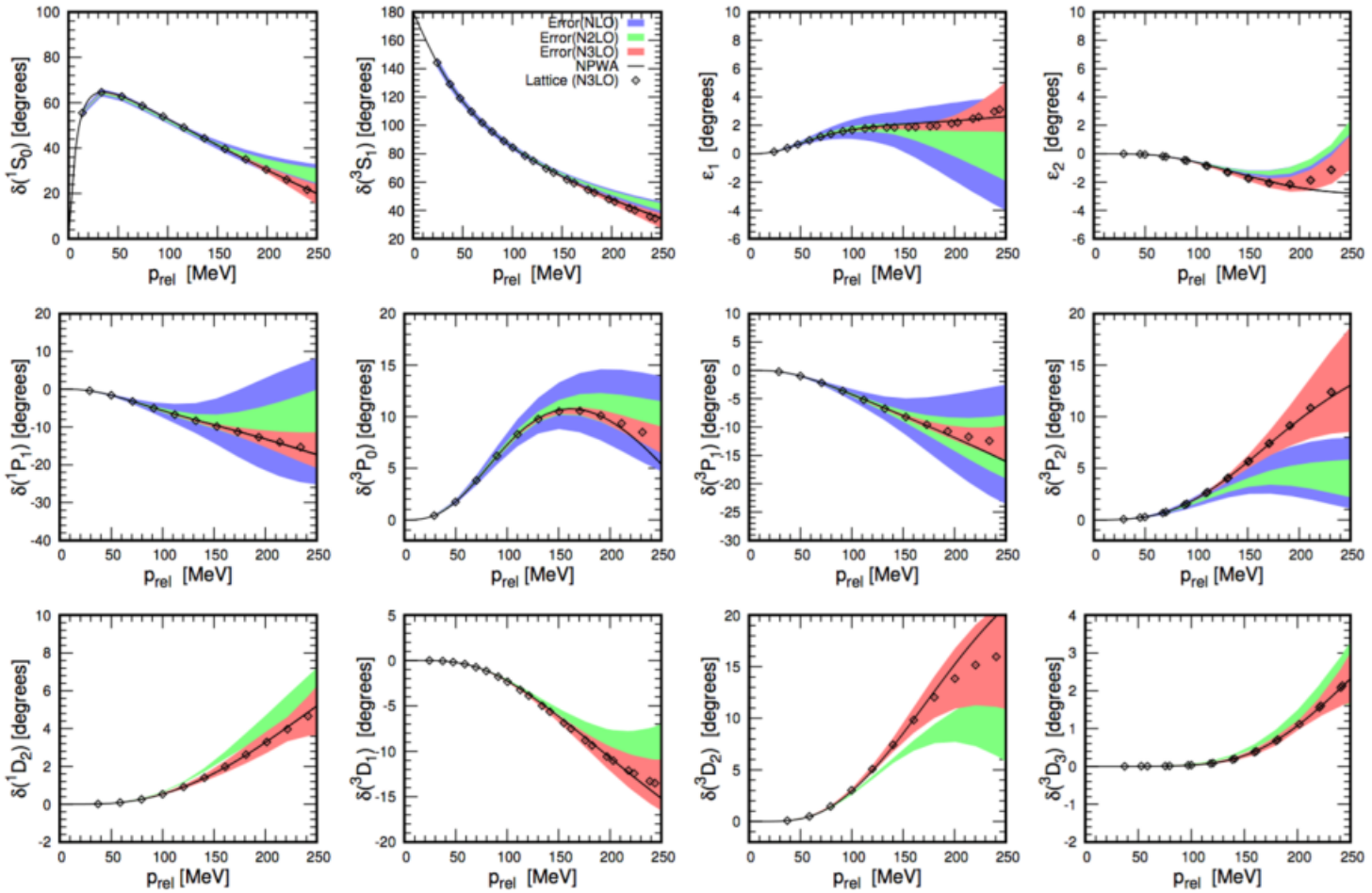
Spherical wall method:

$$R_\ell^{(p)}(r) = N_\ell(p)\times\begin{cases}\cot\delta_\ell(p)\,j_\ell(p\,r) - n_\ell(p\,r)\\ \cot\delta_\ell(p)\,F_\ell(p\,r) + G_\ell(p\,r)\end{cases}$$

Nucl. Phys. A 424, 47-59 (1984), Eur. Phys. J. A 34, 185-196 (2007).



Chiral nuclear force up to N^3LO: fit on the lattice



fit to N^2LO: Alarcon, Du, Klein, Lahde, Lee, Ning Li, B.L., Luu, Meissner, EPJA 53, 83 (2017)

fit to N^3LO: Ning Li, Elhatisari, Epelbaum, Lee, B.L., Meissner, PRC 98, 044002 (2018)

Lattice EFT: A many-body EFT solver

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

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

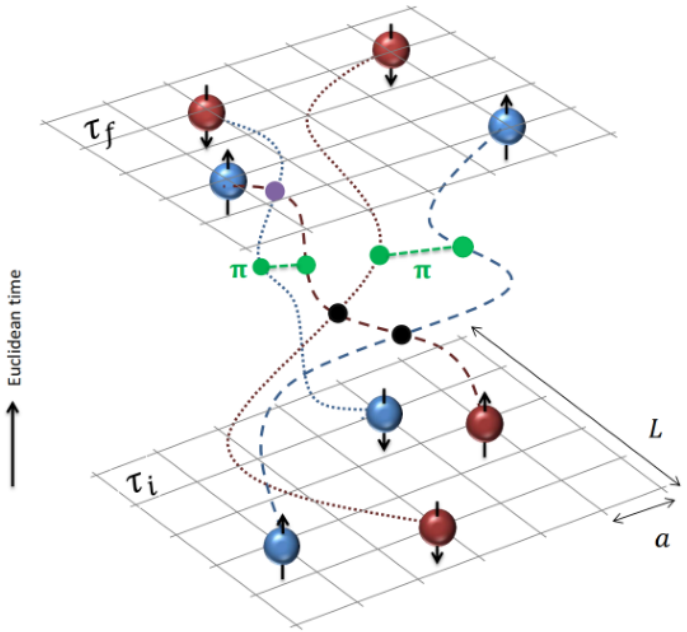
with $|\Psi_A\rangle$ representing A *free* nucleons.

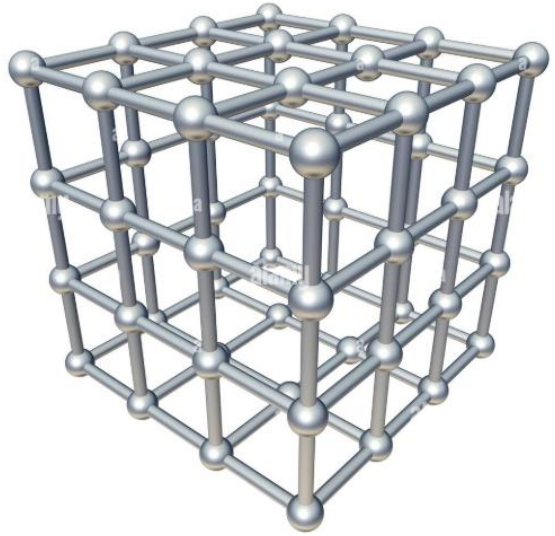
- Expectation value of any operator $\mathscr{O}$:

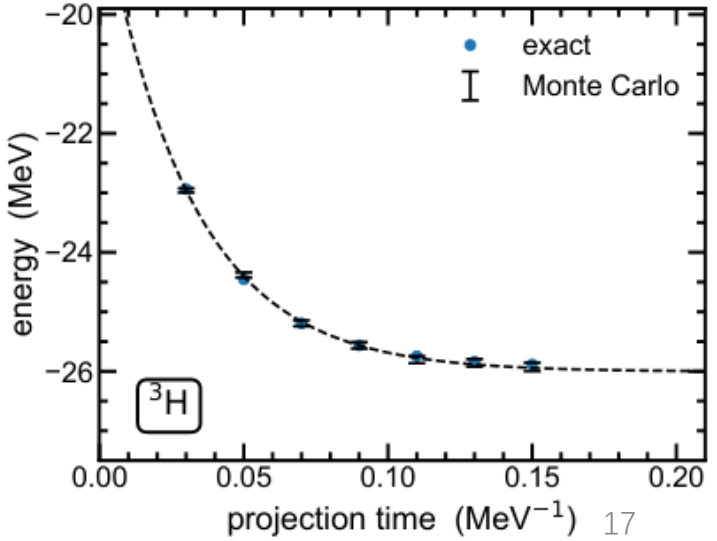
$$\langle O\rangle = \lim_{\tau\to\infty} \frac{\langle\Psi_A|\exp(-\tau H/2)\mathscr{O}\exp(-\tau H/2)|\Psi_A\rangle}{\langle\Psi_A|\exp(-\tau H)|\Psi_A\rangle}$$

- 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

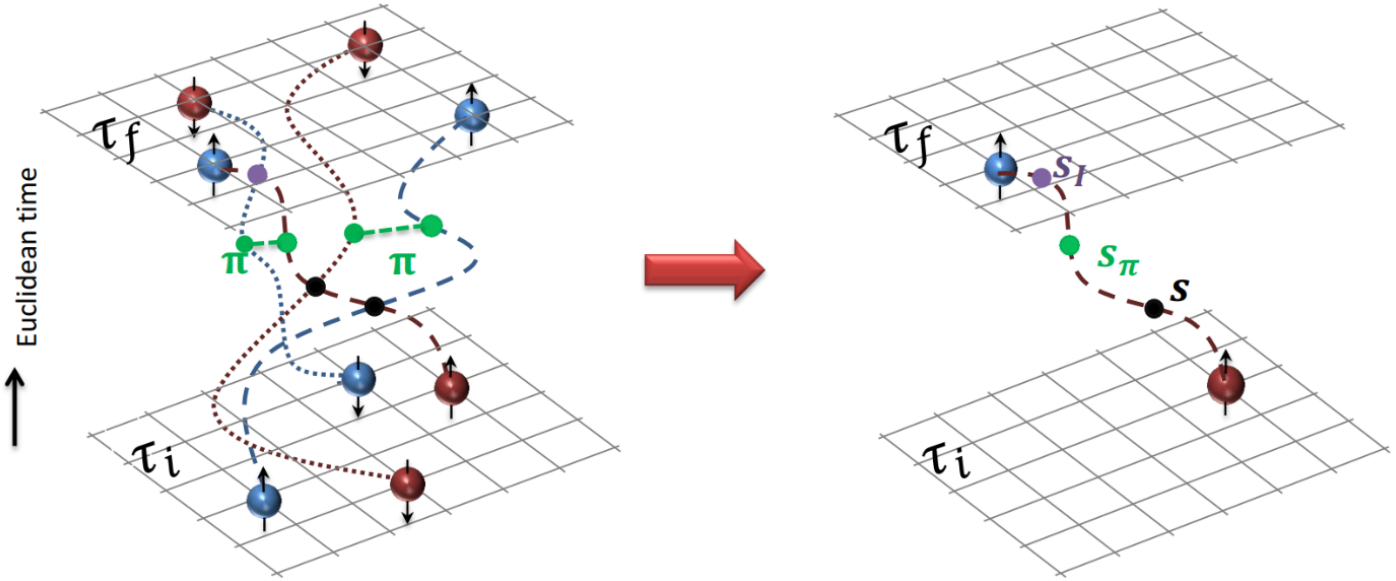
- Quantum correlations between nucleons are represented by fluctuations of the auxiliary fields.

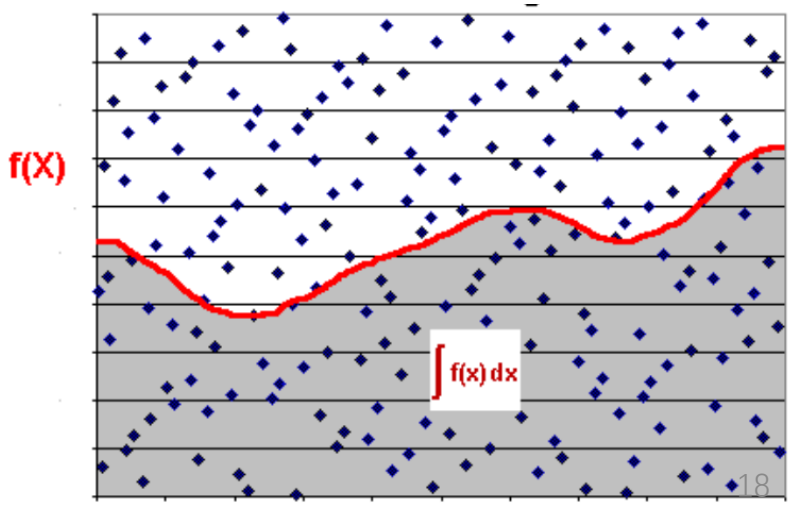
$$:\exp\left[-\frac{a_t C}{2}(\psi^\dagger\psi)^2\right]:=\frac{1}{\sqrt{2\pi}}\int ds:\exp\left[-\frac{s^2}{2}+\sqrt{-a_t C}s(\psi^\dagger\psi)\right]:$$

- 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. ⟸**No *N*-*N* interaction**

Solve a general Hamiltonian with 5 steps:

1. Rewrite expression into a path integral
2. For each field configuration, calculate the amplitude.
3. Integrate out the field variables using Monte Carlo algorithms.
4. Take the limit $\tau \to \infty$
5. Take the limit $L \to \infty$





Quantum Monte Carlo

- Solve **quantum many-body problem** using **stochastic sampling**
  - Optimization in high-dimensional parameter space ← e.g., neuron network
  - High-dimensional integrals
- QMC methods for condensed matter, nuclear physics, atomic-molecular physics, high-energy physics, etc.
- Compute integrals using **importance sampling**

$$S = \int_a^b f(x)dx = \int_a^b p(x)\frac{f(x)}{p(x)}dx = E_{x\sim p(x)}[\frac{f(x)}{p(x)}]$$

- Key point: Generate a set of samples with probability distribution *p(x)*
- If *p(x)* is simple (e.g., Gaussian, uniform, etc.), direct sampling
- If *p(x)* is complex, use **Metropolis algorithm**

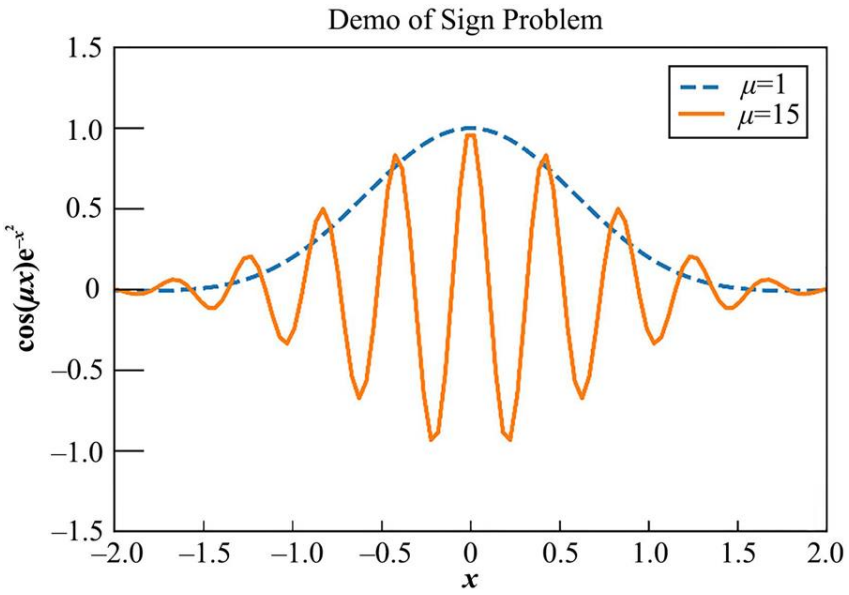
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Sign problem in quantum Monte Carlo

$$\frac{\int f(x)dx}{\int g(x)dx} = \frac{\int |g(x)| \frac{f(x)}{|g(x)|} dx}{\int |g(x)| \frac{g(x)}{|g(x)|} dx} = \frac{\left\langle \frac{f(x)}{|g(x)|} \right\rangle_{p(x)\propto|g(x)|}}{\left\langle \frac{g(x)}{|g(x)|} \right\rangle_{p(x)\propto|g(x)|}}$$

- **Sign** problem arises for **repulsive interactions** or **unbalanced fermions**
  - Coulomb interaction
  - Hard core in NN potentials
  - Tensor forces
  - Three-body forces
  - Unpaired pinholes
  - …
- Very few interactions and systems can be simulated directly
  - Large statistical errors
  - Signal-noise issue
  - Bad scaling → errors increase exponentially with system size
  - No universal solution → NP-hard problem M. Troyer and U.-J. Wiese, PRL94, 170201 (2005)

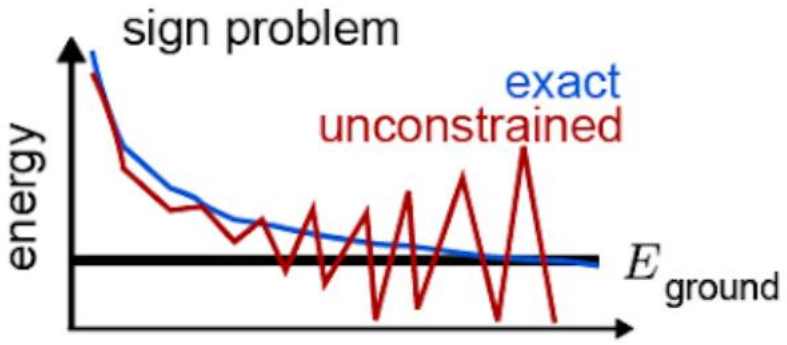


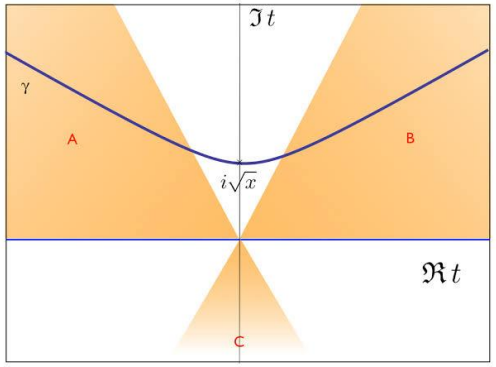


Sign problem in quantum Monte Carlo

- **Quantum Monte Carlo** transform the **quantum many-body problems** into **high-dimensional integrals**
- QMC Statistical error ~$O(N^{-1/2})$ ← **Polynomial scaling!**

- **Sign problem** occurs when the integrand is **NOT** positive definite
- **Sign problem scales exponentially** with particle number
  - Solutions: Constrained-path, fixed-nodes, Lefschetz thimble, etc.
  - Rely on approximations or induces systematic biases
    ← **Not exact even with infinite number of samples!**





No-free-lunch theorem

Examples of sign-problem-free QMC

Sign-problem-free algorithms exist but mostly confined to specific models

- **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)

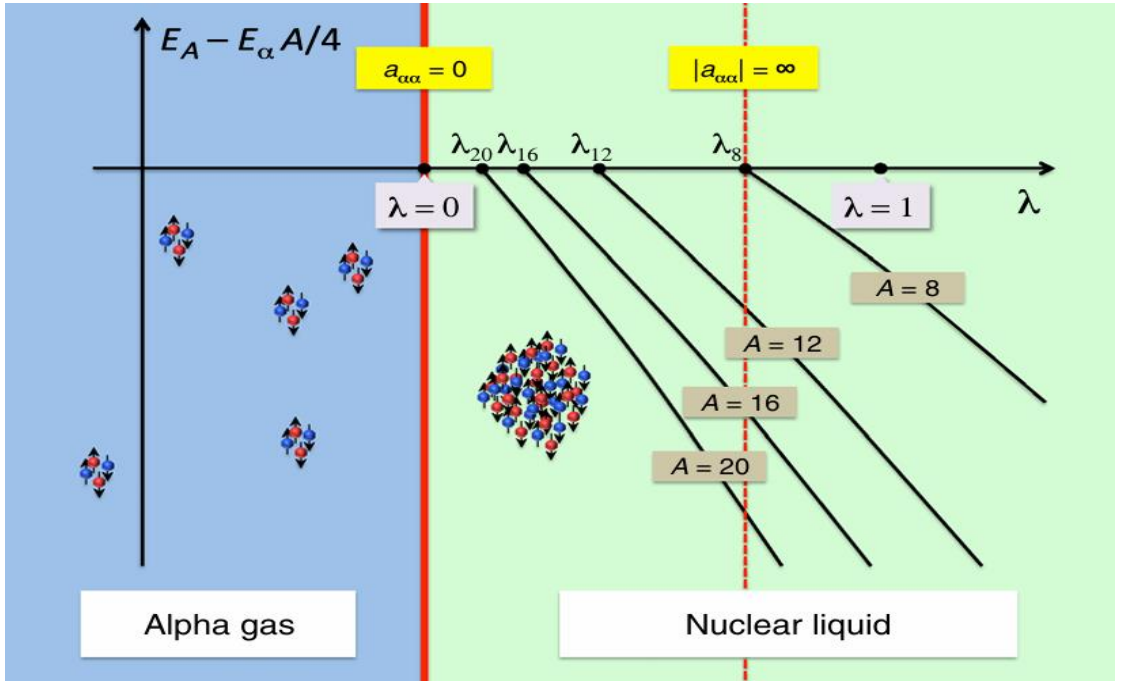
Nuclear binding near a quantum phase transition

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

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

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

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



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)

“Essential element” Hamiltonian as zeroth order

- **Wigner-SU(4) symmetry** + **paired fermions**
  = Immunity to sign problem
  Wigner, Phys. Rev. 51, 106 (1937)

- Also inspired by the **unexpected effectiveness** of the **locality** in nuclear forces
  Elhatisari et al., PRL 117, 132501 (2016)

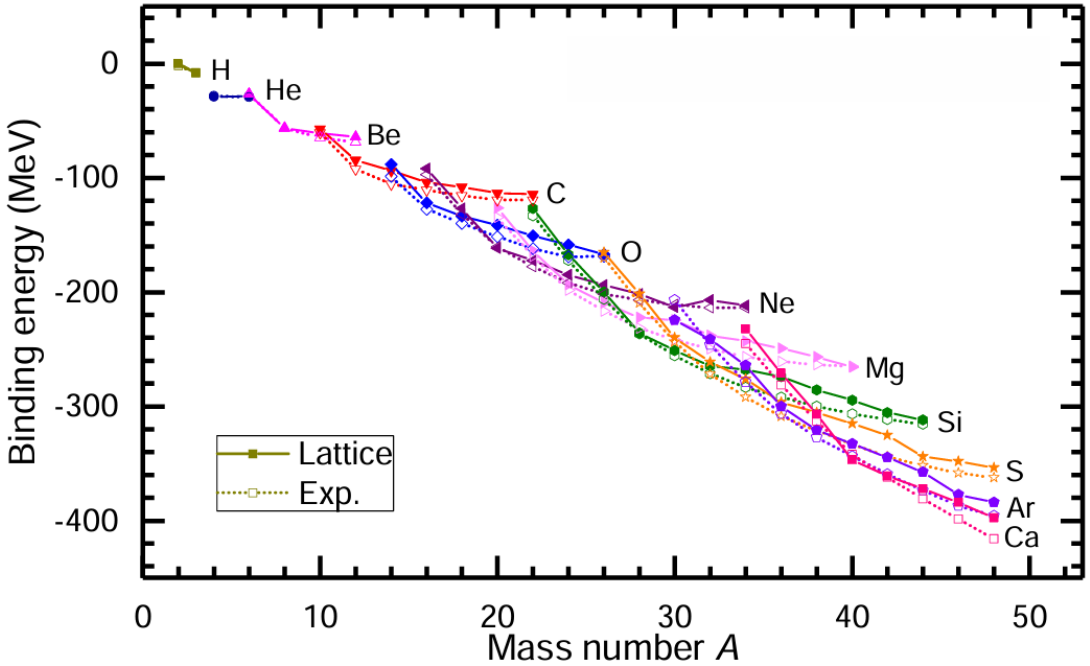
$$H_{\mathrm{SU}(4)} = H_{\mathrm{free}} + \frac{1}{2!}C_2 \sum_{\boldsymbol{n}} \tilde{\rho}(\boldsymbol{n})^2 + \frac{1}{3!}C_3 \sum_{\boldsymbol{n}} \tilde{\rho}(\boldsymbol{n})^3$$

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

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

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

BNL et al., PLB 797, 134863 (2019)

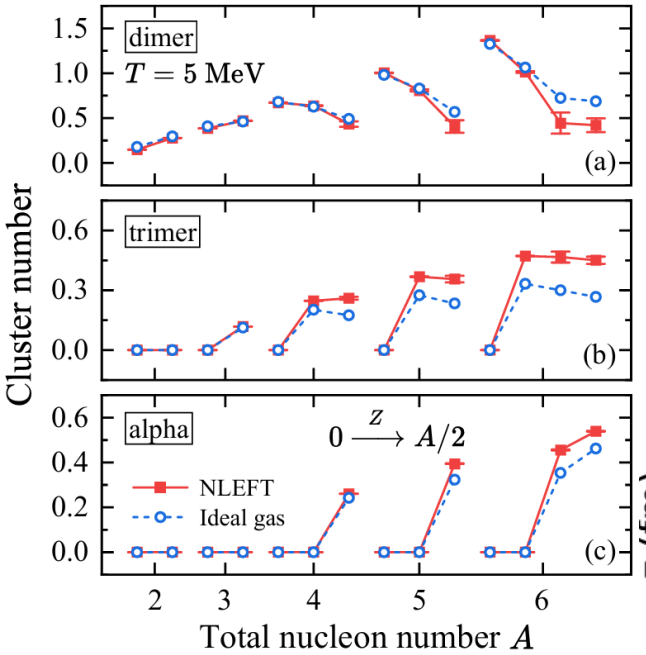


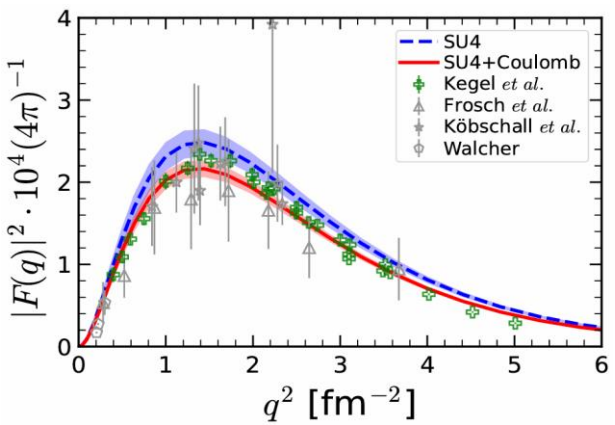
Applicable in nuclear spectroscopy, clustering, thermodynamics, electromagnetic transition, ⋯

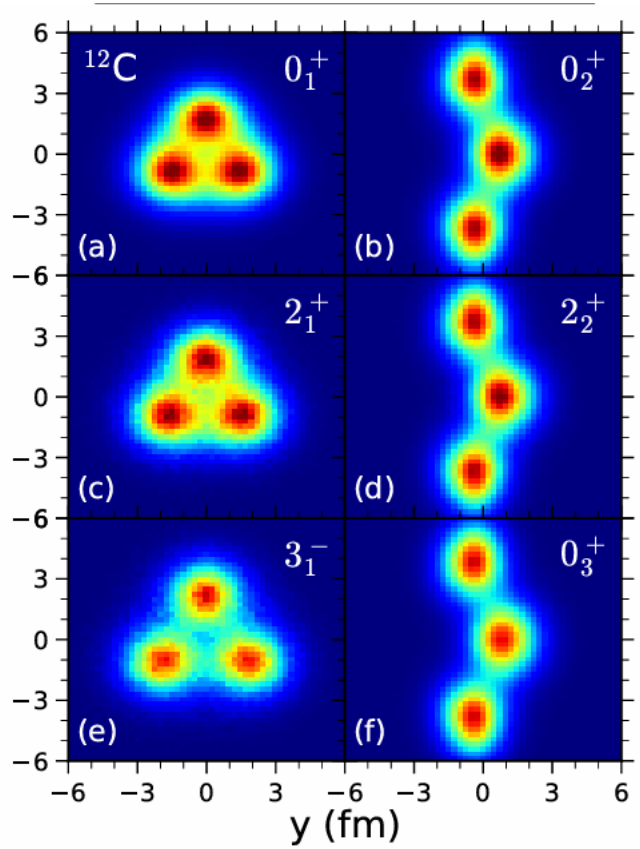
pros: non-perturbative, small statistical errors
cons: low-fidelity, large theory uncertainties

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)
-

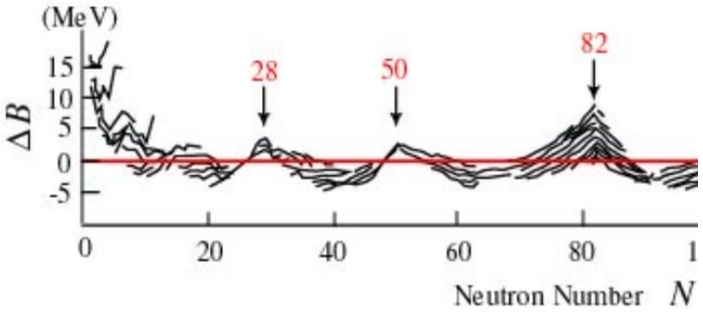






Improved Wigner-SU(4) interaction

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



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

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

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

- **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

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

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

$$M(c) = \exp\left[\sum_{\boldsymbol{n},\boldsymbol{n}'}a_t\frac{\Psi^\dagger(\boldsymbol{n})\nabla^2_{\boldsymbol{n}\boldsymbol{n}'}\Psi(\boldsymbol{n}')}{2M} + \sum_{\boldsymbol{n}}\sqrt{-a_tC_2}c(\boldsymbol{n})\left(\overline{\rho}(\boldsymbol{n}) + \frac{C_s}{2C_2}\overline{\rho}_s(\boldsymbol{n})\right)\right]$$

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

- 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:

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

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

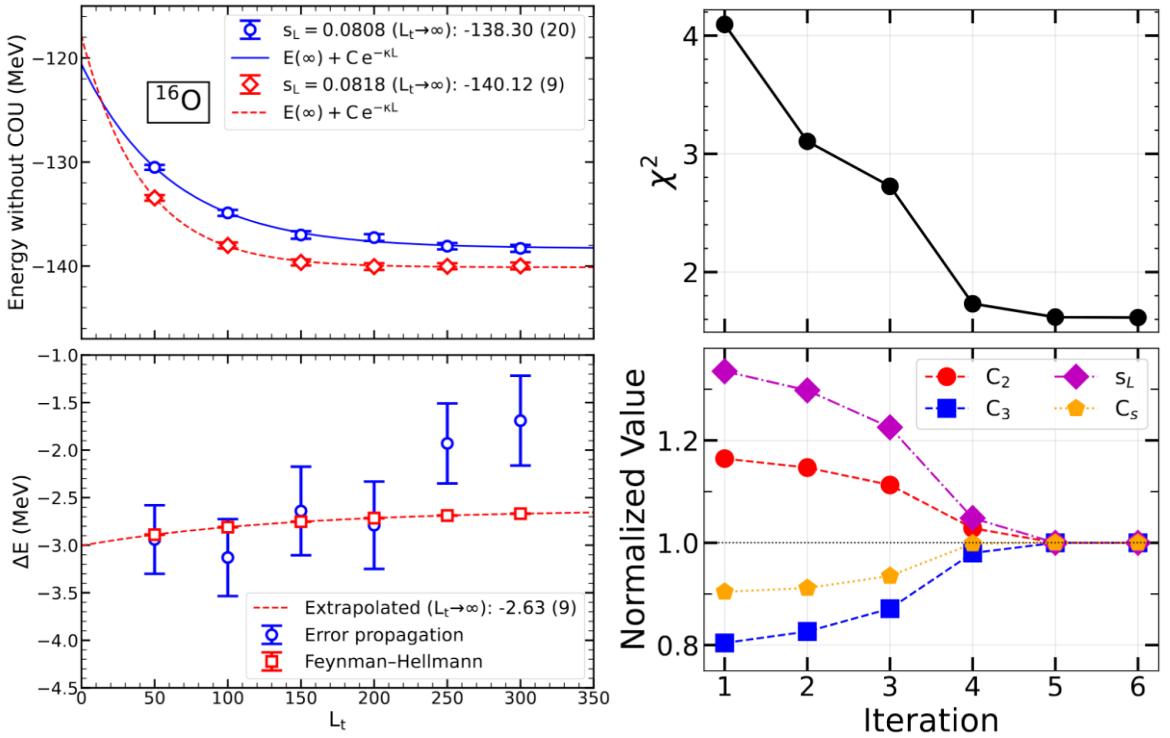
$$\chi^2 = \sum_A \left[\frac{E(A) - E_{\rm exp}(A)}{\Delta(A)} \right]^2$$

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

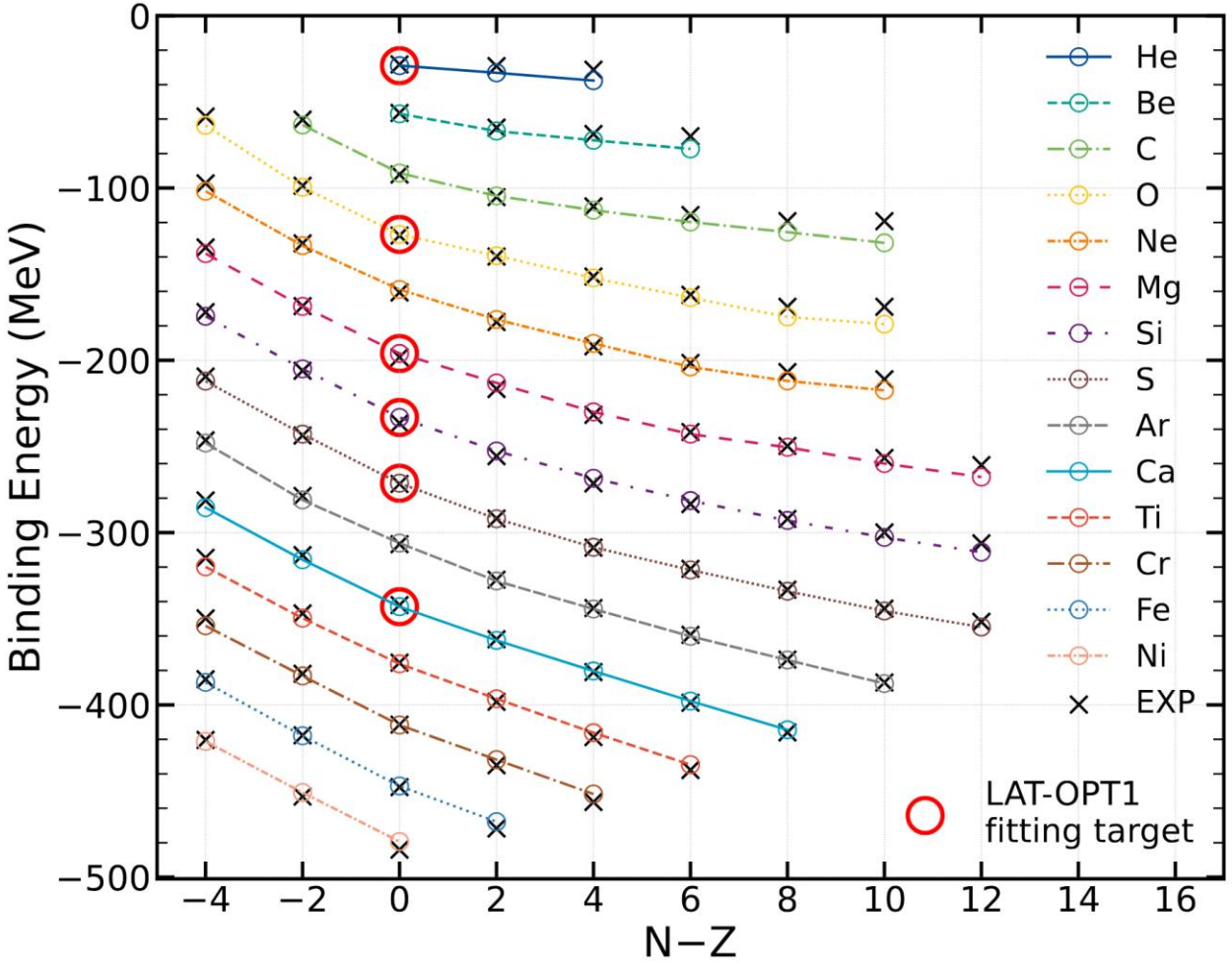
$$\partial E(A)/\partial x = \langle \Phi | H(x+\delta) - H(x) | \Phi \rangle / \delta$$

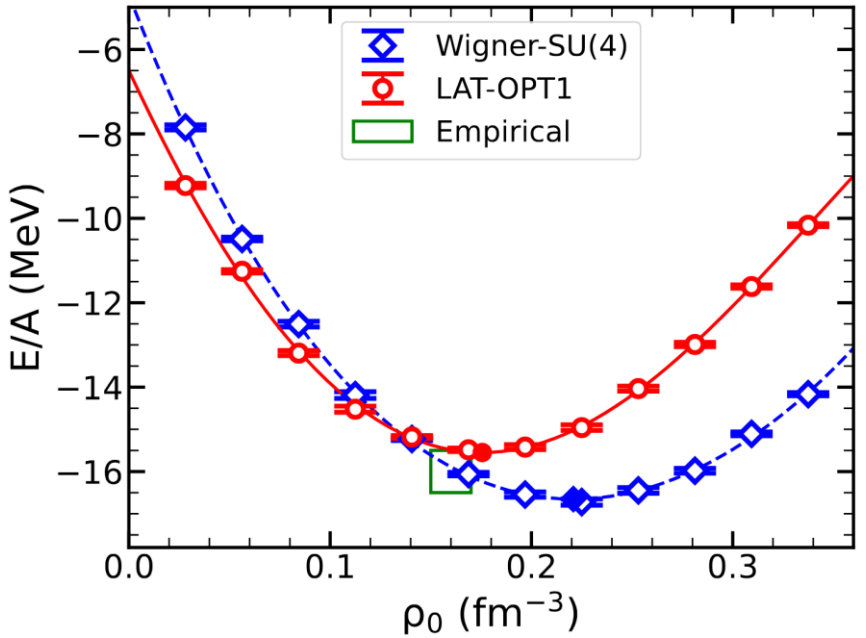
- Typically converge within 10 iterations
  ← **precise and unbiased** derivative computation is essential!

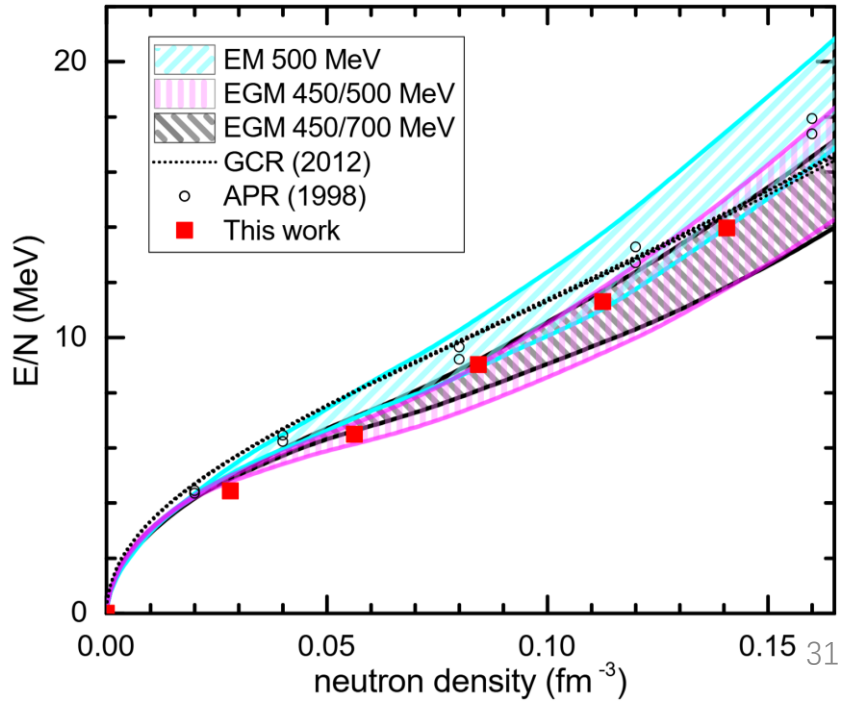
$C_2 = -4.410 \times 10^{-7}$ MeV^{-2}, $C_3 = 1.561 \times 10^{-15}$ MeV^{-5}, $C_s = 8.590 \times 10^{-12}$ MeV^{-4}, $s_{\rm L} = 0.081$, $s_{\rm NL} = 0.45$ "LAT-OPT1"



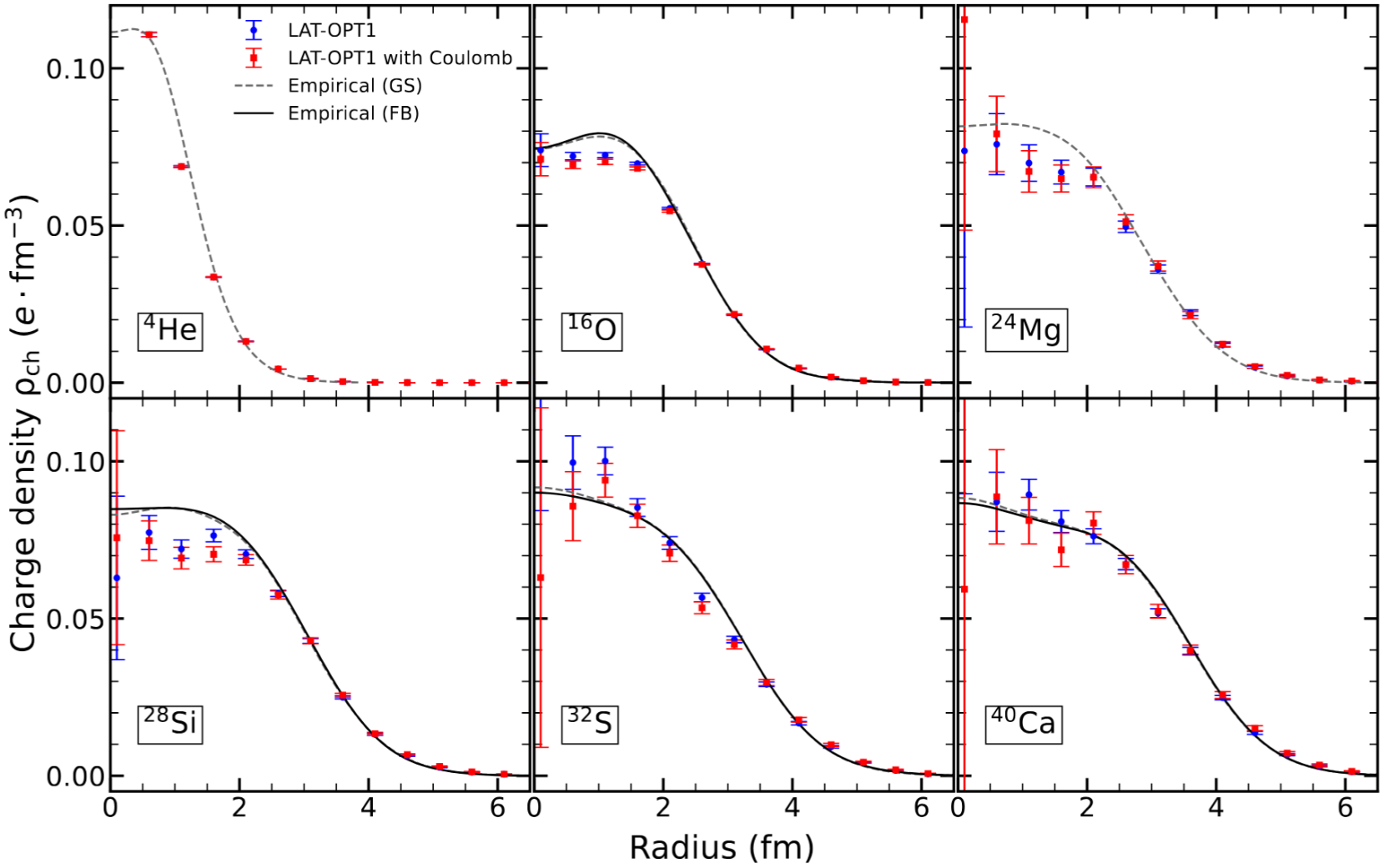
Results from LAT-OPT1







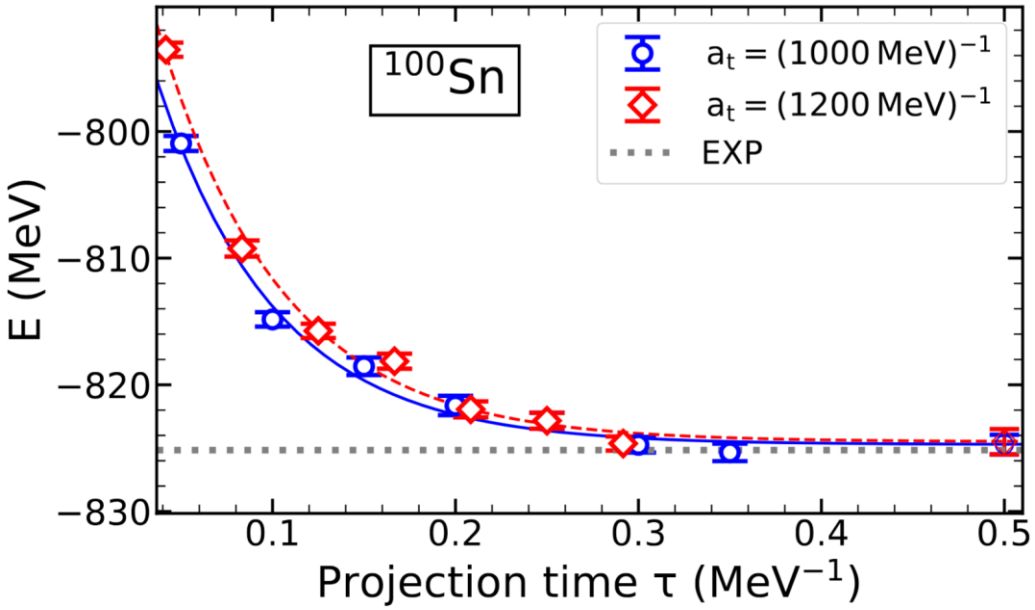
Results from LAT-OPT1: Charge densities



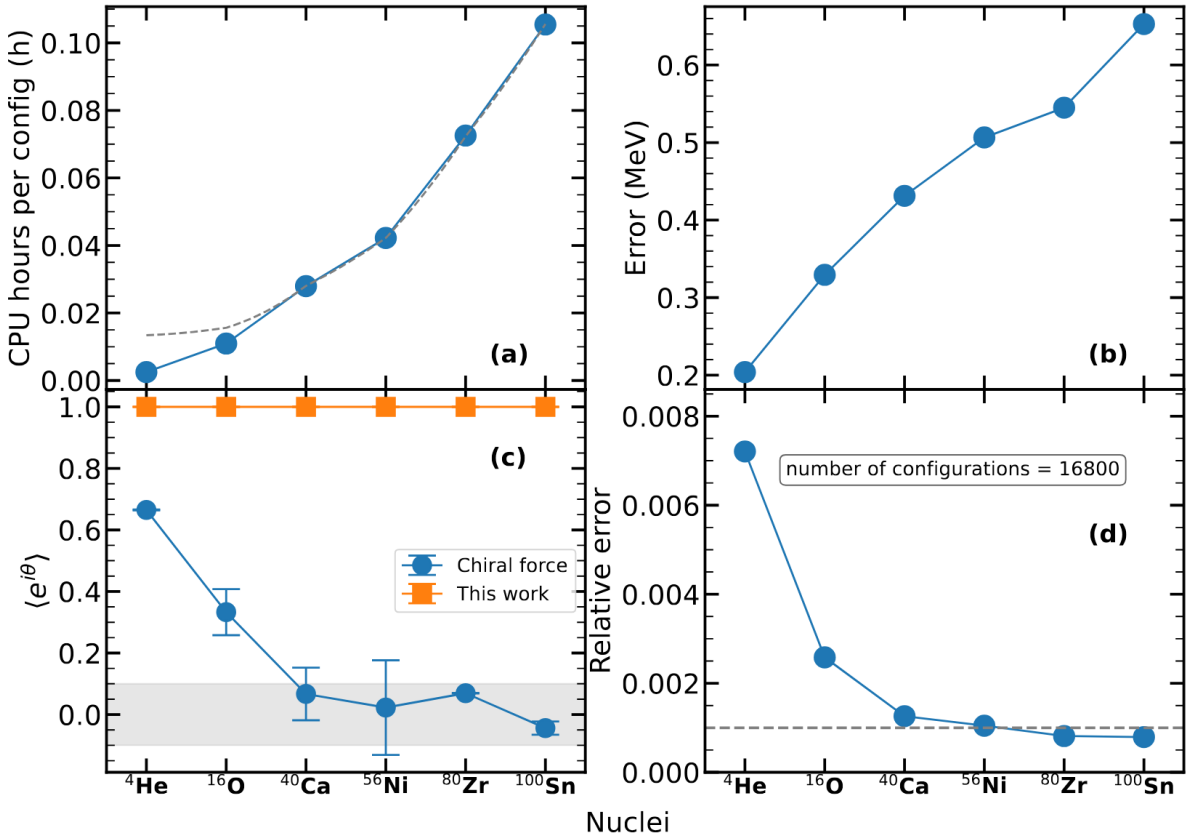
- Charge densities calculated using **pinhole algorithm**
  Elhatisari et al., PRL119, 222505 (2017)
- **Pinhole algorithm** induce **mild sign problem**, not available for A>=40. See **partial pinhole algorithm** for a solution
  Zheng-Xue Ren et al., PRL135-152502 (2025)

Results from LAT-OPT1: Heavy nuclei

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

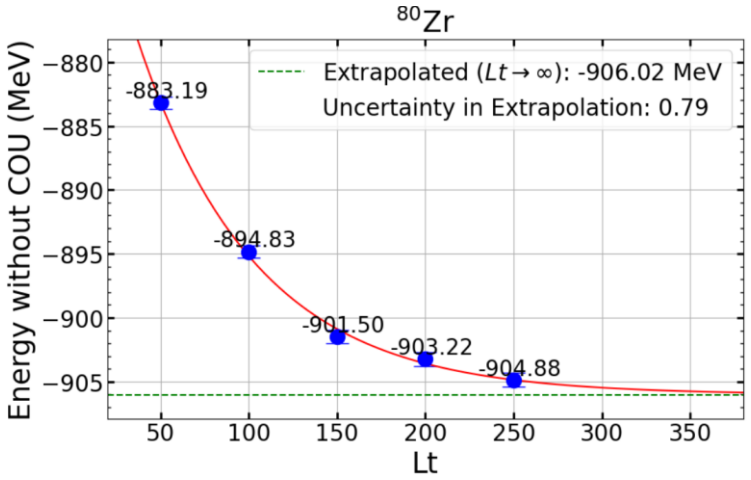


Extract binding energy of ^{100}Sn with **~1 MeV precision** using **~30000 CPU hours**
(10 days on AMD EPYC 9554@3.1GHz, 128 CPU cores)



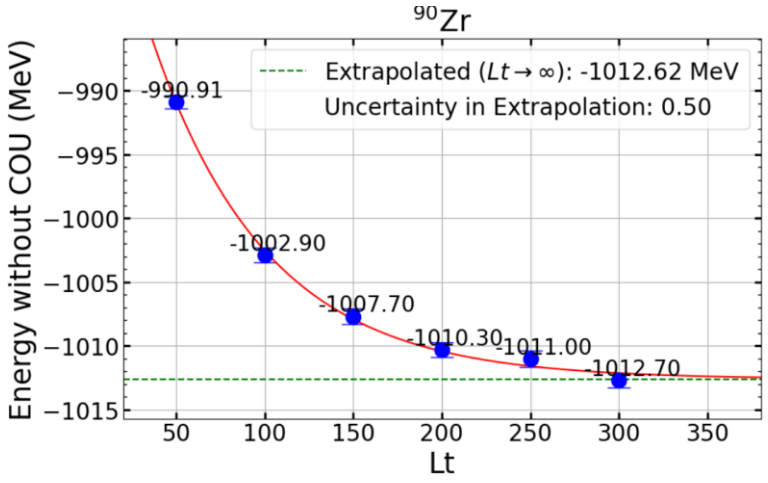
Relative errors <0.1% for heavy nuclei

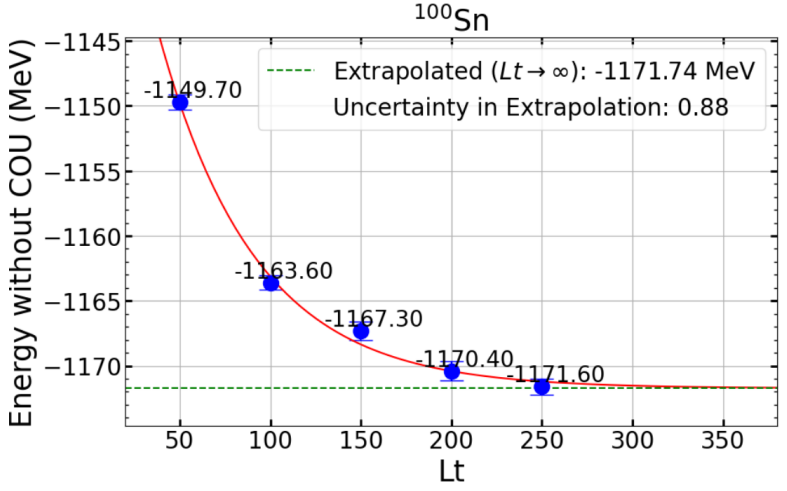
Results from LAT-OPT1: Heavy nuclei

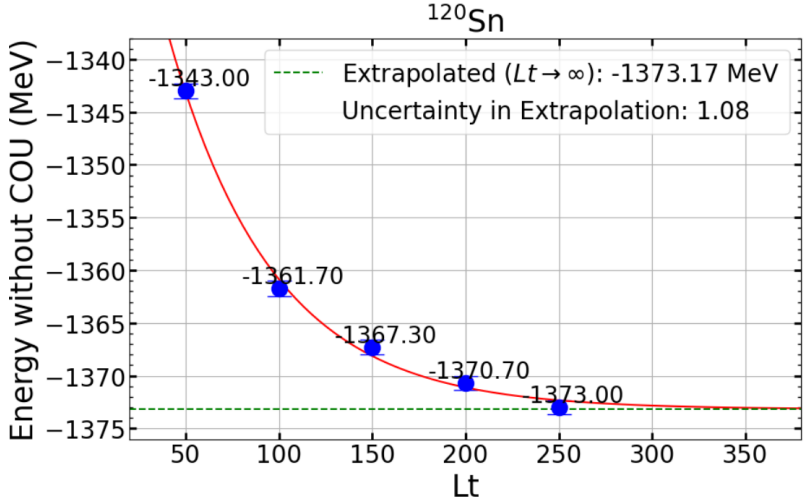


Nucleus	$E_{\rm bind}$ (MeV)	$E_{\rm sl}$ (MeV)	$E_{\rm sl}/E_{\rm bind}$	EXP (MeV)
^{4}He	$-29.0(2)$	-0.3	0.010	-28.3
^{12}C	$-91.3(1)$	-13.3	0.146	-92.2
^{14}C	$-104.6(1)$	-12.7	0.121	-105.3
^{16}O	$-126.9(2)$	-5.6	0.044	-127.6
^{40}Ca	$-343.0(2)$	-13.6	0.040	-342.1
^{48}Ca	$-414.5(3)$	-42.3	0.102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







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

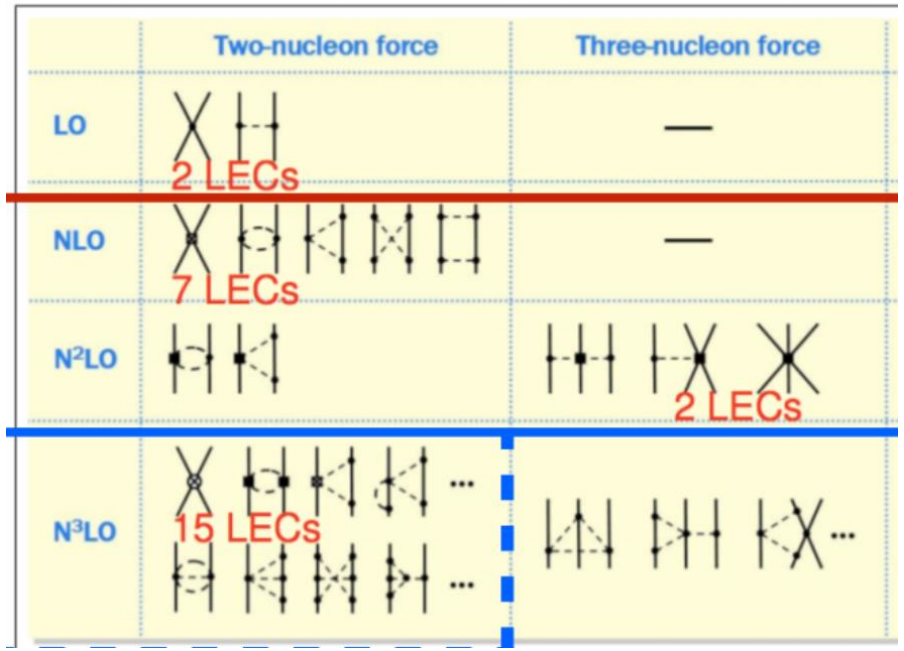
Model	Parameterization	Parameters	σ (MeV)	Nuclei	σ_{all} (MeV)
Macroscopic-microscopic	FRDM [9]	> 30	1.15	69	0.56
Relativistic mean field	PC-PK1 [10]	11	2.25	60	1.52
Skyrme DFT	UNEDF1 [11]	12	3.43	75	1.91
Lattice EFT	Wigner-SU(4) [1]	4	10.21	55	—
Lattice EFT	LAT-OPT1	5	2.93	76	—

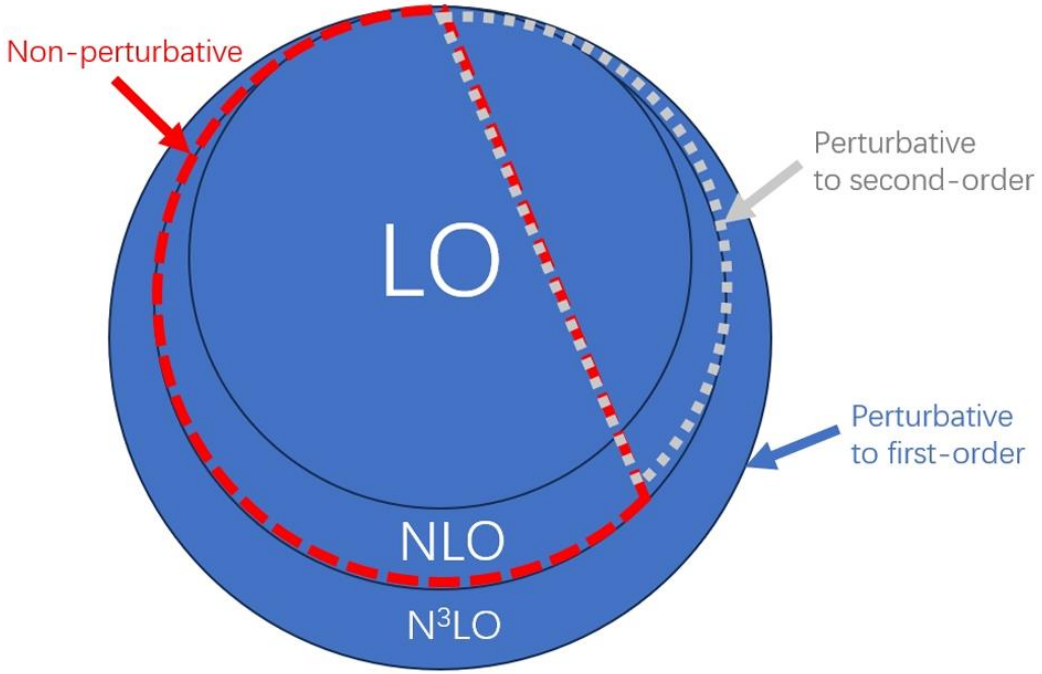
Contents

- Introduction to Nuclear Lattice Effective Field Theory
- Non-perturbative QMC and sign problem
- **Perturbative QMC**
- Renormalization of NLEFT
- Ab initio nuclear thermodynamics
- Summary and perspective

Go beyond leading order

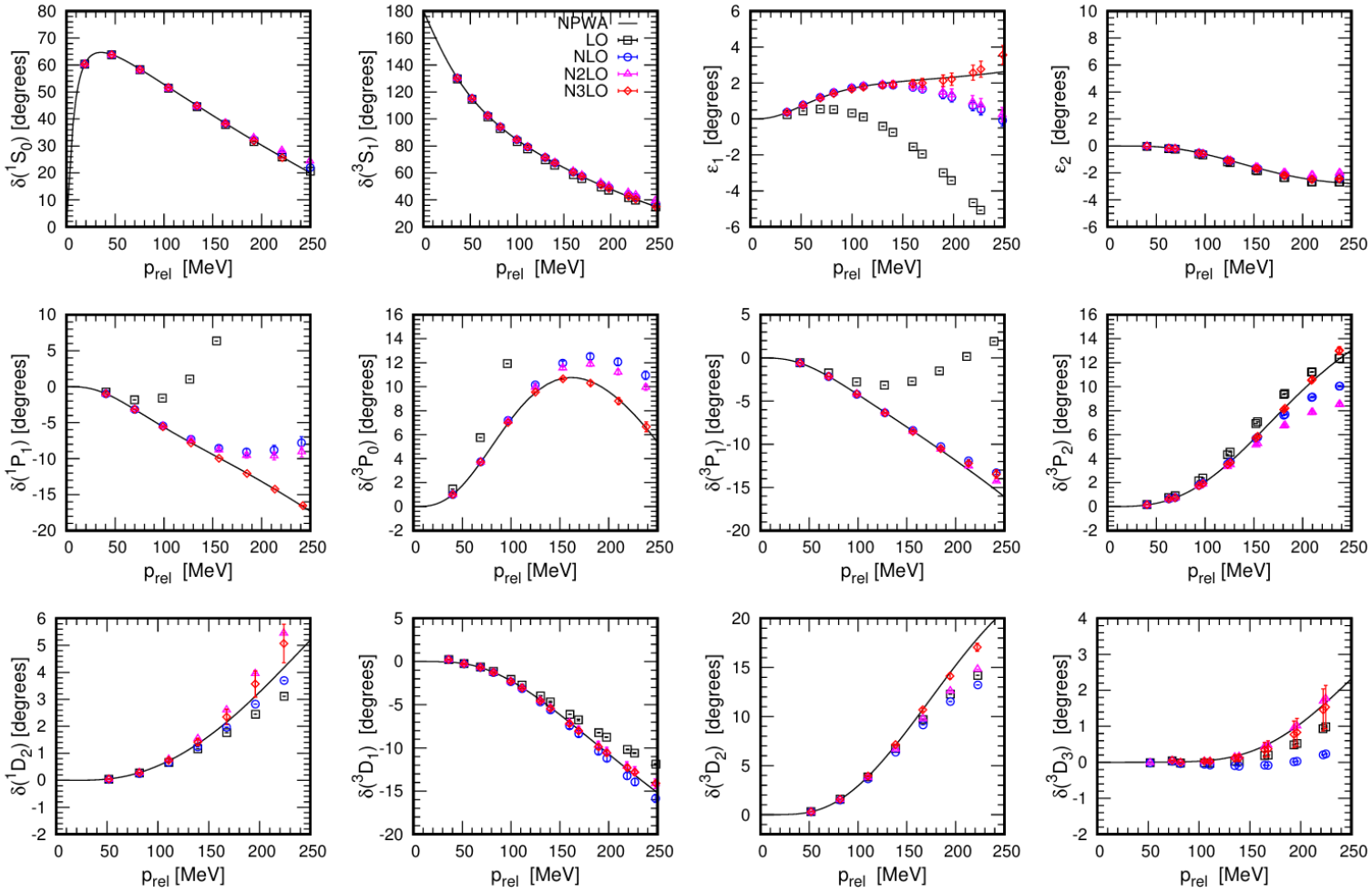
- Complicated structures of the nuclear forces can be included using perturbation theory





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

Precision lattice chiral nuclear forces



Lattice chiral forces determined with A≤3

- Fit to NN phase shifts at **NLO**
  Borasoy et al., EPJA 35, 343 (2008)
- Fit **three-body forces** to triton
  Epelbaum et al., EPJA 41, 125 (2009)
- Precision method for mixing angles
  BNL et al., PLB 760, 309 (2016)
- Fit to NN phase shifts at **N2LO**
  Alarcon et al., EPJA 53, 83 (2017)
- Fit to NN phase shifts at **N3LO**
  Li et al., PRC 98, 044002 (2018)

Pion-exchange potentials are taken from the continuum expressions
Reinert et al., EPJA 54, 86 (2018)

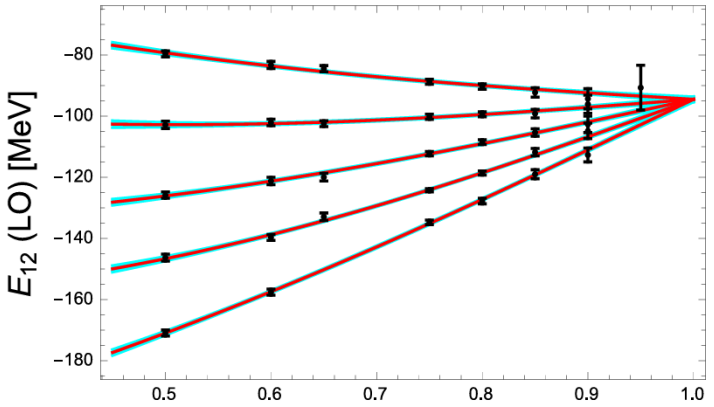
Circumvent sign problem in NLEFT

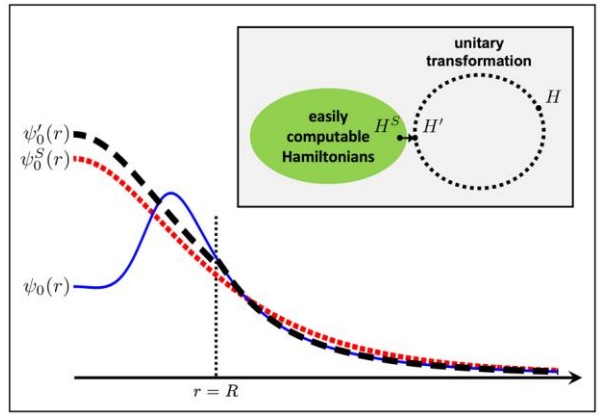
Sign problem is severe for **fermionic systems**

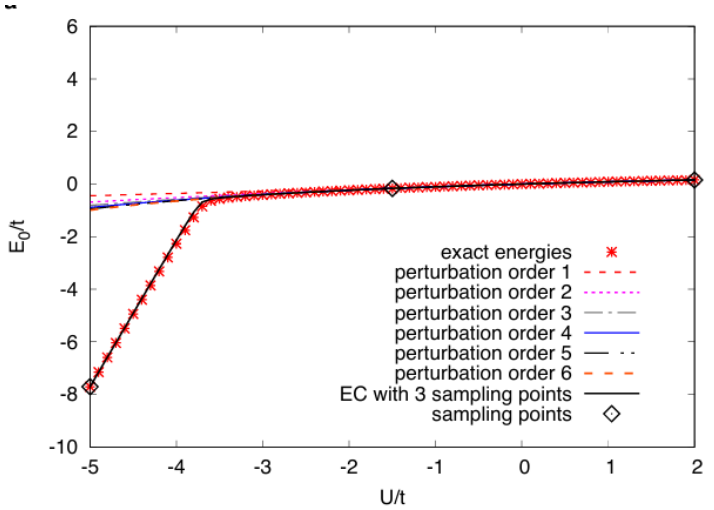
Conventional approach:
Hamiltonian without sign problem (e.g., SU4)
+ first order perturbation theory
Borasoy et al., EPJA 31, 105 (2007)

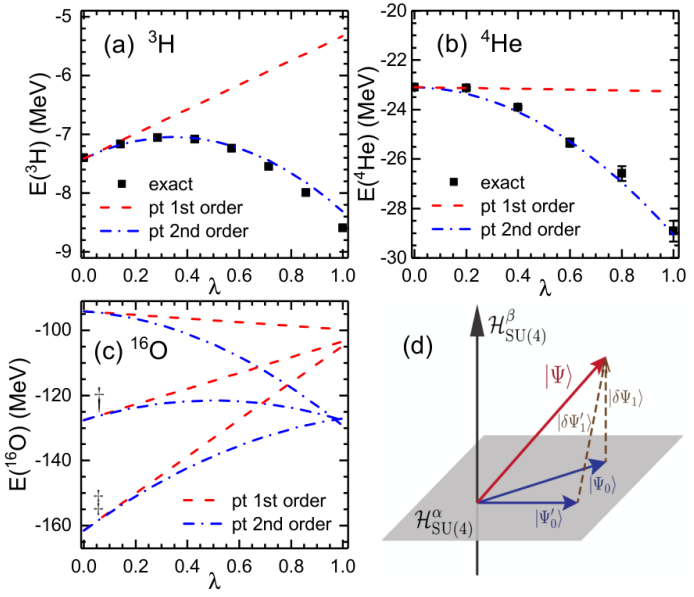
Go beyond the 1st order perturbation theory:

- Symmetry-Sign extrapolation
  Lähde et al., EPJA 51, 92 (2015)
- Eigenvector continuation
  Frame et al., PRL121, 032501 (2018)
- Perturbative quantum Monte Carlo method
  Lu et al., PRL 128, 242501 (2022)
- Wave function matching method
  Elhatisari et al., Nature 630, 59 (2024)
- Rank-one operator method
  Ma et al., PRL 132, 232502 (2024)

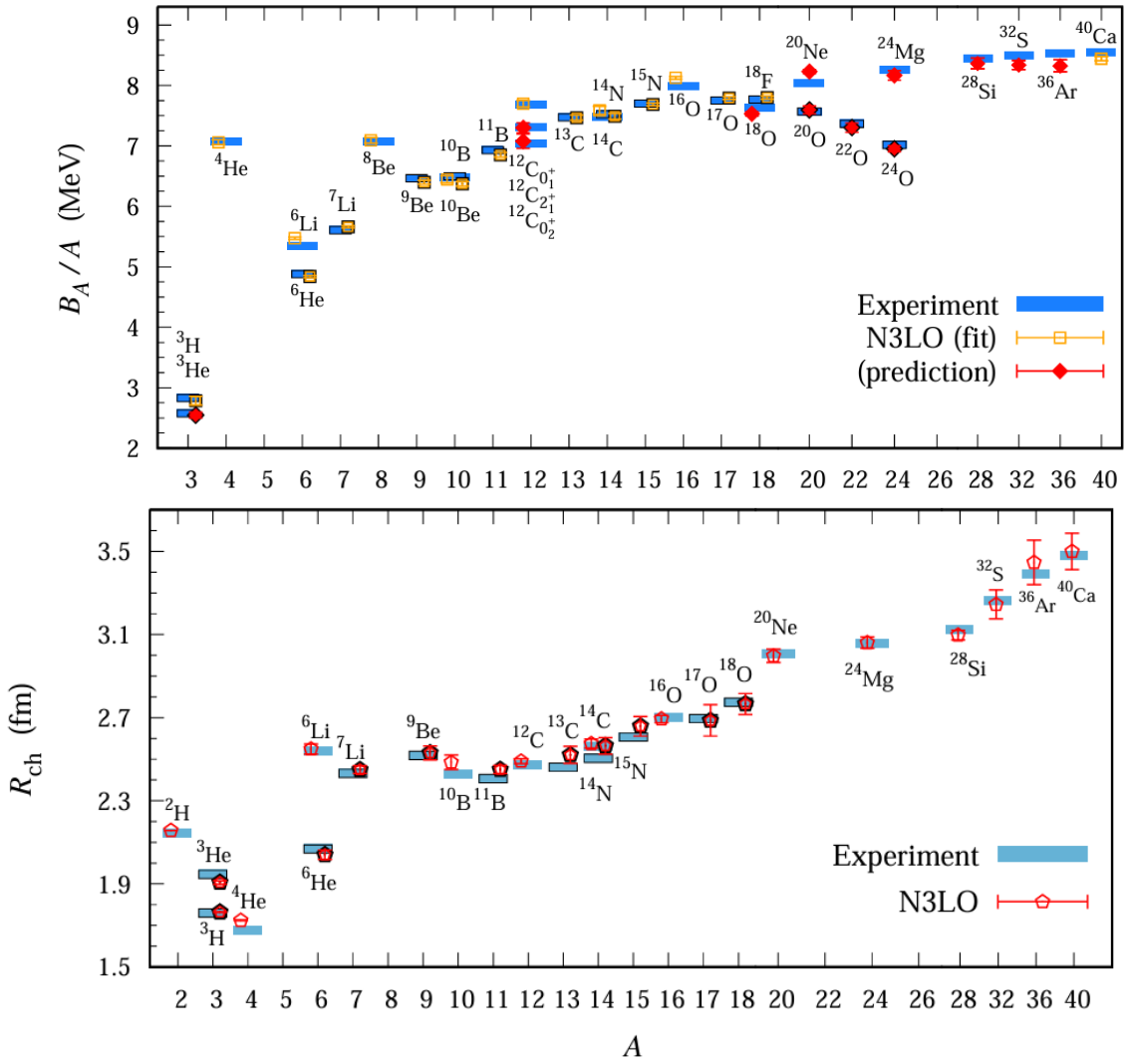


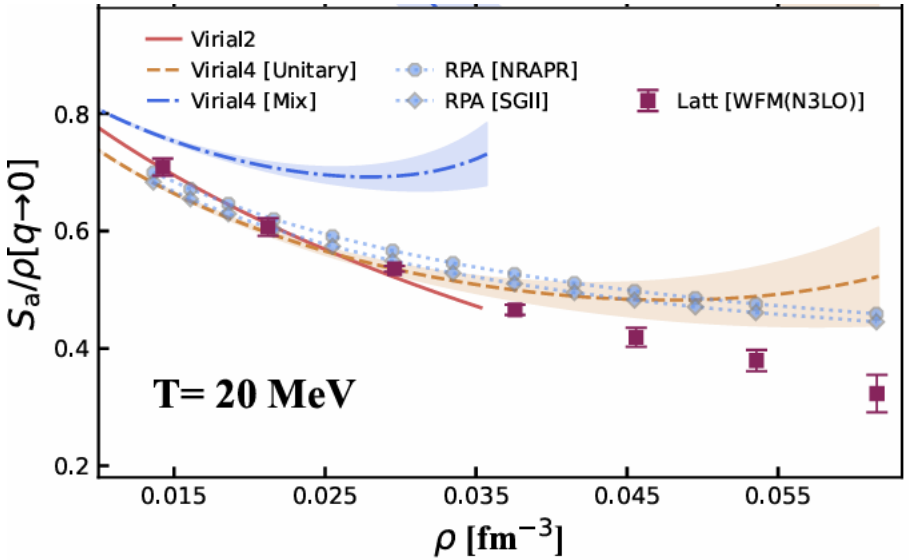






Calculations with high-fidelity nuclear forces

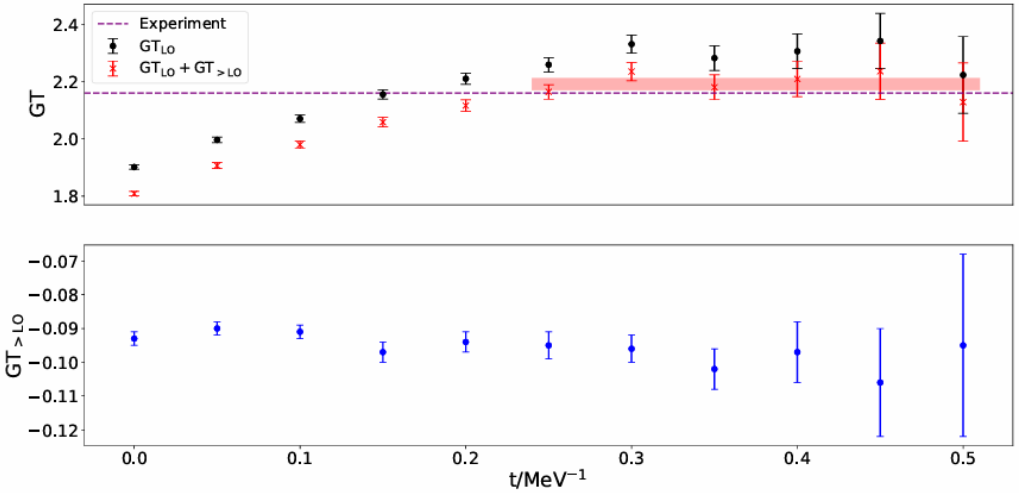


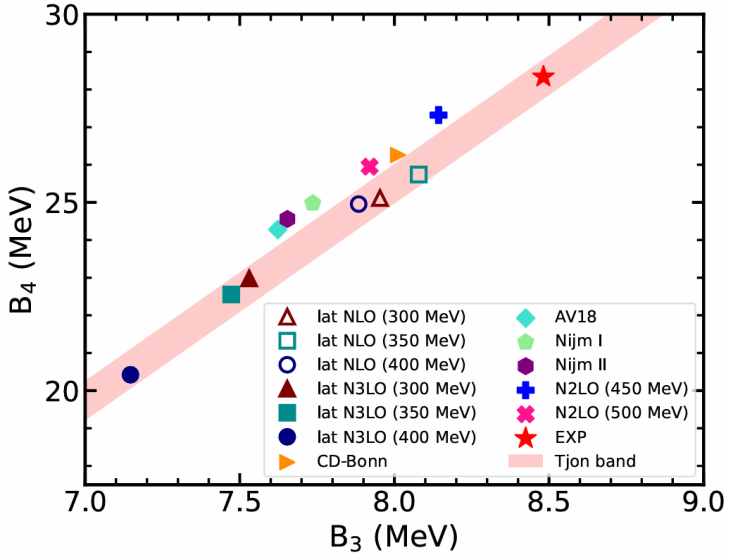


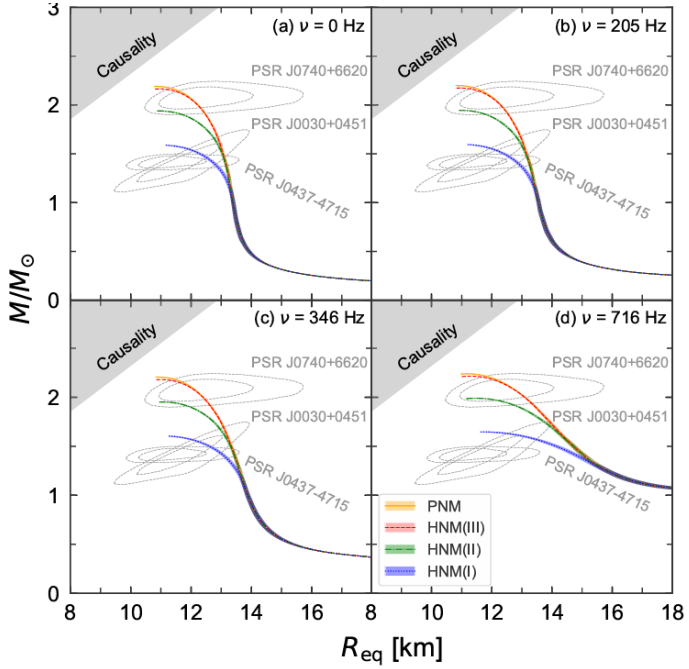
Calculations with N^{3}LO chiral forces:

- 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





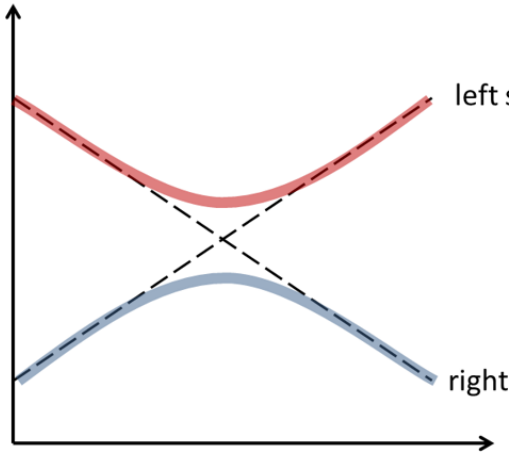


Calculations with N^{3}LO chiral forces (continued):

- 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 ^{6}He
  T. Wang et al., 2503.23840 (2025)

Limitations of first order perturbation theory

- In these cases, we should **not** trust the first order perturbation theory and need to go beyond:
  - First order corrections are too large
  - Hard-core interactions with soft zeroth order
  - States near the bound-continuum threshold
  - Explicit symmetry breaking due to perturbations
  - Near the level crossing



- For improving the precision, we also need higher-order corrections
- Conventional **Rayleigh-Schrödinger perturbation theory** is not applicable for **projection Monte Carlo calculations**

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

Excited states expensive in NLEFT

Perturbative quantum Monte Carlo

- Expand the projected ground states:

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

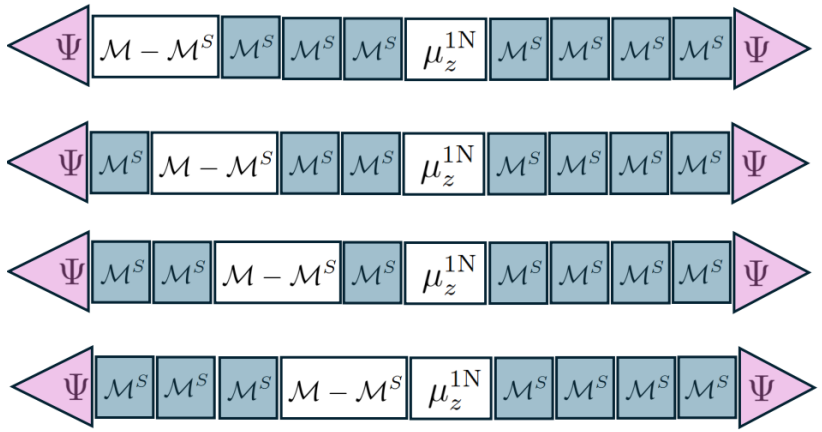
$$|\Psi_0\rangle = \lim_{L_t\to\infty} M_0^{L_t/2}|\Psi_T\rangle,$$

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

- The normalized wave function:

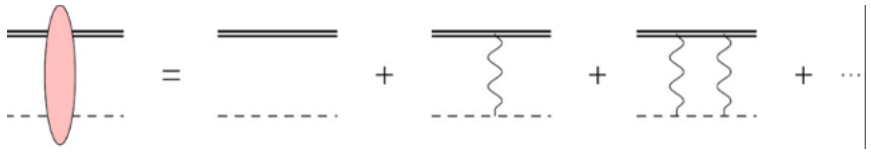
$$|\Psi'\rangle = \frac{|\Psi\rangle}{\sqrt{\langle\Psi|\Psi\rangle}} = \frac{|\Psi_0\rangle}{\sqrt{\langle\Psi_0|\Psi_0\rangle}} + \frac{1}{\sqrt{\langle\Psi_0|\Psi_0\rangle}} \times \left[|\delta\Psi_1\rangle - \frac{\mathrm{Re}\langle\Psi_0|\delta\Psi_1\rangle}{\langle\Psi_0|\Psi_0\rangle}|\Psi_0\rangle\right] + \mathcal{O}(V_C^2)$$

BNL et al., PRL 128, 242501 (2022)



.....

Courtesy of Teng Wang

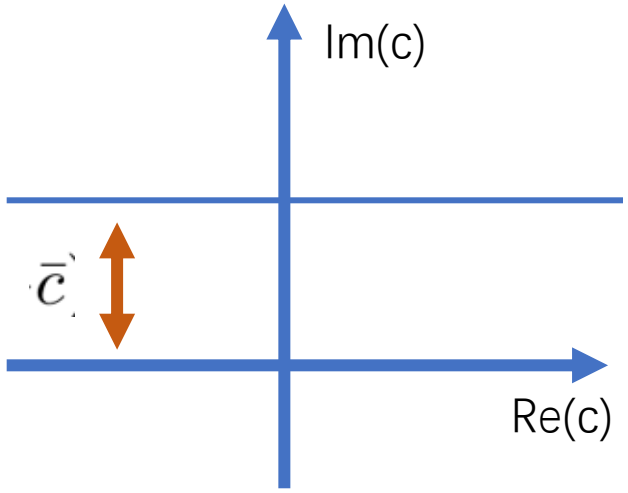


(Imaginary) time-dependent perturbation theory

Evaluation of partial amplitudes

- The partial amplitudes can be evaluated using contour integral

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



- Integral contour shifted with a field

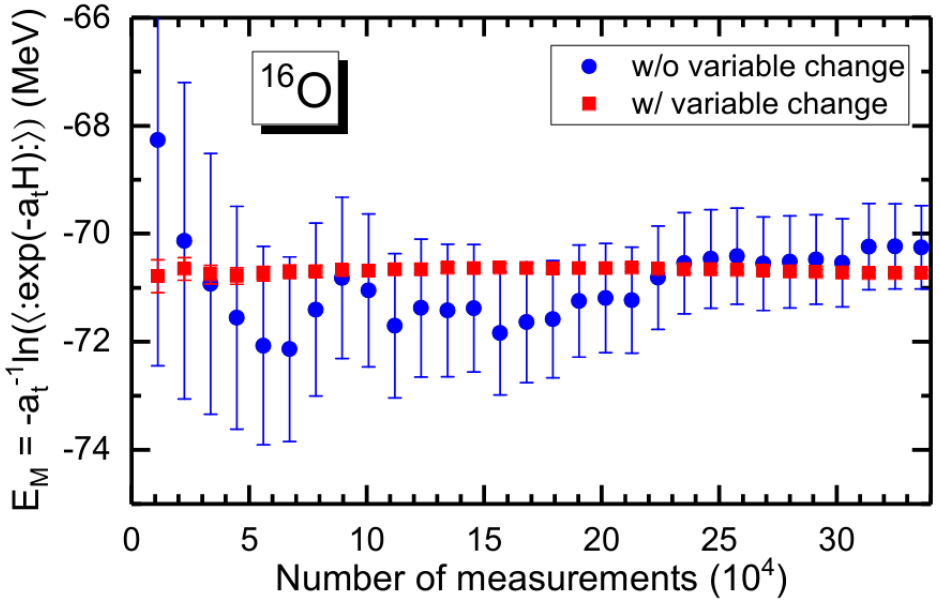
$$\begin{aligned}\bar{c}(\boldsymbol{n}) &= \frac{\partial}{\partial c(\boldsymbol{n})} \ln \langle \cdots M(s_k, c) \cdots \rangle_T \Big|_{c=0} \\ &= \sqrt{-a_t C} \langle \cdots : M_0(s_k) \rho_c(\boldsymbol{n}) : \cdots \rangle_T / \mathcal{M}(1)\end{aligned}$$

$$P(c+\bar{c}) = \exp\left[-(c+\bar{c})^2/2\right]$$
$$M(c+\bar{c}) \approx \exp\left[\bar{c}(c+\bar{c})\right]$$

Linear term in *c* causing sign problem is canceled out

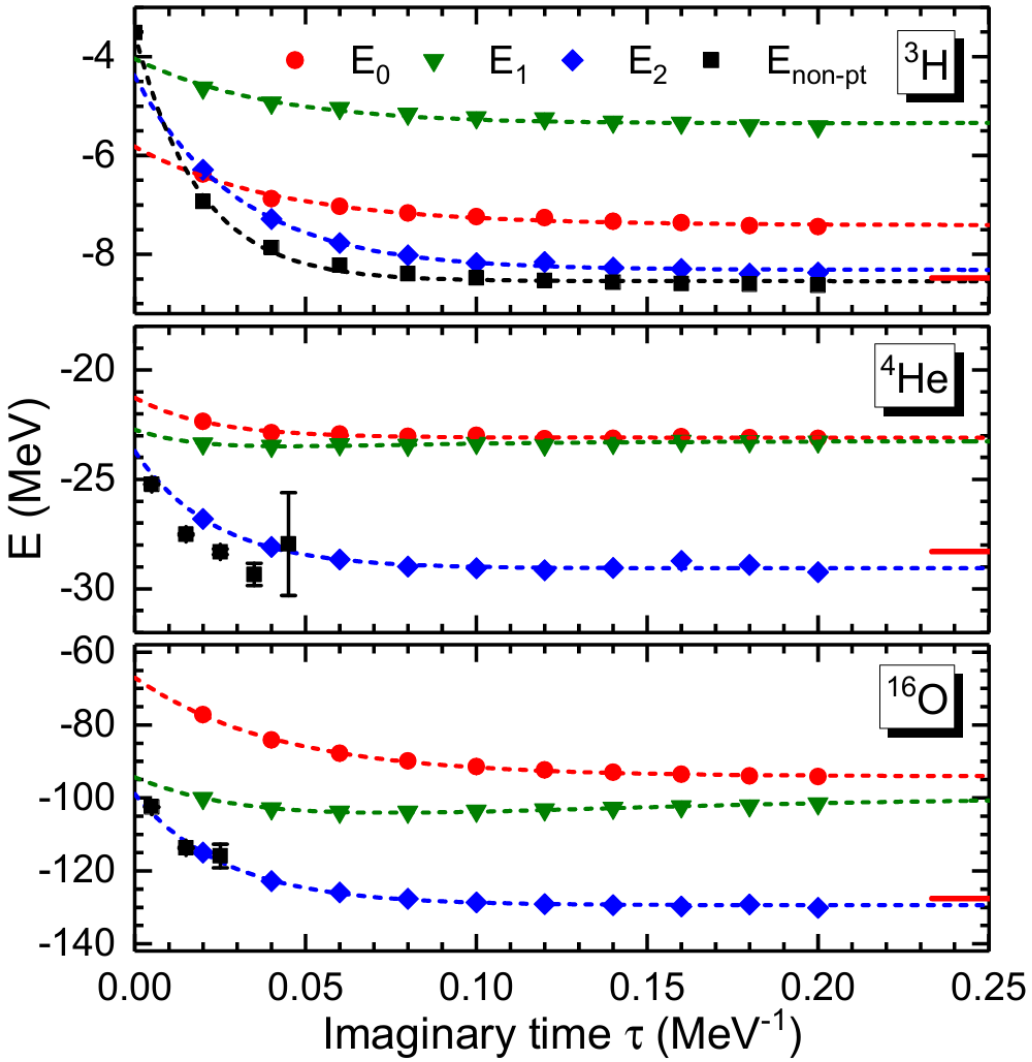
Evaluation of energy corrections

- Complex contour shift reduces statistical errors by more than one order



- Energy corrections at large τ accessible now

$$E_0 = \langle\Psi_0|(K+V_0)|\Psi_0\rangle/\langle\Psi_0|\Psi_0\rangle,$$
$$\delta E_1 = \langle\Psi_0|V_C|\Psi_0\rangle/\langle\Psi_0|\Psi_0\rangle,$$
$$\delta E_2 = \mathrm{Re}(\langle\Psi_0|V_C|\delta\Psi_1\rangle - \delta E_1\langle\Psi_0|\delta\Psi_1\rangle)/\langle\Psi_0|\Psi_0\rangle$$



Partial energy contributions

$$V_{2N} = \Big[B_1 + B_2(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2) + C_1 q^2 + C_2 q^2(\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)$$
$$+ C_3 q^2(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2) + C_4 q^2(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)(\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)$$
$$+ C_5\frac{i}{2}(\boldsymbol{q}\times\boldsymbol{k})\cdot(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2) + C_6(\boldsymbol{\sigma}_1\cdot\boldsymbol{q})(\boldsymbol{\sigma}_2\cdot\boldsymbol{q})$$
$$+ C_7(\boldsymbol{\sigma}_1\cdot\boldsymbol{q})(\boldsymbol{\sigma}_2\cdot\boldsymbol{q})(\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)\Big] f_{2N}(p_1,p_2,p_1',p_2')$$
$$- \frac{g_A^2 f_\pi(q^2)}{4F_\pi^2}\left[\frac{(\boldsymbol{\sigma}_1\cdot\boldsymbol{q})(\boldsymbol{\sigma}_2\cdot\boldsymbol{q})}{q^2+M_\pi^2} + C_\pi'\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\right](\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)$$

- Target interaction = NLO two-body contact terms
  + One-Pion-Exchange Potential
  + N2LO three-body c_E term
  + Coulomb force

  All determined for $A \leq 3$

- Zeroth order interaction = "essential element"

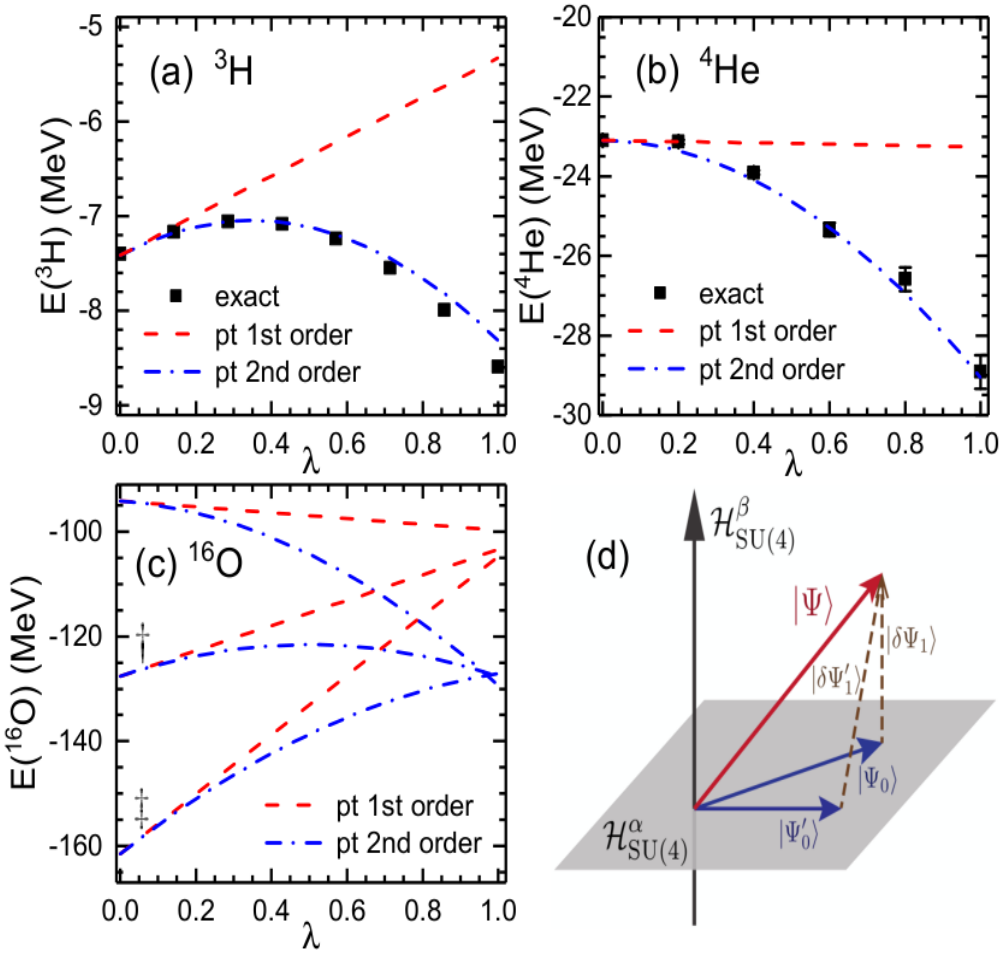
  $H_{\mathrm{N2LO}} = H_{SU4} + (H_{\mathrm{N2LO}} - \mathrm{H}_{SU4})$

- With different strength of the zeroth order interaction, ^{16}O converge to the same energy

- Large second order corrections, account for 20% of total energies. Unusual. Anything wrong?

	E_0	δE_1	E_1	δE_2	E_2	E_{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

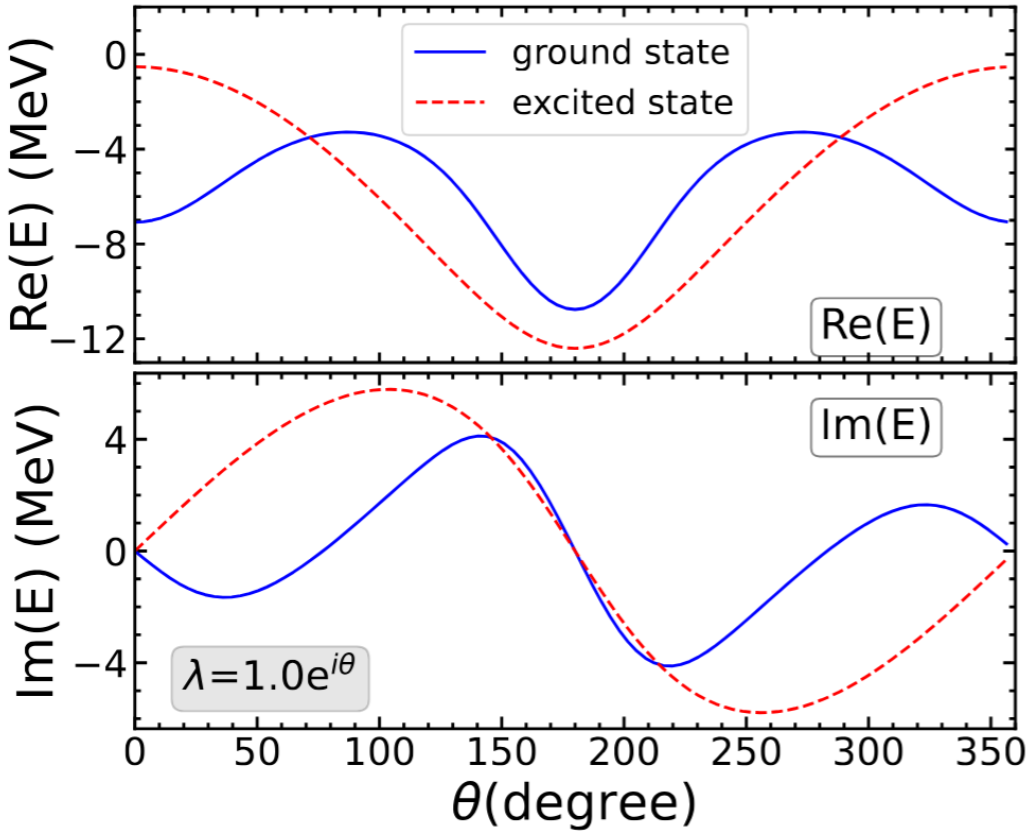
Origin of the large second order corrections

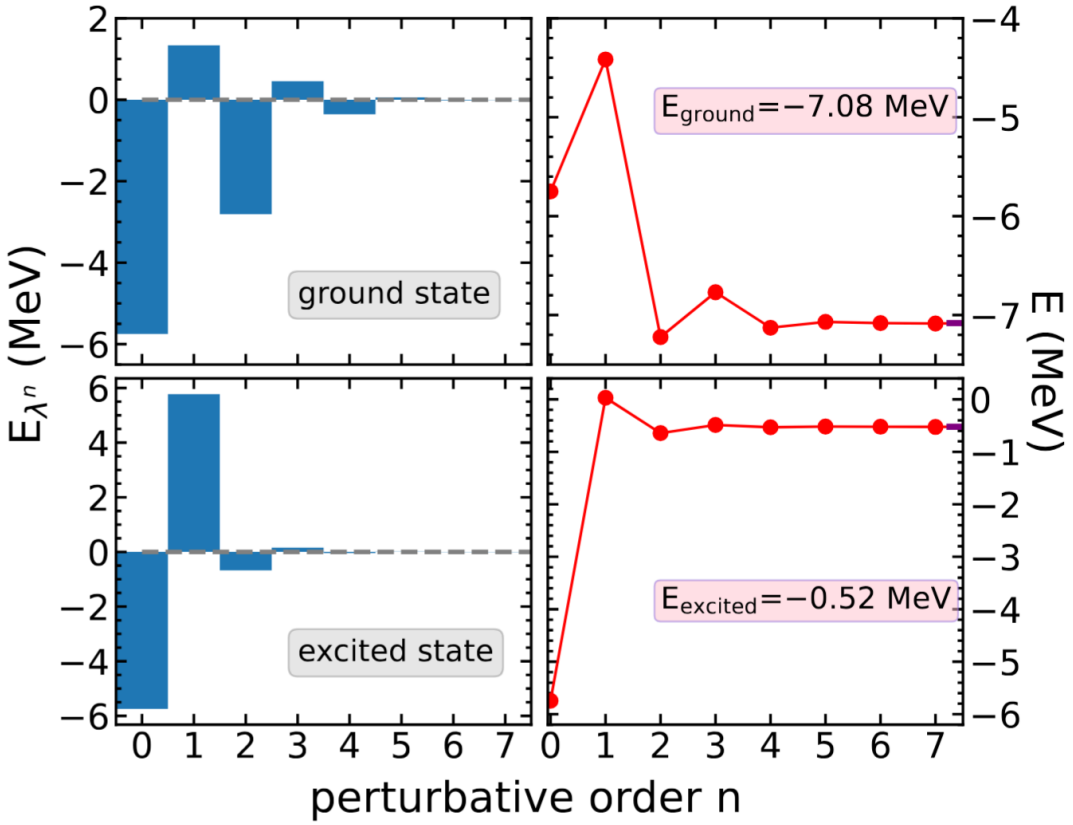


- In perturbative calculations the convergence pattern can be **invalidated** by **symmetry constraints**.
- The **unperturbed Hamiltonian H_0** respects the **SU(4) symmetry**, the wave function must belong to one of its irreducible representations (*irreps*).
- The **full Hamiltonian** breaks the **SU(4) symmetry**, its ground state is a mixture of different SU(4) *irreps*.
- The components of SU(4) *irreps* can only be seen in $|\delta\Psi_1\rangle$ or δE_2.
- This effect is strongest for the OPEP as it breaks both the **Wigner-SU(4)** and the **spin SU(2)** symmetries.

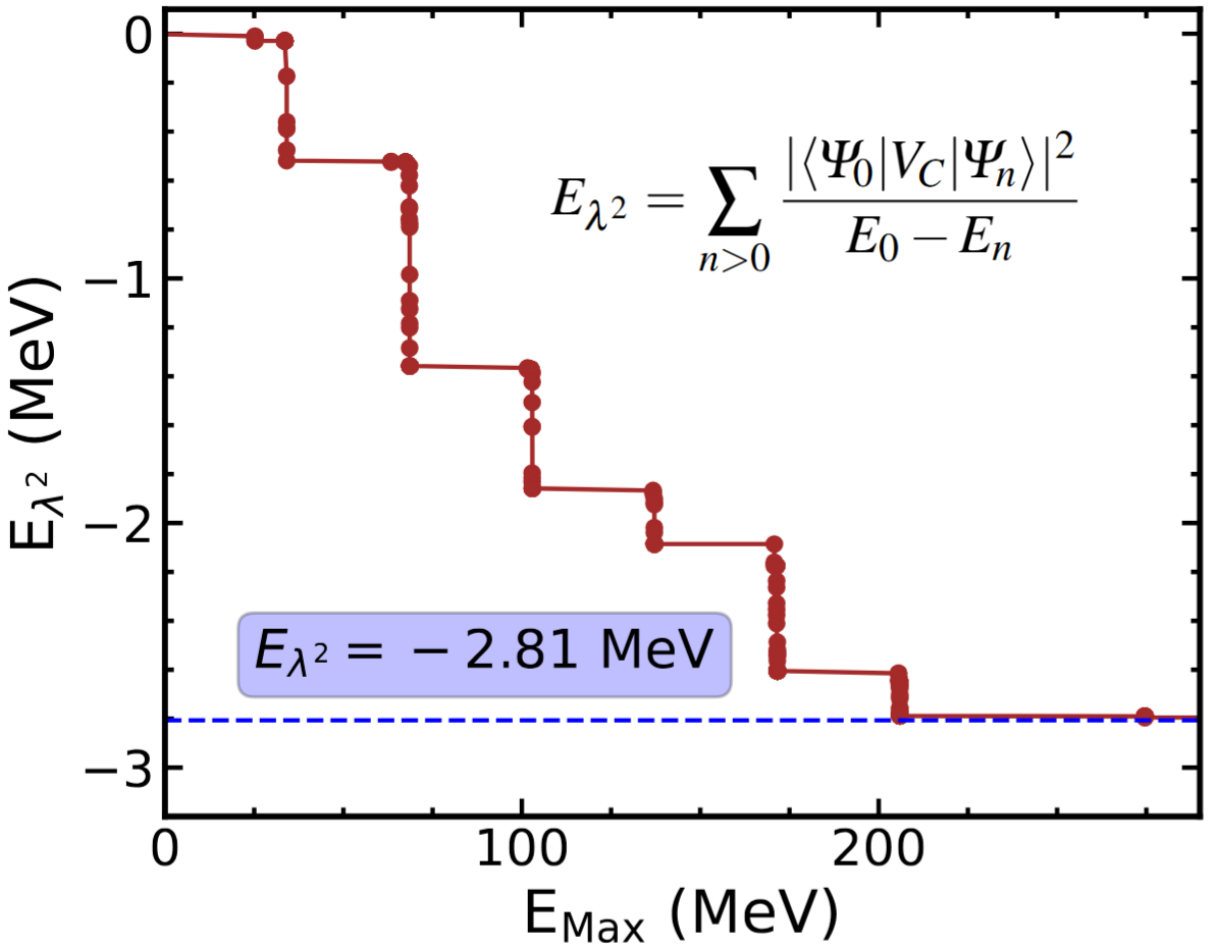
Go beyond second order: ^{2}H in a box

- Deuteron energy can be expanded using Cauchy integral formula $\left.\frac{\partial^n E}{\partial \lambda^n}\right|_{\lambda=0} = \frac{n!}{2\pi i}\oint_{|\lambda|=1}\frac{E(\lambda)}{\lambda^{n+1}}d\lambda$





Comparison with Rayleigh-Schrödinger scheme



- We compare three methods for 2nd correction
  - Perturbative QMC
  - Rayleigh-Schrödinger
  - Cauchy formula
- For ^{2}H in a box all methods agree excellently
- However, R-S method needs hundreds of excited states, converge slowly
- Cauchy formula not applicable for $A > 3$

All state with $E \leq E_{max}$ included
Each point corresponds to a state

Contents

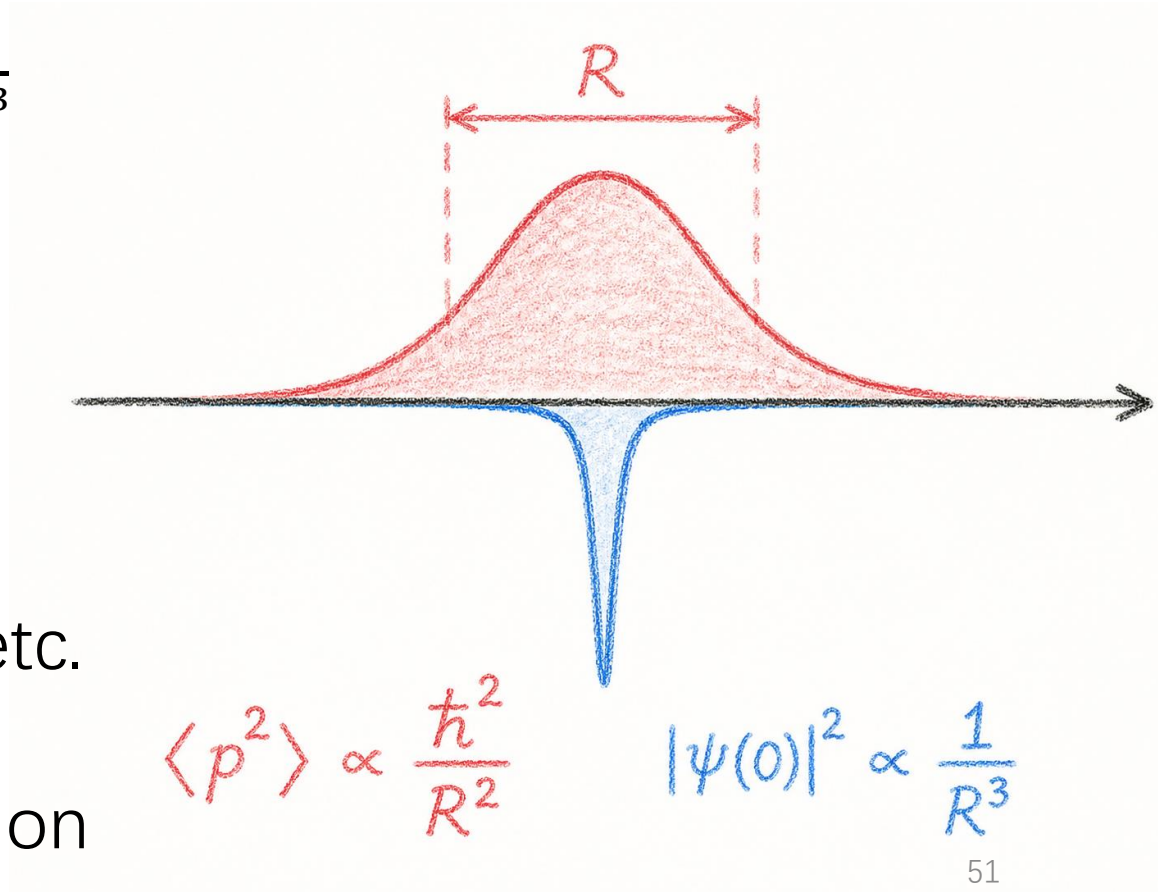
- Introduction to Nuclear Lattice Effective Field Theory
- Non-perturbative QMC and sign problem
- Perturbative QMC
- **Renormalization of NLEFT**
- Ab initio nuclear thermodynamics
- Summary and perspective

Why cutoff matters?

- 3-d attractive Dirac-δ potential has **no stable ground state**
  - Kinetic energy $T \propto \frac{\hbar^2}{2mR^2}$
  - Potential energy $V \propto -|\psi(0)|^2 \propto -\frac{\lambda}{R^3}$
- Total energy $E \sim \frac{\hbar^2}{2mR^2} - \frac{\lambda}{R^3} \to -\infty$

Point particles + zero-range interactions cause infinities!

- Need **regularization**
  ← momentum cutoffs, dim. reg., etc.
- Need **renormalization**
  ← remove regulator after calculation



Historical experiences

- **First renormalized theory: QED**
  1. Apply a momentum cutoff Λ.
  2. Eliminate bare parameters using observables
  3. Send Λ to infinity


Sin-Itiro Tomonaga


Julian Schwinger


Richard P. Feynman

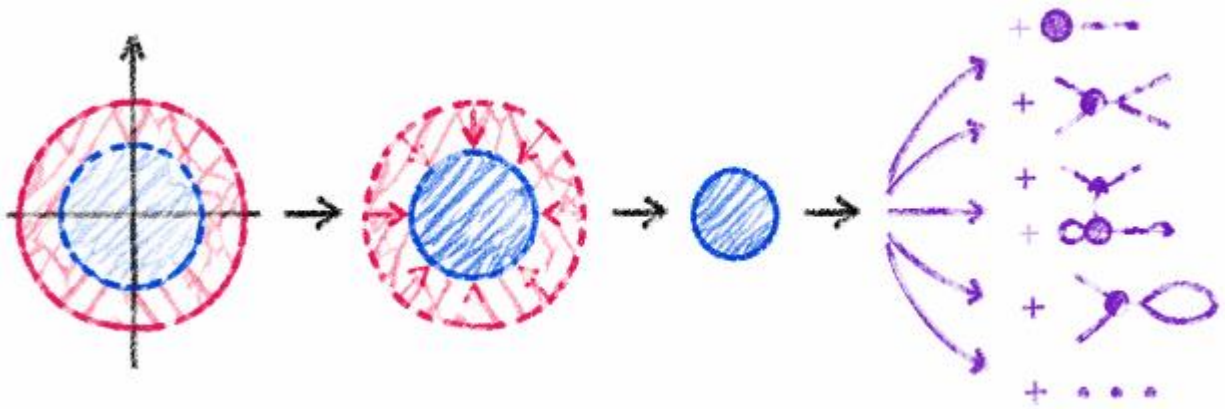
Infinities in QED originate from the assumption of **point-particles**

Why a simple form factor is not satisfactory? ← Model dependence

Dual role of cutoff

- Feynman, Schwinger and Tomonaga's view point:
  - For a given Lagrangian, absorb infinities into bare parameters
    → Safe to send $\Lambda \to \infty$
- Wilson's viewpoint:
  - Variation of Λ induces infinite contact terms
    → Predictions independent of Λ

Both procedures eliminate the dependences on Λ





Disaster of using arbitrary cutoff

- Calculate difference

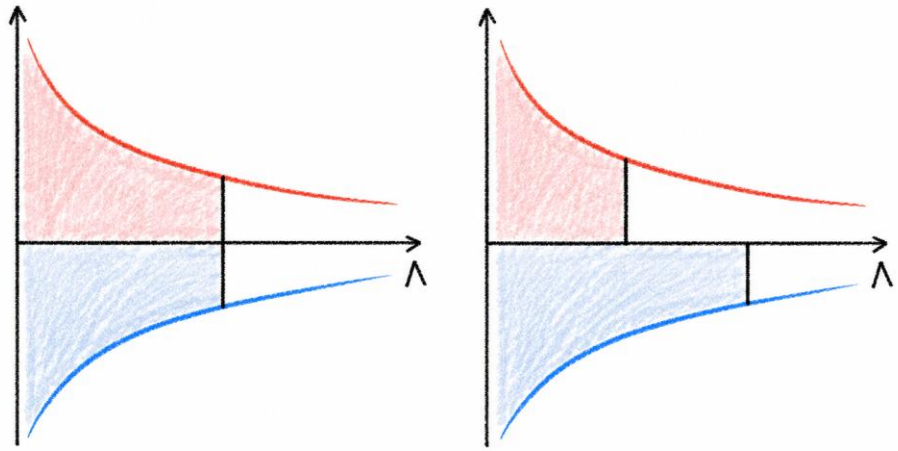
$$I = \int_0^\infty \frac{p^2 dp}{p^2+M^2} - \int_0^\infty \frac{p^2 dp}{p^2+M'^2} = \int_0^\infty \frac{(M'^2-M^2)p^2 dp}{(p^2+M^2)(p^2+M'^2)} = \frac{\pi}{2}(M'-M)$$

- Impose inconsistent cutoff Λ, Λ':

$$I = \lim_{\Lambda,\Lambda'\to\infty} \left[\int_0^\Lambda \frac{p^2 dp}{p^2+M^2} - \int_0^{\Lambda'} \frac{p^2 dp}{p^2+M'^2}\right] = \int_\Lambda^{\Lambda'} \left[\frac{p^2 dp}{p^2+M^2} - \frac{p^2 dp}{p^2+M'^2}\right]$$

$$= \frac{\pi}{2}(M'-M) + \Lambda - \Lambda'$$

- Predictions of field theory relies on **cancelations** between terms
- Inconsistent cutoffs lead to **arbitrary** predictions



Chiral EFT as *ab initio* foundation

Eur. Phys. J. A (2020) 56:95
https://doi.org/10.1140/epja/s10050-020-00101-3

Review

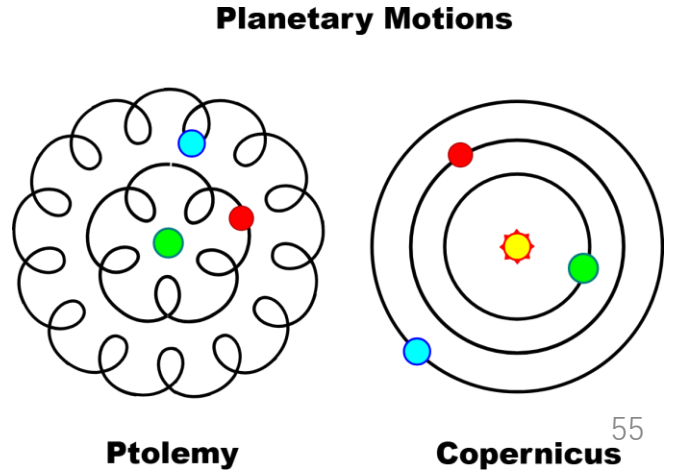
Can chiral EFT give us satisfaction?

R. Machleidt[a], **F. Sammarruca**[b]

Department of Physics, University of Idaho, Moscow, ID 83844, USA

the nuclear theory of the past was nothing but an omnium-gatherum of models. This is very unsatisfactory in view of the traditional goal of theoretical physics, namely, to develop theories that are reductionist, unifying, and fundamental. However, the gap between the jumble of nuclear models and the holy grail of theory is so wide that there is no hope to overcome it any time soon. This is where the notions of emergence

calculations. However, in spite of the considerable progress made possible by chiral EFT, complete satisfaction cannot be claimed until outstanding problems – the renormalization issue being the most important one – are finally settled.



Is chiral EFT prediction cutoff-dependent?

- Two-body scattering

  D. Kaplan et al., Phys. Lett. B 424, 390 (1998)

  A. Nogga et al., Phys. Rev. C 72, 054006 (2005)

  E. Epelbaum et al., Nucl. Phys. B 925, 161 (2017)

- Three- and four-body systems

  P. Bedaque et al., Phys. Rev. Lett. 82, 463 (1999)

  L. Platter et al., Phys. Lett. B 607, 254 (2005)

- Medium-mass nuclei and nuclear matter

  A. Dyhdalo et al., Phys. Rev. C 94, 034001 (2016)

  C.-J. Yang et al., Phys. Rev. C 103, 054304 (2021)

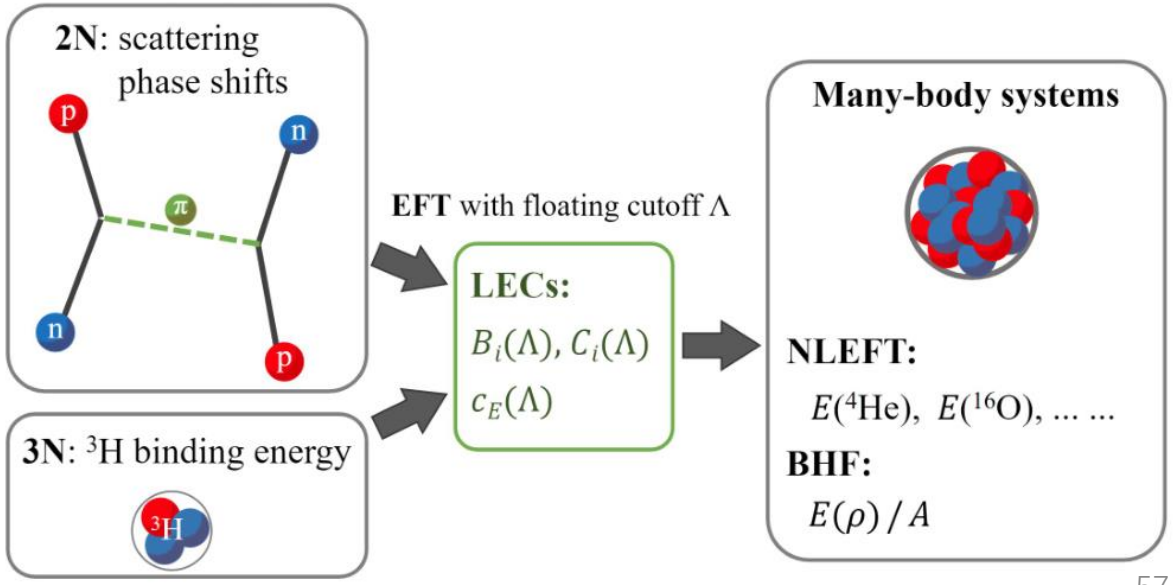
- Most RG studies focus on **few-body systems**
- Many-body calculations often use EFTs as **phenomenological forces**
  → fit to NN phase shifts and finite nuclei, with **fixed cutoff**
- Proving **cutoff-independence** of many-body predictions is the first step towards a **model-independent EFT framework**

Challenges: Non-perturbative interaction & Many-body problem

Re-examination of EFT principles

- **Principles of applying effective field theory to many-body systems**
  - Write down all vertices respecting symmetries
  - Truncate momenta consistently
  - Do calculations
  - Examine cutoff-dependences of observables

- Not systematically examined for medium-mass nuclei & nuclear matter



Chiral interaction and lattice regulator

$$
\begin{aligned}
V_{Q0} &= \left[B_1 + B_2(\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)\right] f_{2\mathrm{N}}(\{p_i, p_i'\}), \\
V_{Q2} &= \Big[C_1 q^2 + C_2 q^2 (\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) + C_3 q^2 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) \\
&\quad + C_4 q^2 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) \\
&\quad + C_5 \frac{i}{2} (\boldsymbol{q} \times \boldsymbol{k}) \cdot (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) + C_6 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{q})(\boldsymbol{\sigma}_2 \cdot \boldsymbol{q}) \\
&\quad + C_7 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{q})(\boldsymbol{\sigma}_2 \cdot \boldsymbol{q})(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2)\Big] f_{2\mathrm{N}}(\{p_i, p_i'\}),
\end{aligned}
$$

$$
V_{3\mathrm{N}} = \frac{c_E}{2 F_\pi^4 \Lambda_\chi} f_{3\mathrm{N}}(\{p_i, p_i'\})
$$

$$
V_{1\pi} = -\frac{g_A^2 f_\pi(q^2)}{4 F_\pi^2} \left[\frac{(\boldsymbol{\sigma}_1 \cdot \boldsymbol{q})(\boldsymbol{\sigma}_2 \cdot \boldsymbol{q})}{q^2 + M_\pi^2} + C_\pi' \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \right] (\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2)
$$

$$
V_{\mathrm{CSB}}^{\mathrm{pp}} = c_{\mathrm{pp}} \left(\frac{1 + \tau_{1z}}{2} \right) \left(\frac{1 + \tau_{2z}}{2} \right) f_{2\mathrm{N}}(\{p_i, p_i'\})
$$

$$
V_{\mathrm{CSB}}^{\mathrm{nn}} = c_{\mathrm{nn}} \left(\frac{1 - \tau_{1z}}{2} \right) \left(\frac{1 - \tau_{2z}}{2} \right) f_{2\mathrm{N}}(\{p_i, p_i'\})
$$

We apply a global lattice-inspired regulator

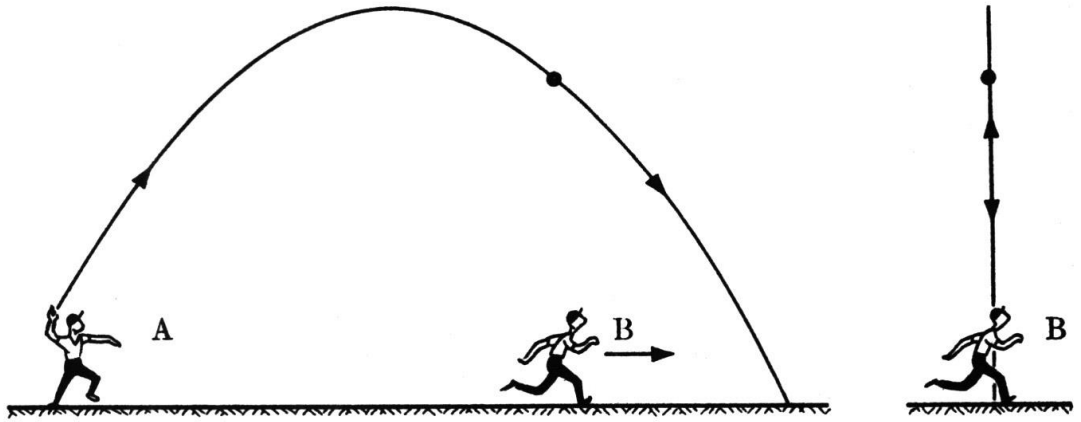
$$
f_{2\mathrm{N}}(\{p_i, p_i'\}) = \exp\left[-\sum_{i=1}^{2} \left(p_i^6 + p_i'^6 \right) / (2\Lambda^6) \right]
$$

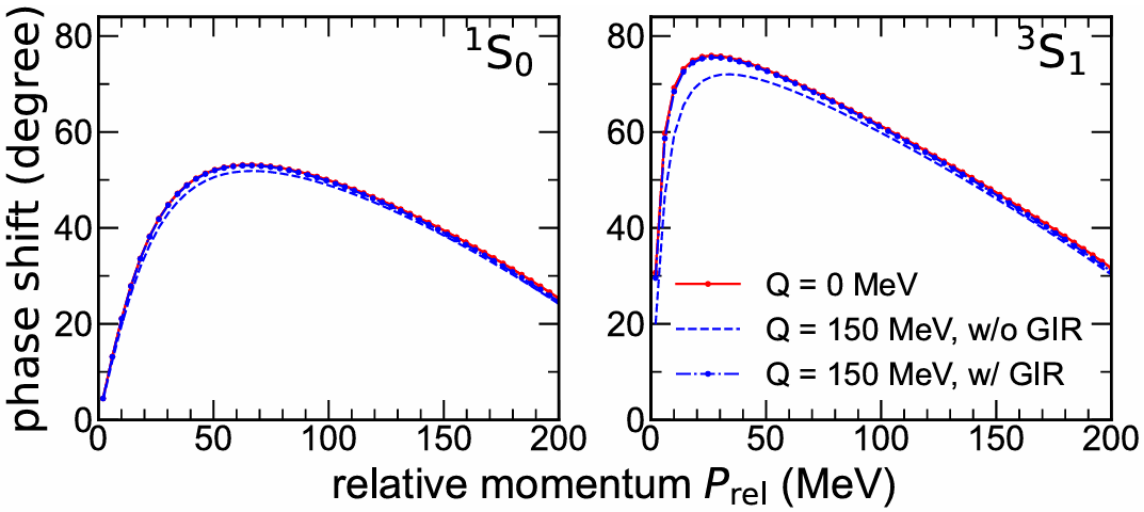
Truncation over absolute momentum induces Galilean-invariance breaking terms

$$
V_{\mathrm{GIR}} = \left[g_1 Q^2 + g_2 Q^2 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) \right] f_{2\mathrm{N}}(\{p_i, p_i'\})
$$

2NF fitted to NN scattering phase shifts
3NF fitted to ^{3}H binding energy
GIR fitted to symmetry constraints

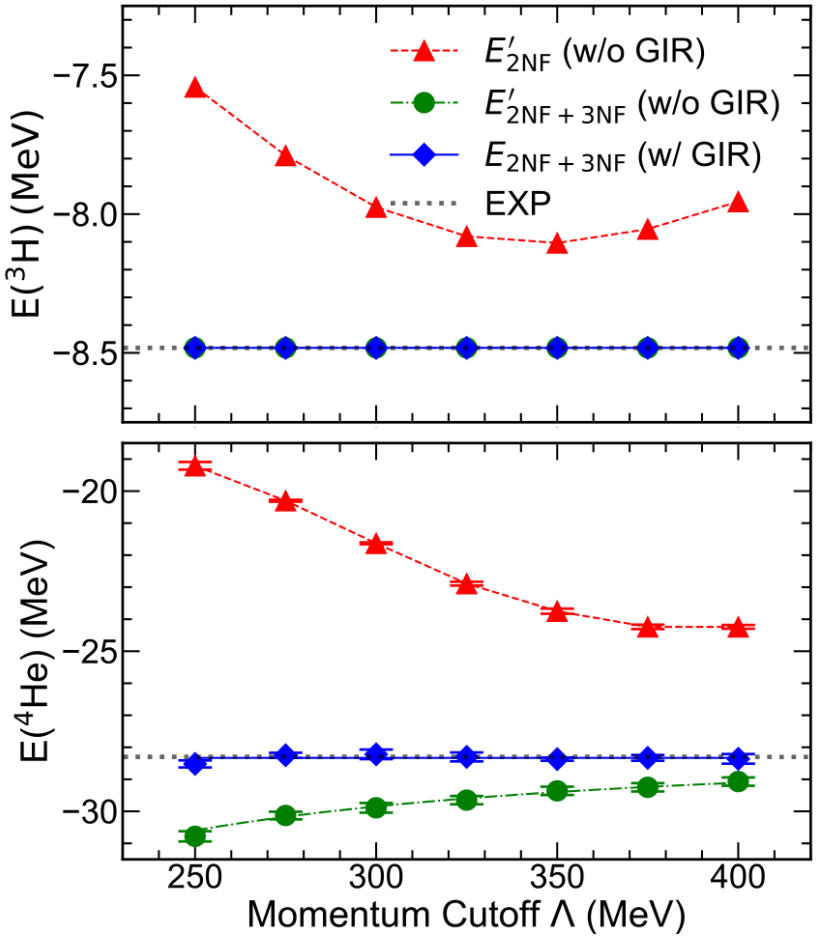
Galilean invariance restoration

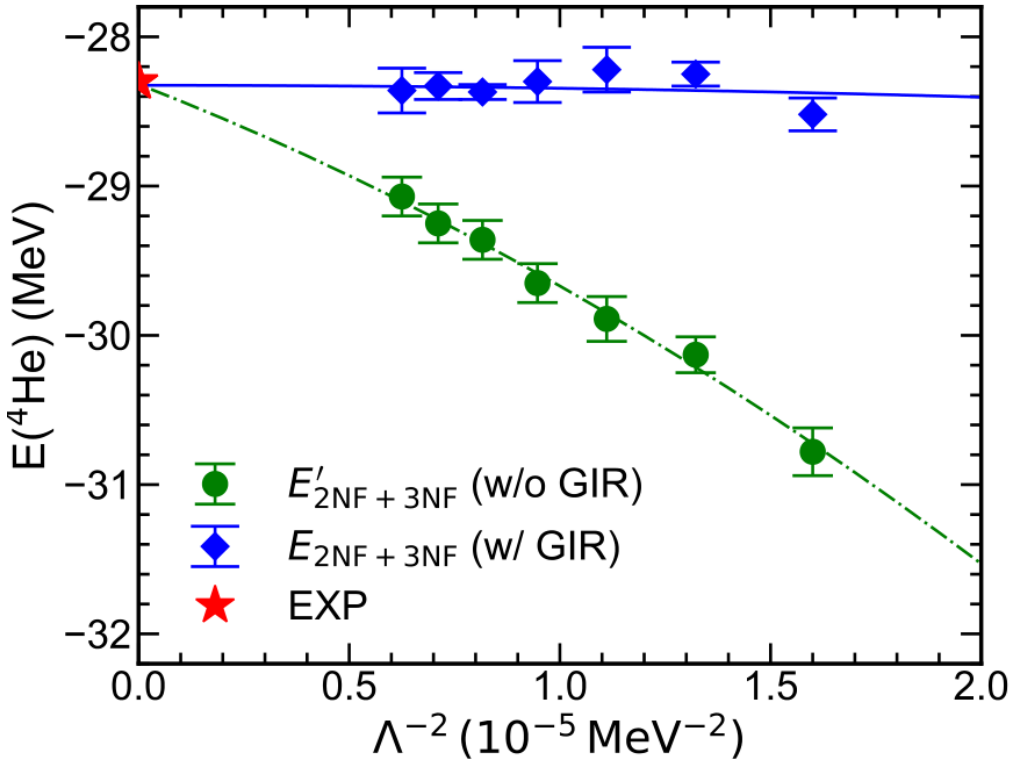




- Galilean invariance
  → Observables only depend on **relative momenta**
- Galilean invariance restoration (GIR) terms
  $V_{\mathrm{GIR}} = \left[g_1 Q^2 + g_2 Q^2 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)\right] f_{2\mathrm{N}}(\{p_i, p_i'\})$
  Center of mass momentum $\boldsymbol{Q} = \boldsymbol{p}_1 + \boldsymbol{p}_2 = \boldsymbol{p}_1' + \boldsymbol{p}_2'$
- Systematic determination of GIR terms
  Li et al., Phys. Rev. C 99,064001 (2019)
- Role of GIR terms in renormalizing 1-d bosons
  Klein et al., Eur. Phys. J. A 54, 233 (2018)
- Wavefunction matching with GIR terms
  Elhatisari et al., Nature 630, 59 (2024)

Binding energy of ^{4}He





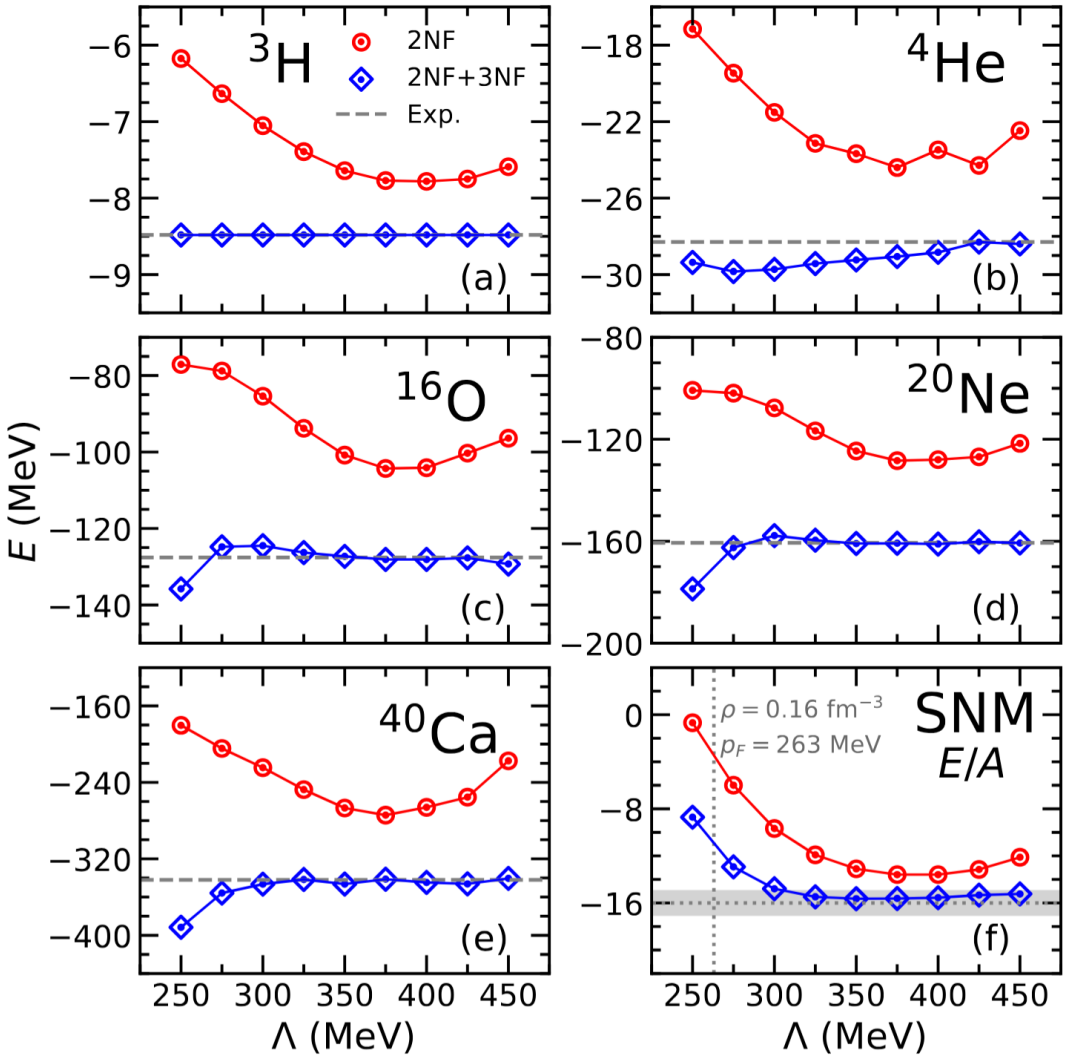
Symmanzik improvement

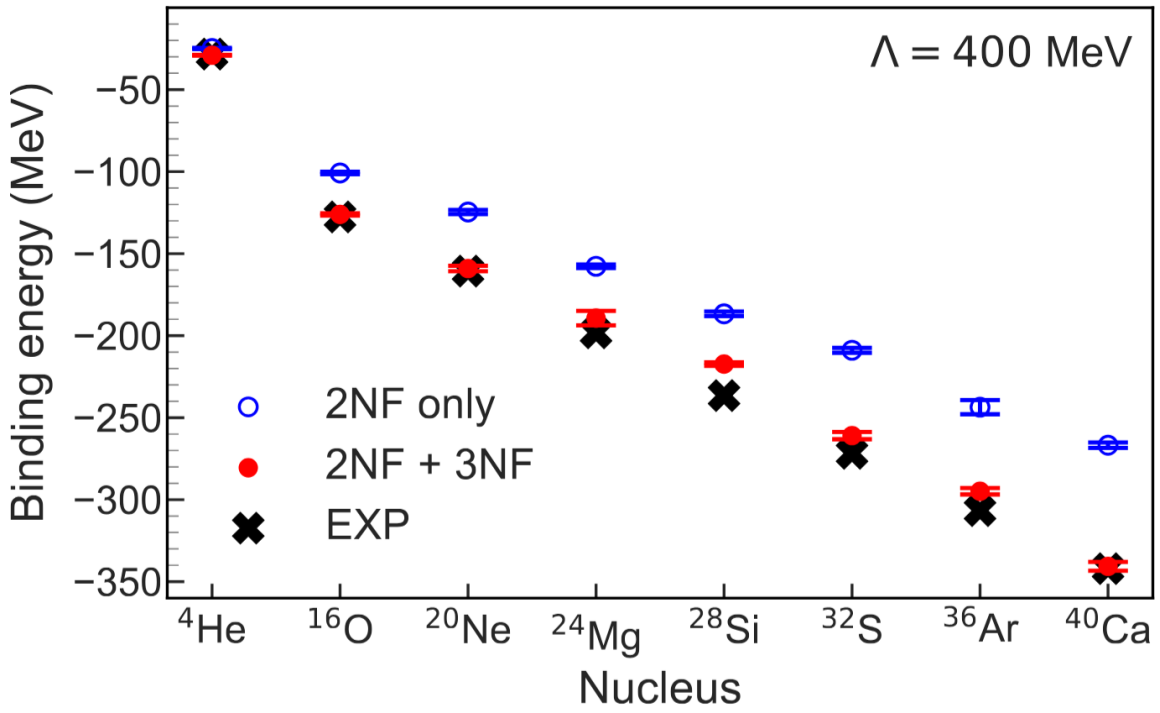
Restore symmetries using counter terms

K. Symanzik, Nucl. Phys. B 226, 187 (1983); Nucl. Phys. B 226, 205 (1983)

Observation of renormalization group invariance in symmetry-restored nuclear lattice effective field theory, J. Shi, C. Wang and BL, Phys. Lett. B 874, 140303 (2026)

Binding energies of medium-mass nuclei

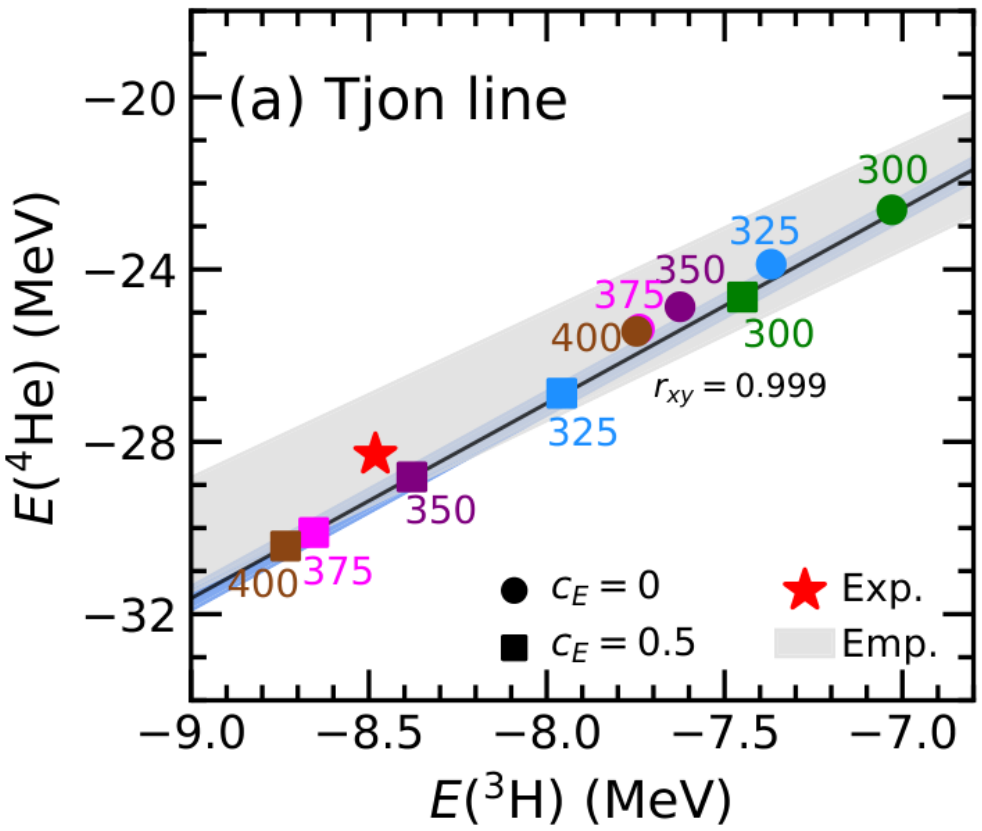




Excellent reproduction of experiments & RG invariance with a single adjustable 3NF

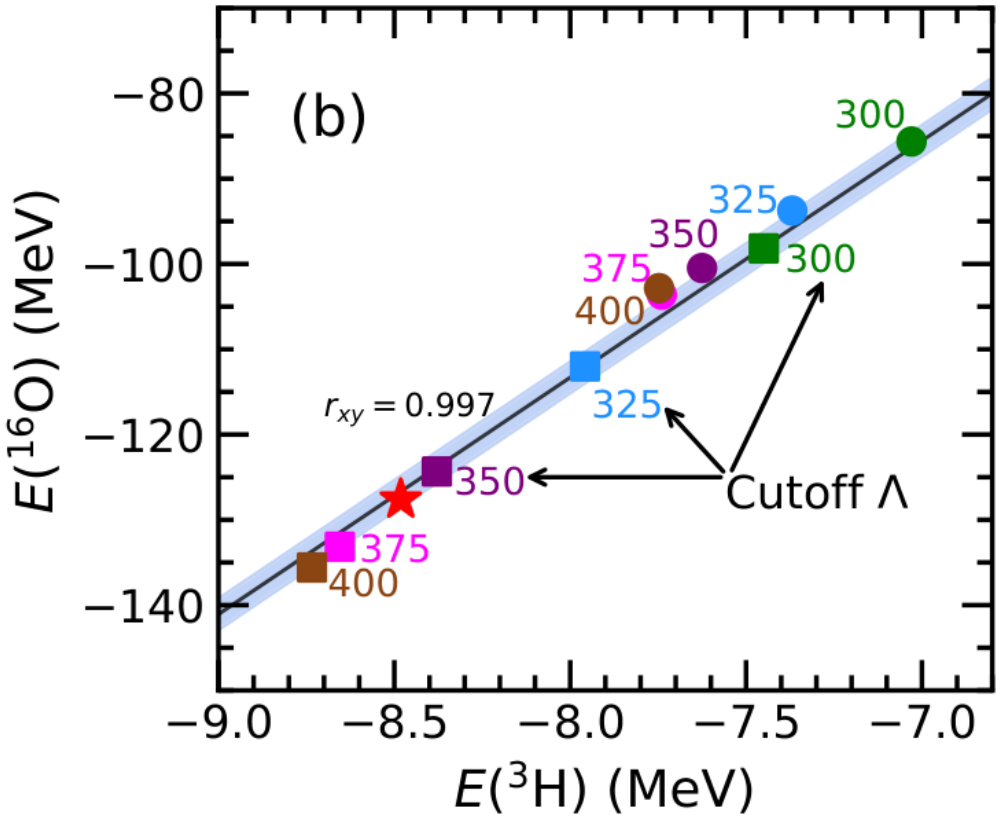
Preliminary, C. Wang, J. Shi, BL

Correlations beyond lightest nuclei



Tjon line discovered 50 years ago

J. Tjon, Phys. Lett. B 56, 217 (1975)

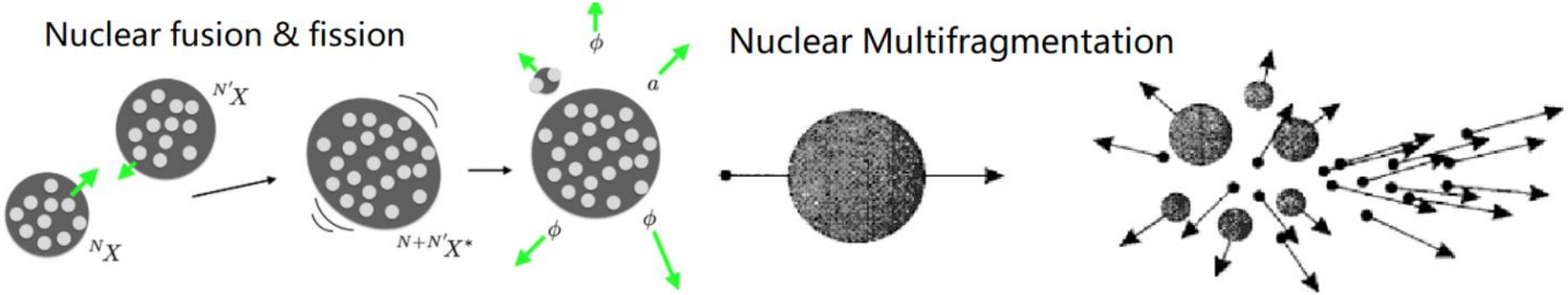


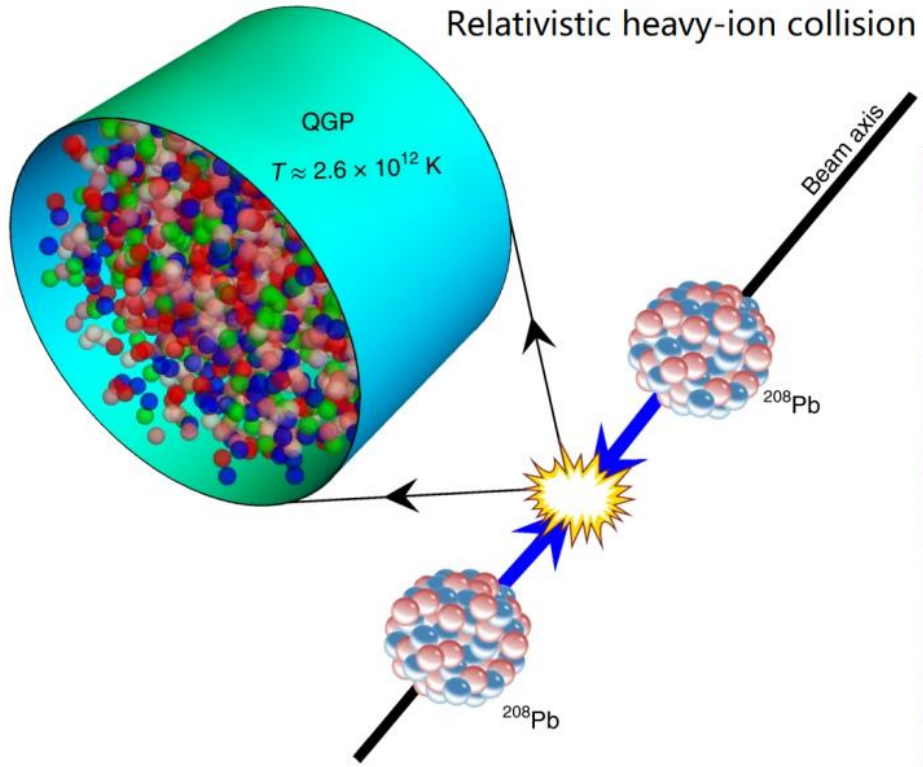
A single 3NF is sufficient to cancel cutoff-dependence

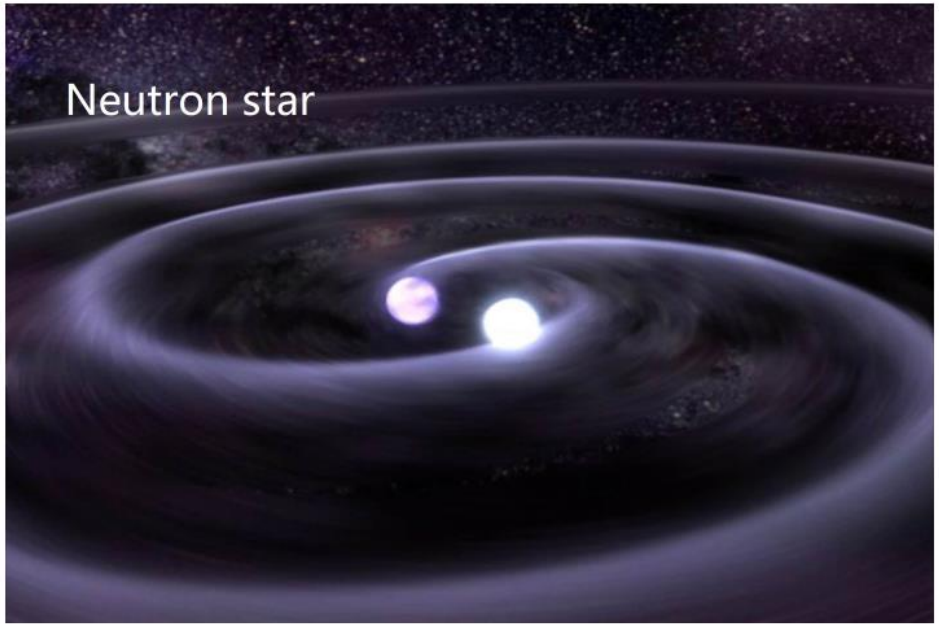
Contents

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- Non-perturbative QMC and sign problem
- Perturbative QMC
- Renormalization of NLEFT
- **Ab initio nuclear thermodynamics**
- Summary and perspective

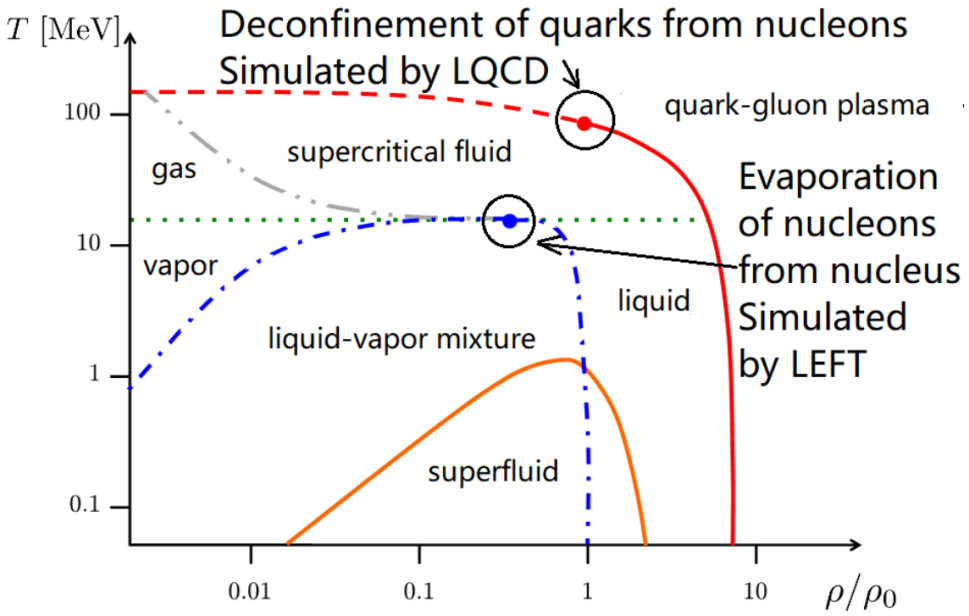
Hot nucleus

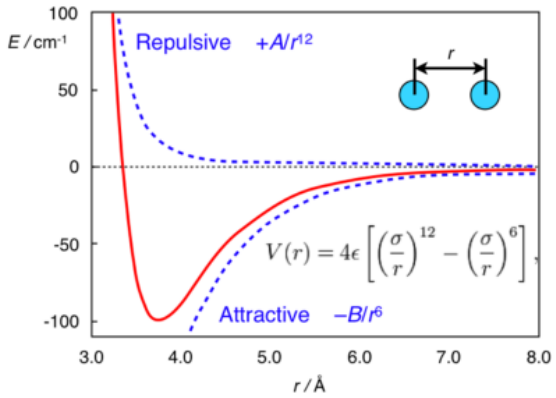

Nuclear fusion & fission
$N'X$
NX
$N+N'X^*$
ϕ
a
ϕ
ϕ
Nuclear Multifragmentation

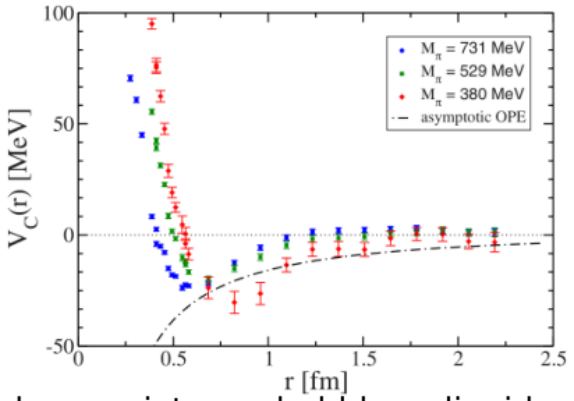

Relativistic heavy-ion collision
QGP
$T \approx 2.6 \times 10^{12}$ K
Beam axis
^{208}Pb
^{208}Pb

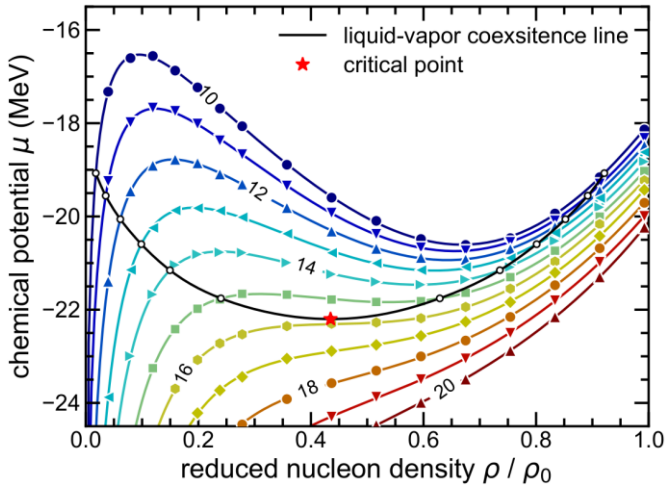

Neutron star

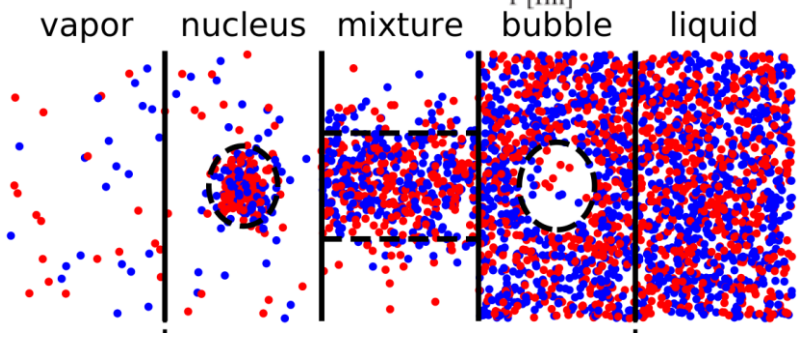
Nuclear thermodynamics from lattice EFT











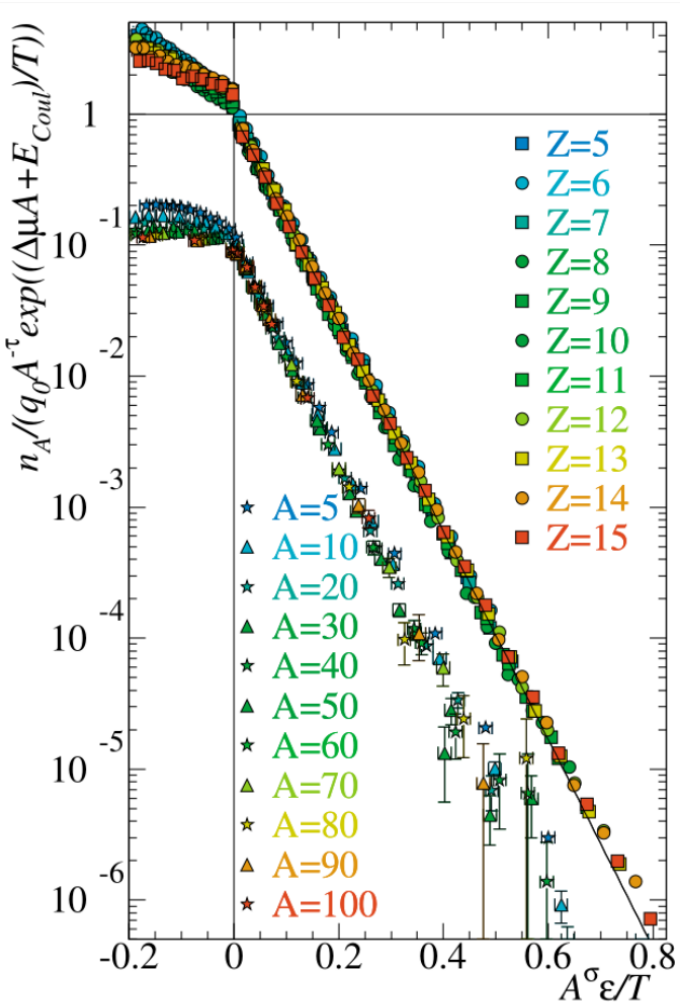
nuclear liquid v.s. normal liquid
nuclear force v.s. van der Waals force
nuclear liquid-gas phase transition
v.s. water liquid-gas phase transition

Ab initio calculation for liquid-gas phase transition in symmetric nuclear matter based on lattice EFT
BNL et al., PRL 125, 192502 (2020)

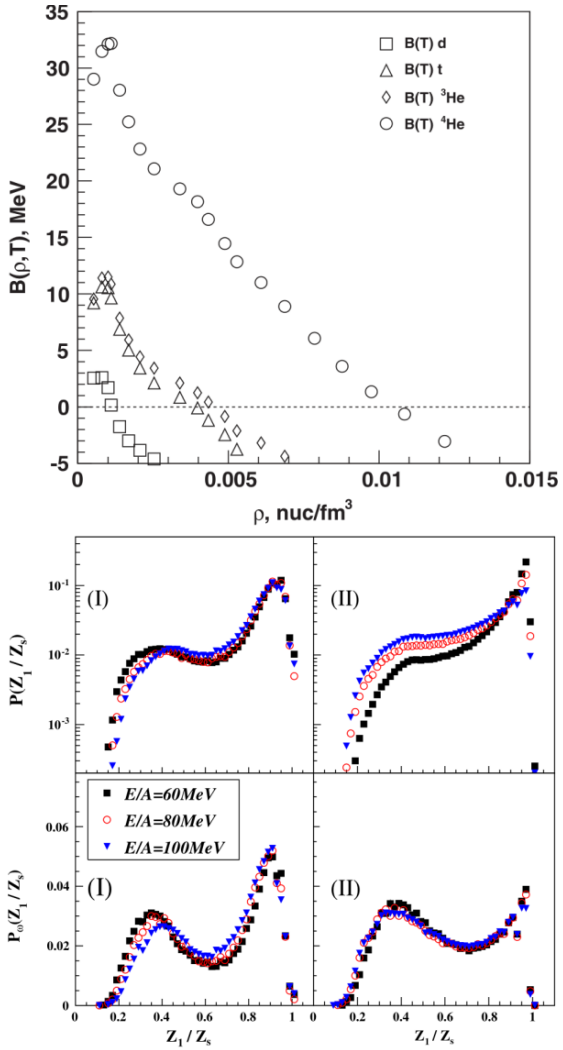
10~1000 times speed up with new Pinhole-trace algorithm



Nuclear Multifragmetation



JB Elliott, et al., PRL 88, 042701 (2002)



Interplay between quantum mechanics & thermodynamics produces abundant microscopic structures

"Cold clusters in a hot vapor"

Upper: Binding energies of clusters versus density, derived from experiments
K Hagel et al., PRL 108, 062702 (2012)

- Mott points: Temperature/Density where the cluster dissociate
- Consequence of many-body correlations

Lower: Two humped structure in largest fragment mass distribution signifies a phase coexistence E Bonnet et al., PRL 103, 072701 (2009)

- Liquid-Vapor coexsitence: **a single large cluster** + **many small clusters**
- Vapor phase: **many small clusters**

Models for Nuclear Multifragmentation

Progress in Particle and Nuclear Physics 105 (2019) 139–179

Contents lists available at ScienceDirect

Progress in Particle and Nuclear Physics

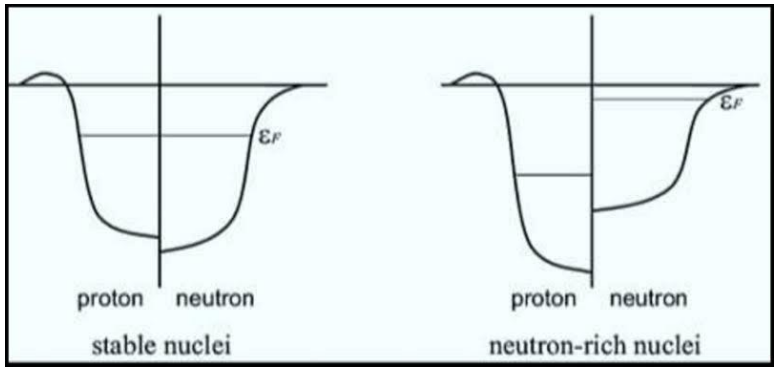
journal homepage: www.elsevier.com/locate/ppnp

Review

Dynamics of clusters and fragments in heavy-ion collisions

Akira Ono

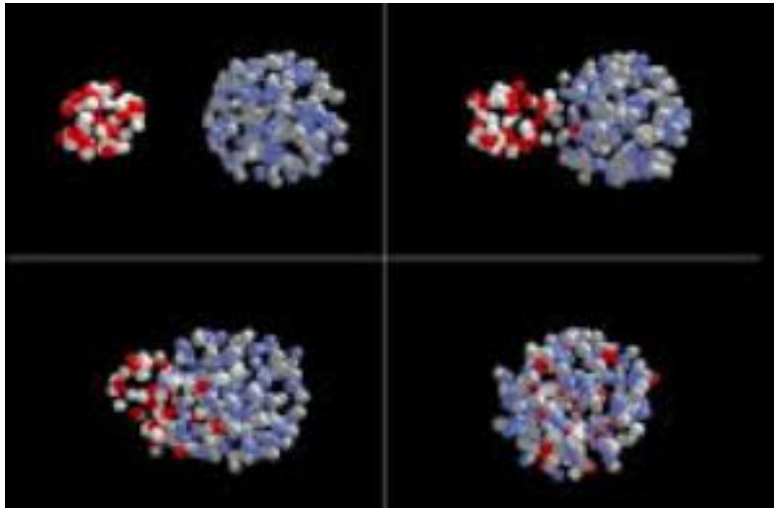
Department of Physics, Tohoku University, Sendai 980-8578, Japan



"Traditionally there are **two types** of transport models. One is the **mean-field models** which are based on the distributions of nucleons moving independently in the mean field. The other is the **molecular dynamics models** which is similar to the A-body classical dynamics but nucleons are represented by Gaussian wave packets."

"Naive statements about the defects of these models are that the **mean-field models lack many-body correlations** and that the **molecular dynamics models are classical**'

"It is **not possible** to exactly solve such quantum many-body problem **from the first principle** with computational facilities available currently or in near future"

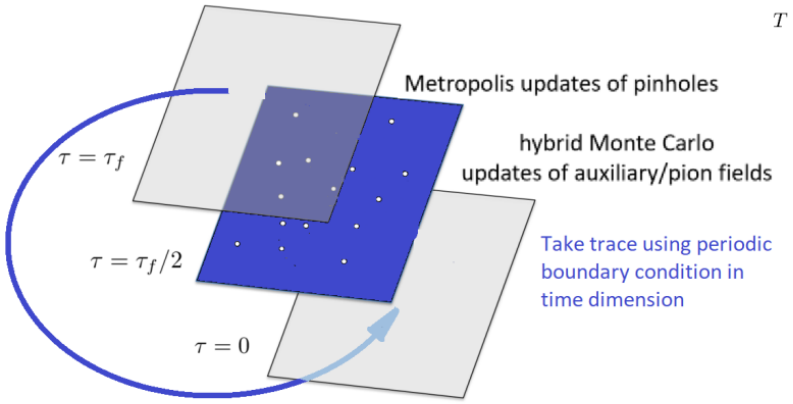


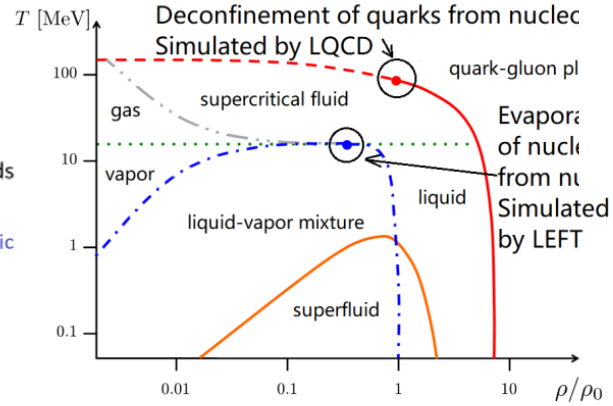
Pinhole trace algorithm

- All we need: **partition function** $Z(T,V,A)=\sum_k\langle\exp(-\beta H)\rangle_k$, sum over all othonormal states in Hilbert space $\mathscr{H}(V,A)$.
- The basis states $|\boldsymbol{n}_1,\boldsymbol{n}_2,\cdots,\boldsymbol{n}_A\rangle$ span the whole A-body Hilbert space. $\boldsymbol{n}_i=(\boldsymbol{r}_i,s_i\sigma_i)$ consists of **coordinate, spin, isospin** of i-th nucleon.
- Cannonical partition function can be expressed in this complete basis:

$$Z_A=\mathrm{Tr}_A\left[\exp(-\beta H)\right]=\sum_{\boldsymbol{n}_1,\cdots,\boldsymbol{n}_A}\int\mathscr{D}s\mathscr{D}\pi\langle\boldsymbol{n}_1,\cdots,\boldsymbol{n}_A|\exp\left[-\beta H(s,\pi)\right]|\boldsymbol{n}_1,\cdots,\boldsymbol{n}_A\rangle$$

- **Pinhole algorithm** + **periodicity in** β = **Pinhole trace**
- Apply **twisted boundary condition** in 3 spatial dimensions to remove finite volume effects. Twist angle θ averaged with MC.



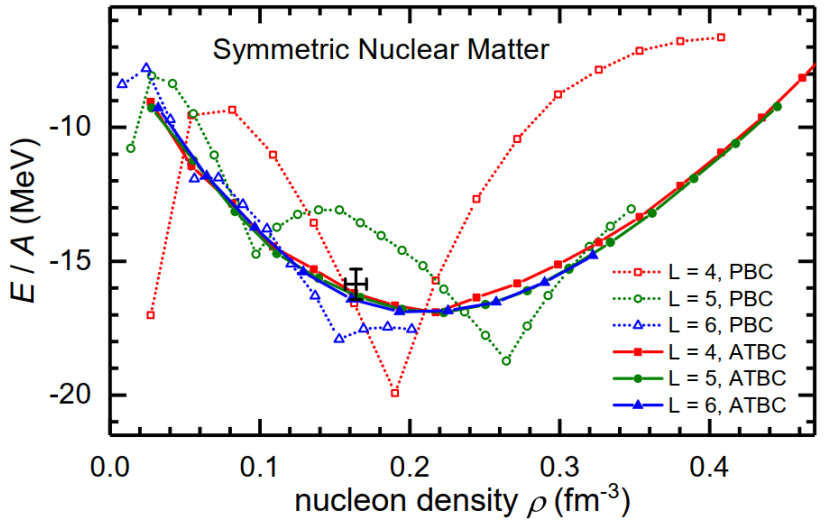


Lu et al., PRL 125, 192502 (2020)

PBC: Periodic Boundary Conditions: $\Psi(x+L)=\Psi(x)$

ATBC: Average Twisted Boundary Conditions: $\Psi(x+L)=e^{i\theta}\Psi(x)$

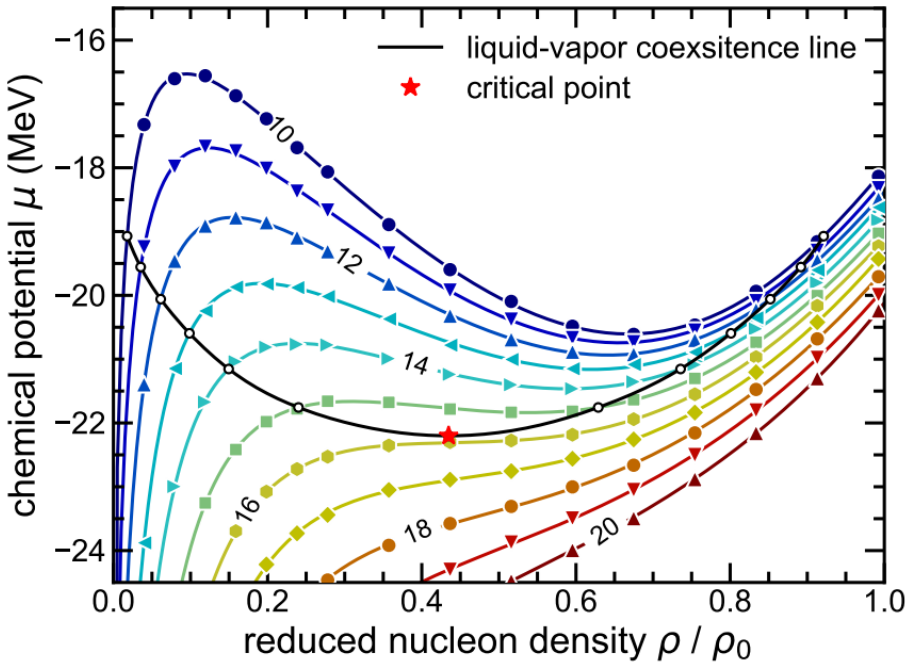
Averaging over θs' to remove fictitious shell effects

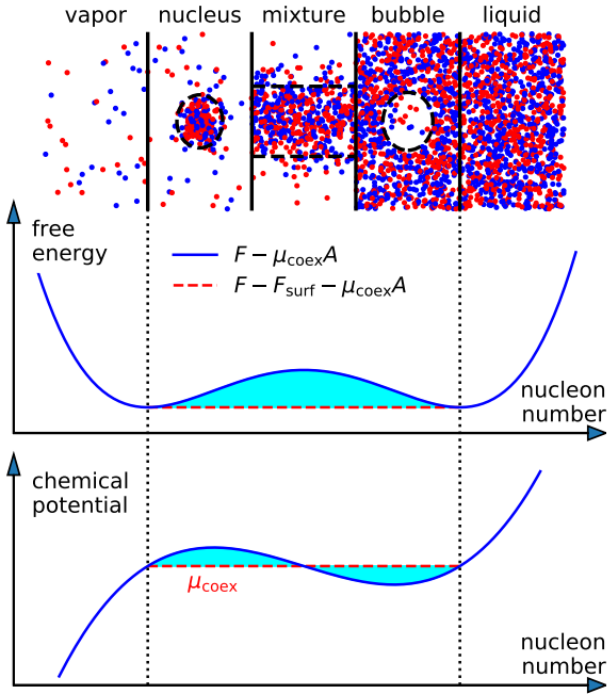


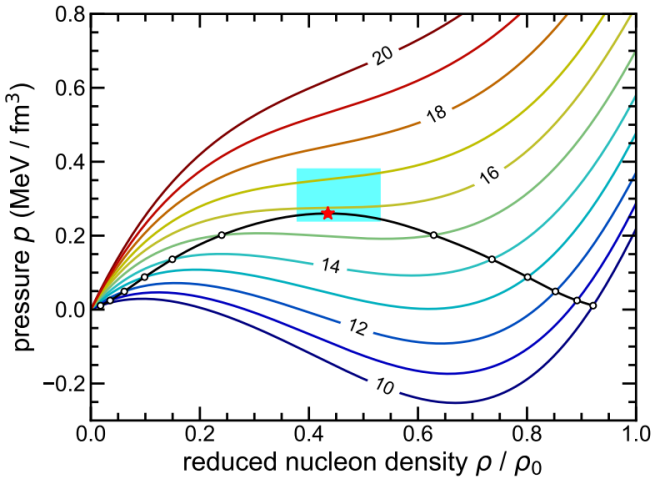
Lu et al., PRL 125, 192502 (2020)

Finite nuclear systems: Liquid-vapor coexistence

- First ***ab initio* calculation** of **nuclear liquid-gas phase transition**.
- Symmetric nuclear matter $N = Z$, lattice spacing $a = 1.32$ fm, volume $V = (6a)^3$, nucleon number $4 \leq A \leq 132$.
- Temperature 10 MeV$\leq T \leq$ 20 MeV, temporal step $\Delta\beta = 1/2000$ MeV^{-1}.
- 288000 independent measurements for every data point.
  Lu et al., PRL 125, 192502 (2020)







	This work	Exp.	RMF(NLSH)	RMF(NL3)
T_c(MeV)	15.80(3)	17.9(4)	15.96	14.64
P_c(MeV/fm^3)	0.260(3)	0.31(7)	0.26	0.2020
ρ_c(fm^{-3})	0.089(1)	0.06(1)	0.0526	0.0463
ρ_0 (fm^{-3})	0.205(0)	0.132		
ρ_c/ρ_0	0.43	0.45		

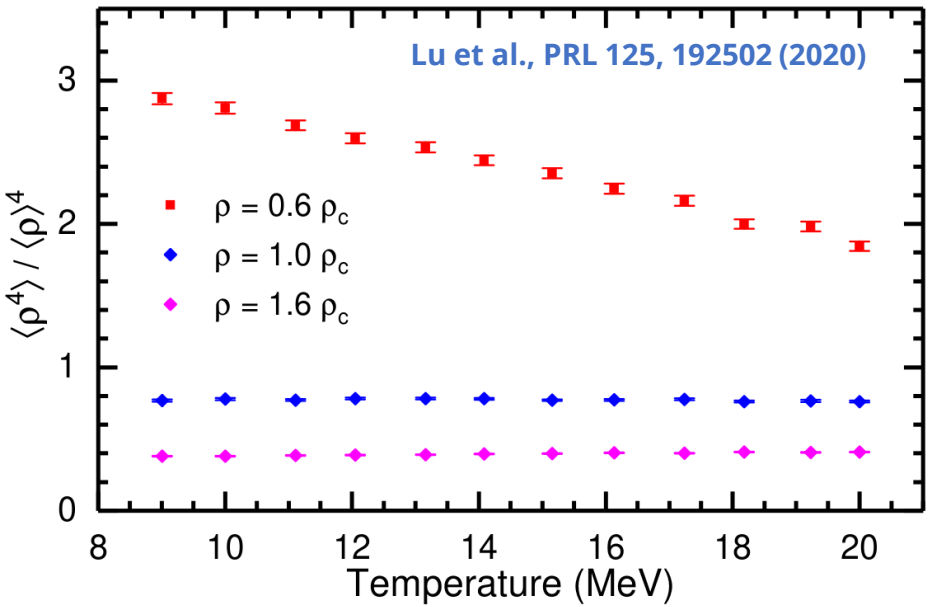
Lu et al., PRL 125, 192502 (2020)

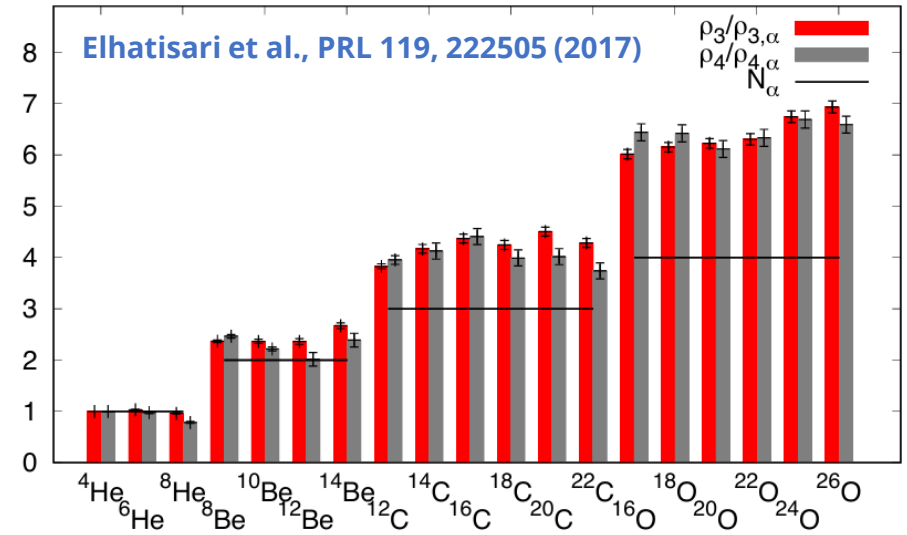
- **Pressure** $p = \int \rho d\mu$ along every isotherm (Gibbs-Duhem equation)

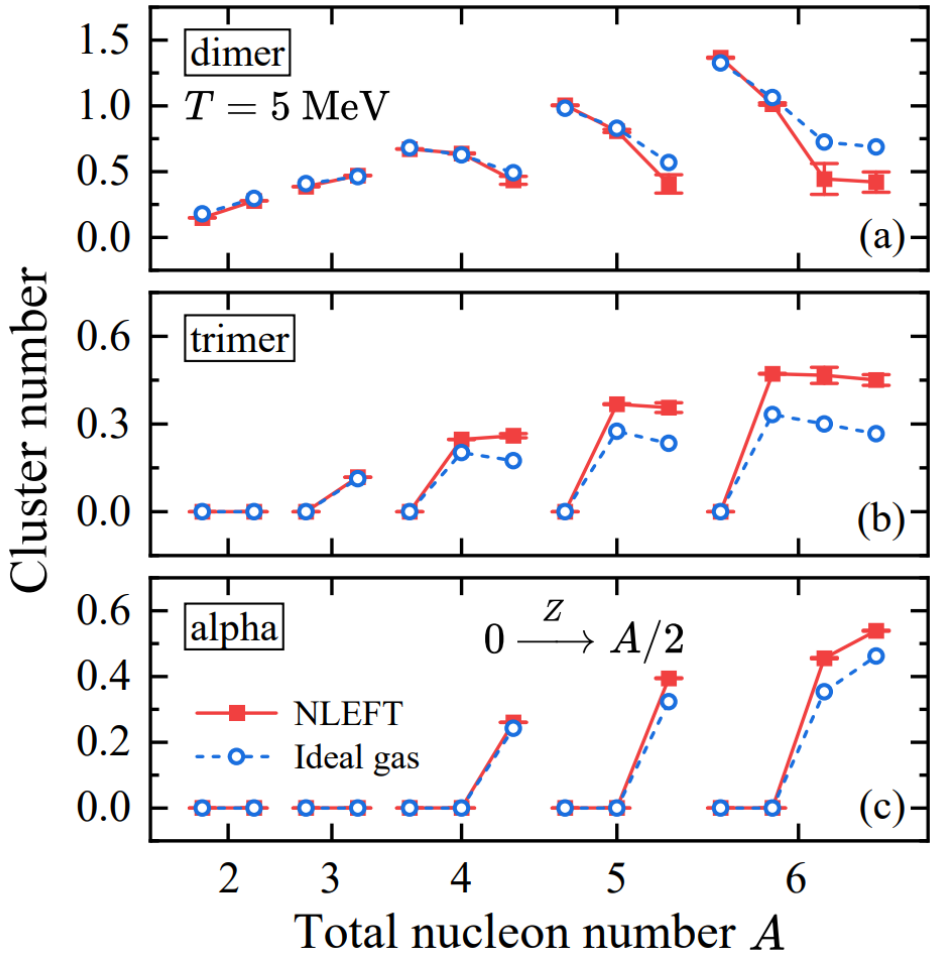
Clustering in ground states and hot nuclear matter

Many clustering indicator can be built from wave functions.
Works for ground states / excited states / finite temperature.

Monitoring how clustering evolves with N/Z, ρ, T, ⋯







$$G_{11}(n) = L^3 \sum_{\{\sigma_i\tau_i\}} :\rho_{\sigma_1\tau_1}(0)\rho_{\sigma_2\tau_2}(\boldsymbol{n}):,$$

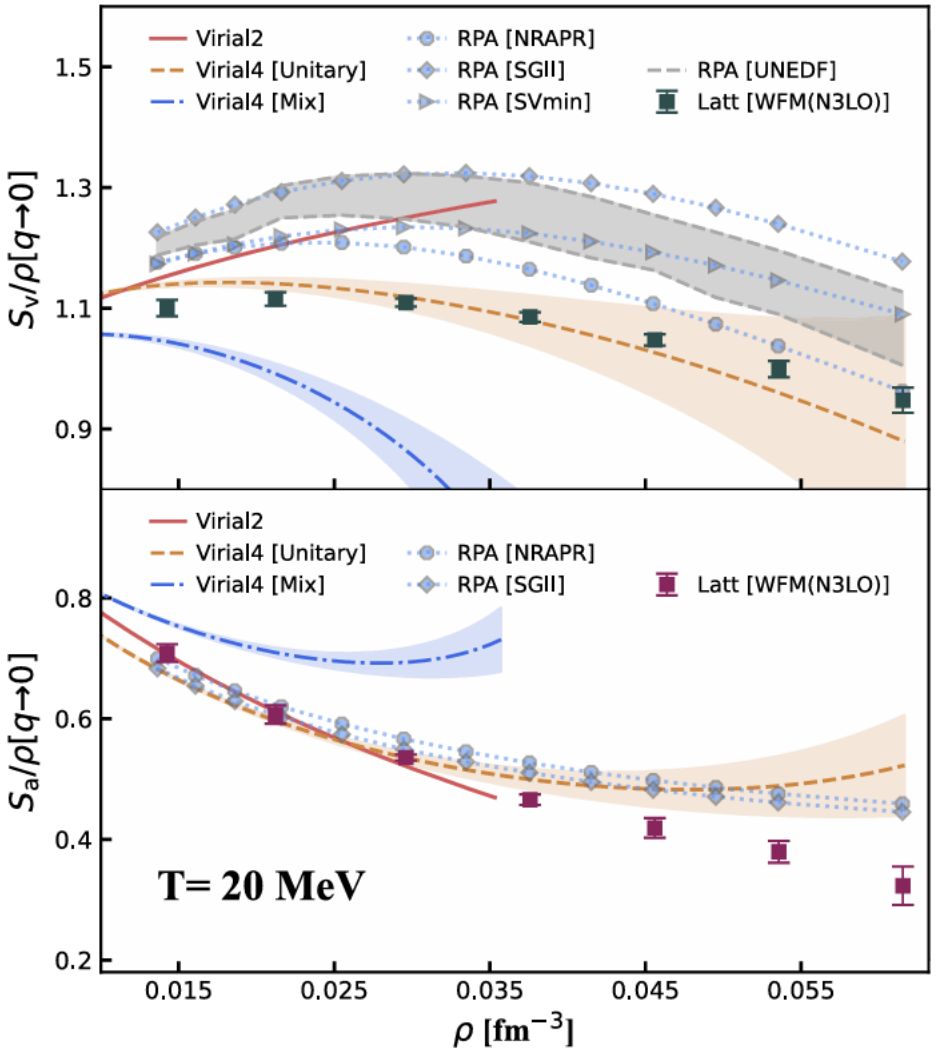
$$G_{21}(n) = L^3 \sum_{\{\sigma_i\tau_i\}} :\rho_{\sigma_1\tau_1}(0)\rho_{\sigma_2\tau_2}(0)\rho_{\sigma_3\tau_3}(\boldsymbol{n}):,$$

$$G_{31}(n) = L^3 \sum_{\{\sigma_i\tau_i\}} :\rho_{\sigma_1\tau_1}(0)\rho_{\sigma_2\tau_2}(0)\rho_{\sigma_3\tau_3}(0)\rho_{\sigma_4\tau_4}(\boldsymbol{n}):,$$

$$G_{22}(n) = L^3 \sum_{\{\sigma_i\tau_i\}} :\rho_{\sigma_1\tau_1}(0)\rho_{\sigma_2\tau_2}(0)\rho_{\sigma_3\tau_3}(\boldsymbol{n})\rho_{\sigma_4\tau_4}(\boldsymbol{n}):.$$

Ren et al., PLB 850, 138463 (2024)

Correlations in hot nuclear matter

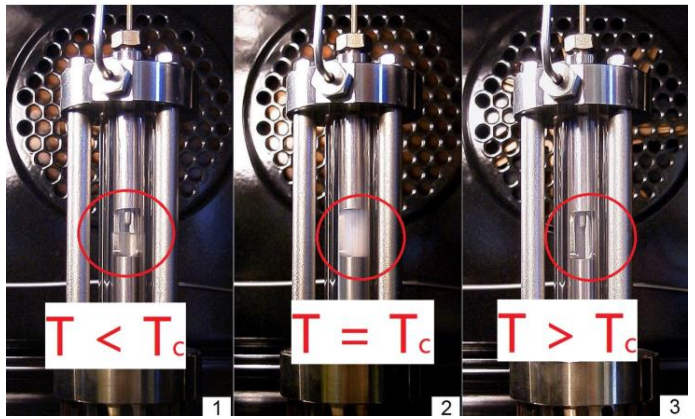


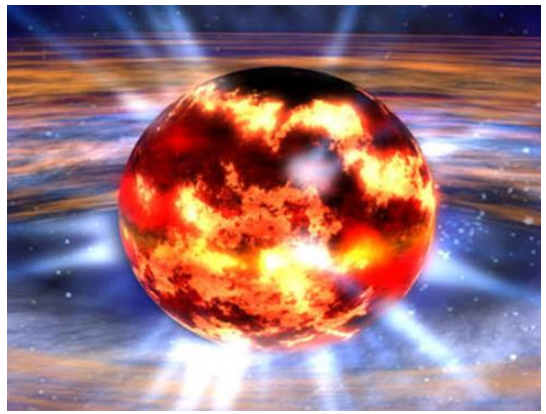
- Structure factors are Fourier transforms of correlation functions

$$S_V(\boldsymbol{q}) = \int d^3r[\langle\hat{\rho}(\boldsymbol{r}+\boldsymbol{r}')\hat{\rho}(\boldsymbol{r}')\rangle - \rho_0^2]e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}$$

$$S_a(\boldsymbol{q}) = \int d^3r[\langle\hat{\rho}_z(\boldsymbol{r}+\boldsymbol{r}')\hat{\rho}_z(\boldsymbol{r}')\rangle - \rho_{z0}^2]e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}$$

- Key for modeling Core-collapse supernovae explosions via neutrino-nucleon scattering
- Lattice EFT provides ab initio calculation with a N^{3}LO chiral interaction based on a rank-one operator method
  Ma et al., PRL 132, 232502 (2024)





Contents

- Introduction to Nuclear Lattice Effective Field Theory
- Non-perturbative QMC and sign problem
- Perturbative QMC
- Renormalization of NLEFT
- Ab initio nuclear thermodynamics
- **Summary and perspective**

Summary and Perspective

- Nuclear Lattice Effective Field Theory is a unified framework for **building NN interactions**, **solving many-body Schrodinger equations** and **extracting observables**.
- Two fundamental challenges in NLEFT calculations
  - Monte Carlo sign problem ← statistical errors
  - Renormalization group invariance (cutoff-independences) ← systematic errors
- Simulation with sign-problem-free interaction + perturbation theory
  - Sign-problem-free interaction with phenomenological precision
  - Second-order perturbative algorithm
- Observation of RG-invariance with precision calculations
- Algorithm enabling applications to finite-temperature systems