Ab initio nuclear physics from the Lattice Effective Field Theory

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Nuclear Lattice EFT Collaboration

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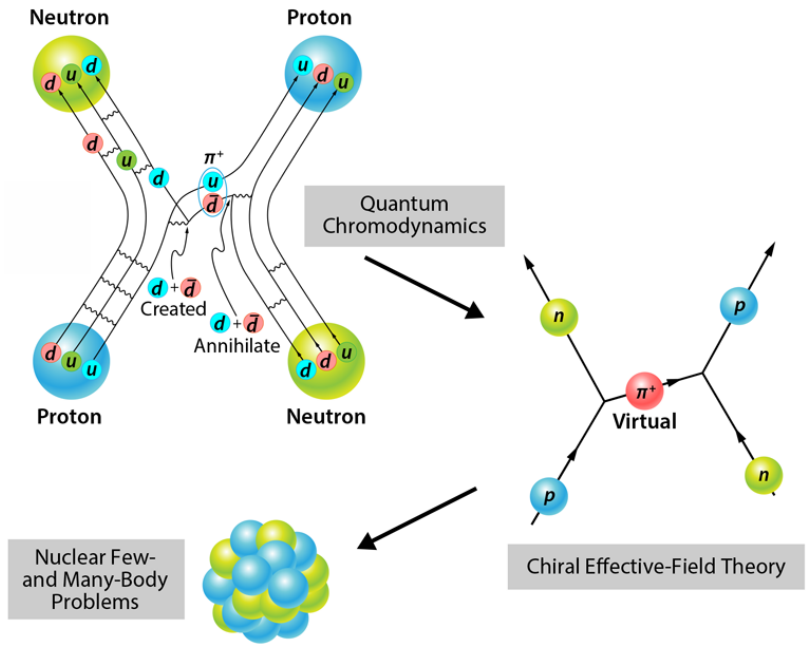
Chiral effective field theory

Chiral EFT: The low-energy equivalence of the QCD

Weinberg (1979,1990,1991), Gasser, Leutwyler (1984,1985)

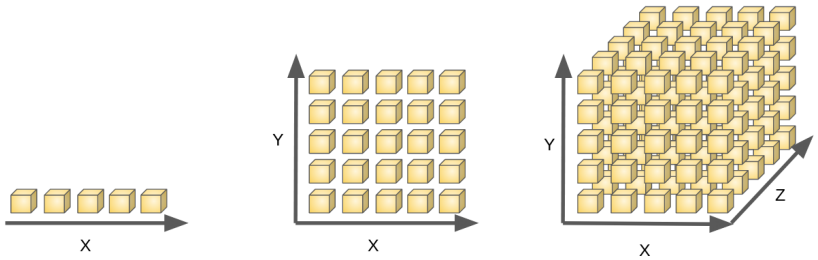
- Proton (uud), neutron (udd), pion ($u\bar{d}$)
- Spontaneously broken chiral symmetry: $SU(2)_L \times SU(2)_R \to SU(2)_V$
- Goldstone theorem implies a light pion: Long-range part of the nuclear force
- Contact terms: Short-range part of the nuclear force
- Hard scale: $\Lambda_\chi \sim 1$ GeV: Chiral EFT works for momentum $Q \ll \Lambda_\chi$

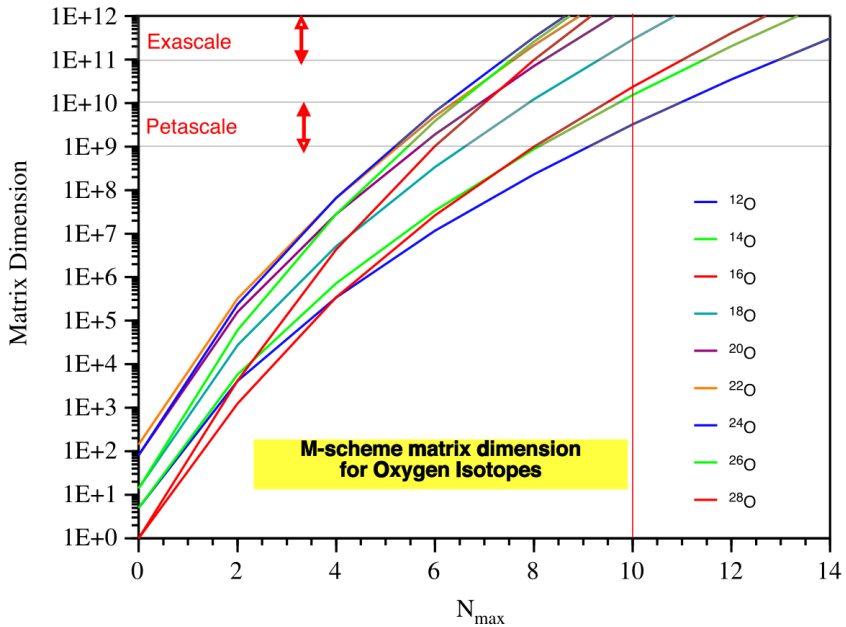


Quarks confined in nucleons and pions

Dimensionality curse in nuclear many-body problems

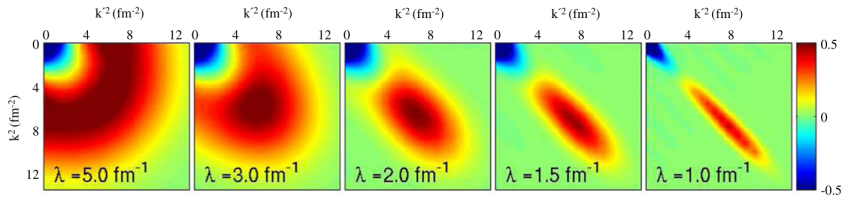
Exponential increase of resources



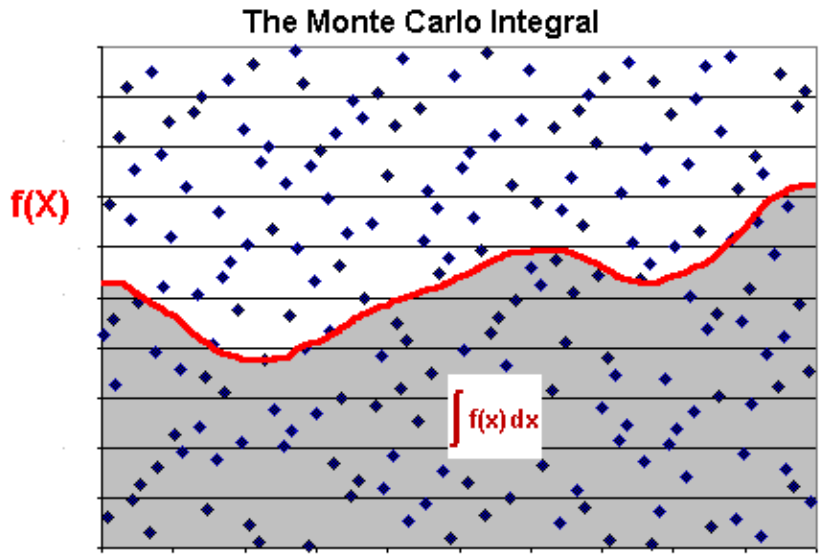


PRC 101, 014318 (2020)

Solution 1: Reduce effective Hilbert space with SRG evolution



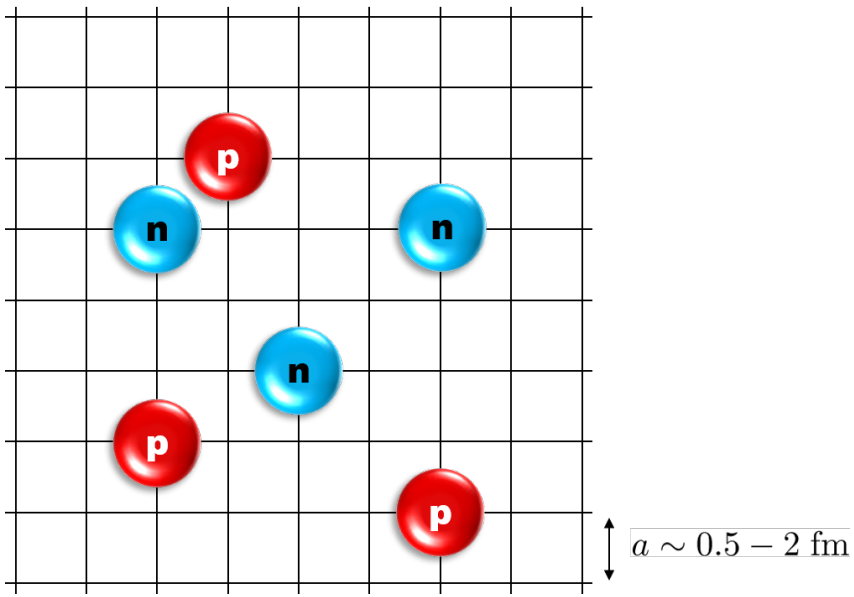
Solution 2: Monte Carlo algorithms



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)

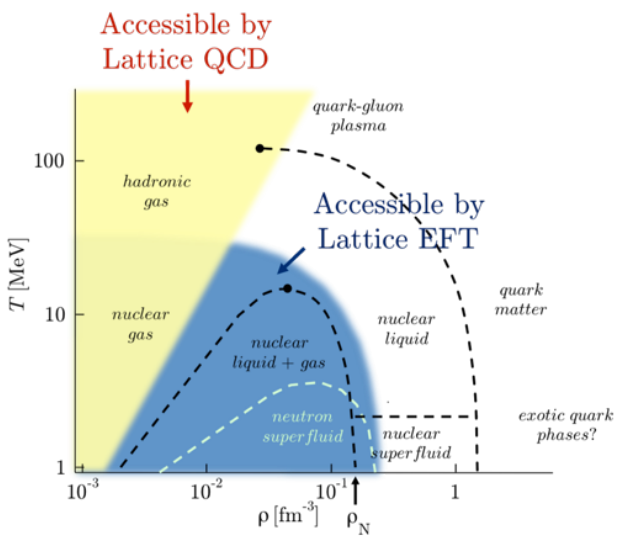
- Discretized chiral nuclear force
- Lattice spacing $a \approx 1$ fm $= 620$ MeV (∼chiral symmetry breaking scale)
- Protons & neutrons interacting via **short-range, δ-like** and **long-range, pion-exchange** interactions
- Exact method, polynomial scaling ($\sim A^2$)

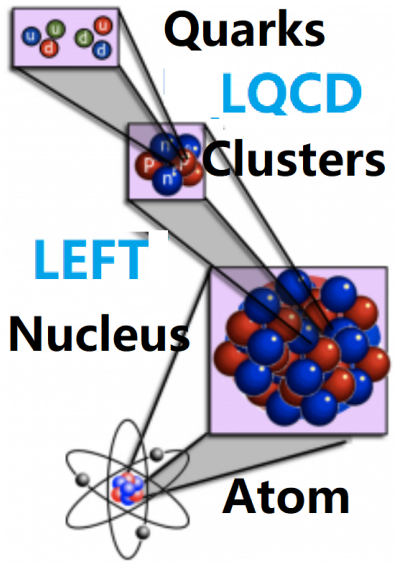


Lattice adapted for nucleus

Comparison to 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

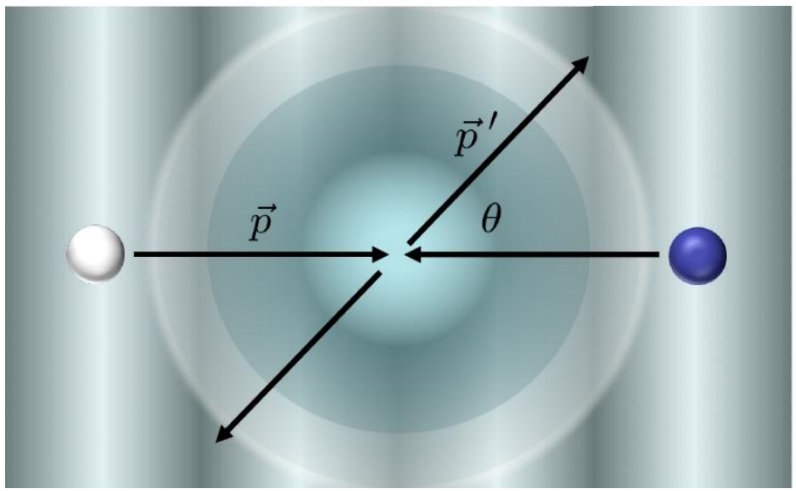




N-N scattering in the center of mass frame

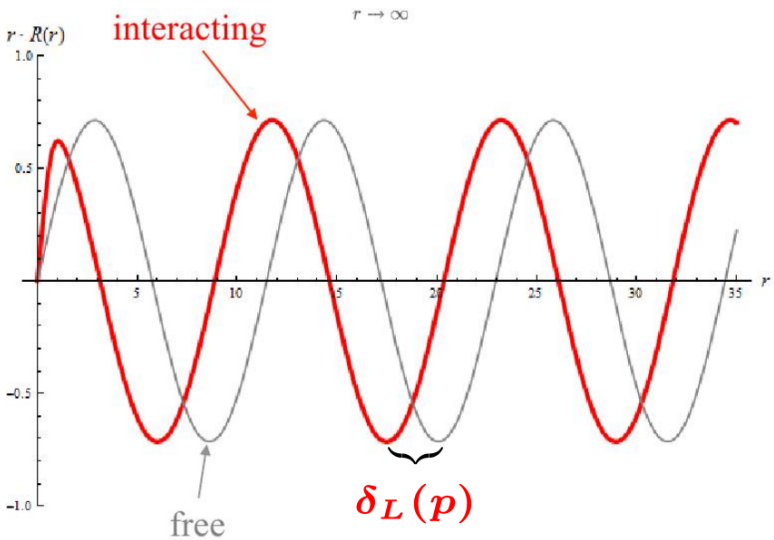
For scattering in the **continuum**:

- Partial wave expansion:
  $\psi(\boldsymbol{r}) = \sum_{J=0}^{\infty} \psi_J(r) P_J(\cos\theta)$
- Asymptotically ($r > R_{\text{force}}$):
  $\psi_J(r) \to A h_J^+(kr) - B h_J^-(kr)$
- Phase shift: $e^{2i\delta} = B/A$



For scattering in a **finite volume**:

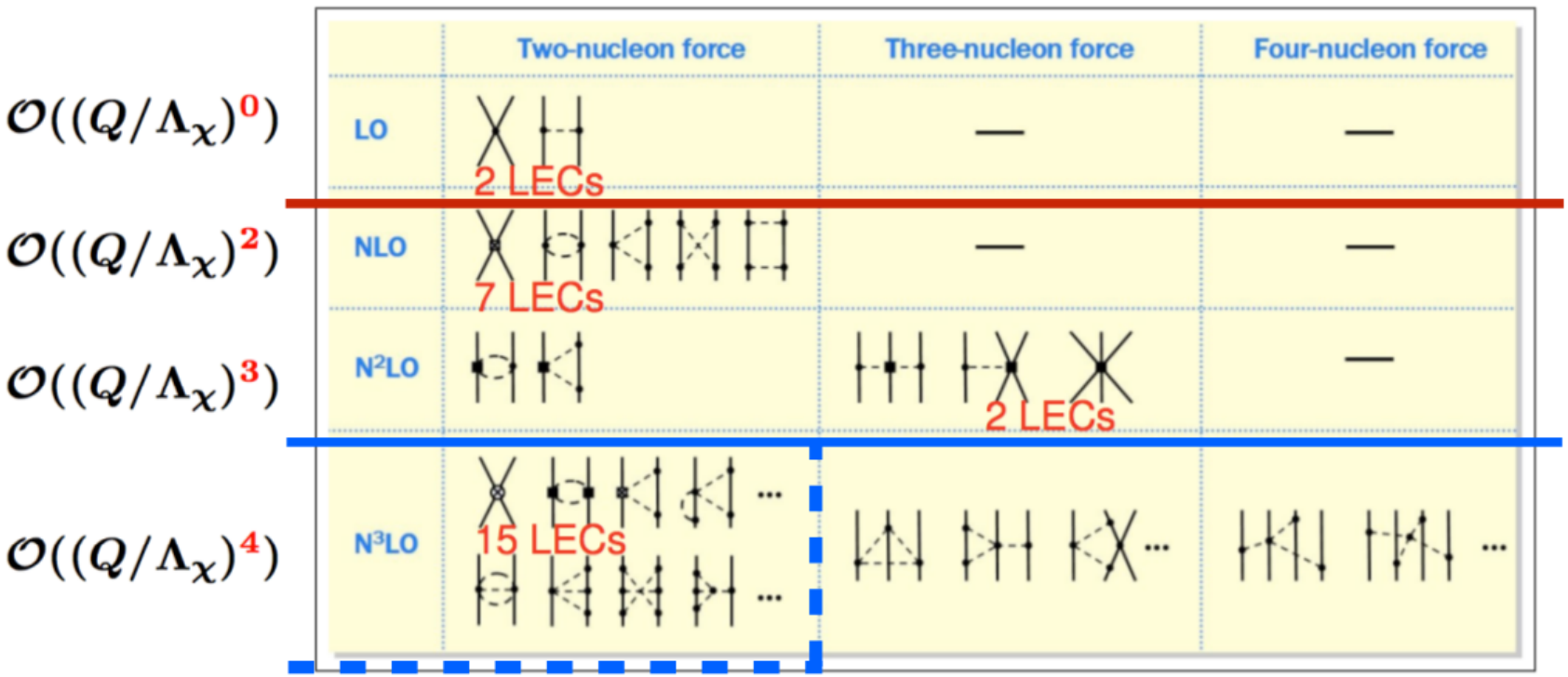
- Luescher's formula:
  $e^{2i\delta} = \frac{Z_{00}(1;q^2)+i\pi^{3/2}q}{Z_{00}(1;q^2)-i\pi^{3/2}q}, \quad \boldsymbol{q} = \frac{2\pi \boldsymbol{n}}{L}$
  $Z_{00}(s,q^2) = \frac{1}{\sqrt{4\pi}} \sum_{\boldsymbol{n}} \frac{1}{(\boldsymbol{n}^2-\boldsymbol{q}^2)^s}$
- Standard tool in LQCD
  Beane et al., Int. J. Mod. Phys. E 17(2008) 1517
- Not applicable in LEFT: noisy data, need higher precision



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



Euclidean time projection

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

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

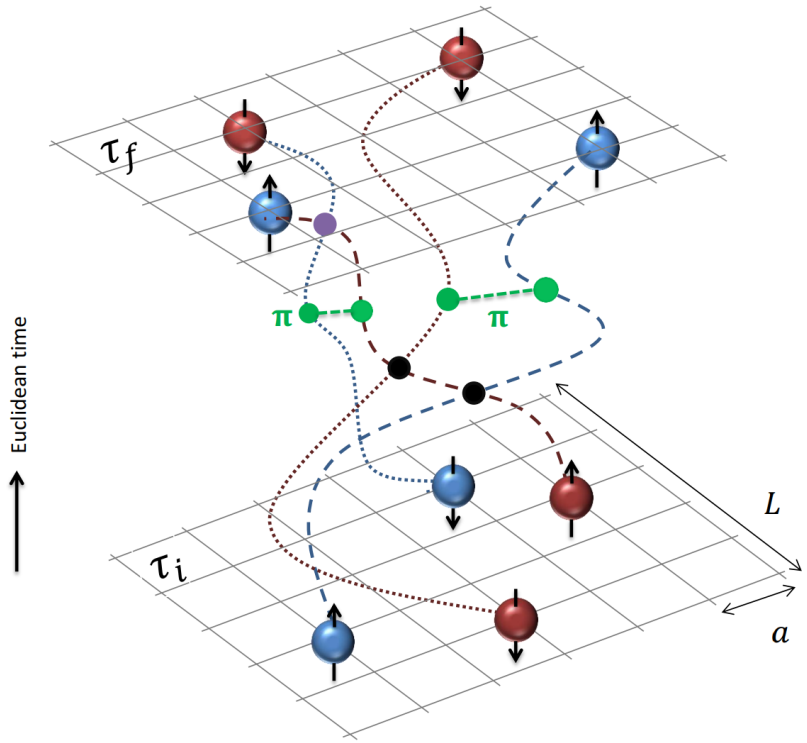
with $|\Psi_A\rangle$ representing A *free* nucleons.

- 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:

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



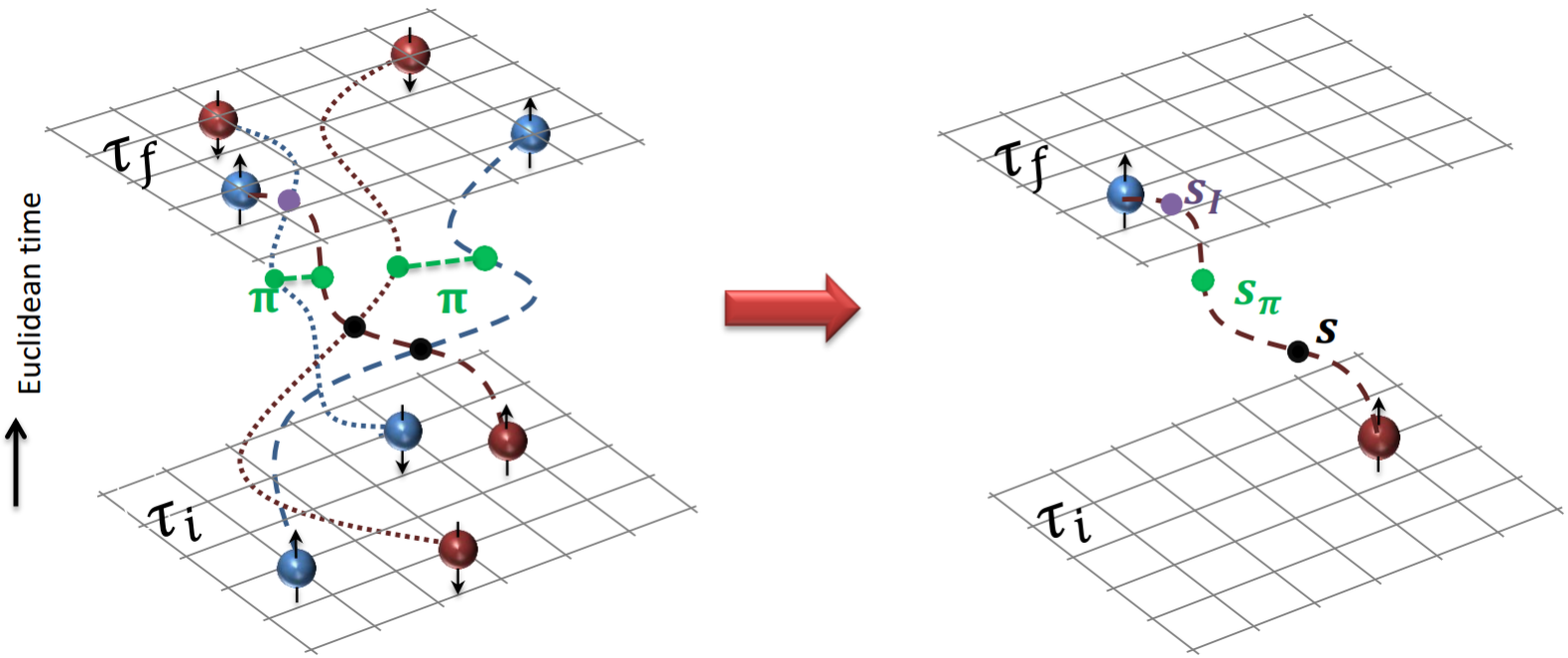
All possible configurations in $\tau \in [\tau_i, \quad \tau_f]$ are sampled.
Complex structures like nucleon clustering emerges naturally.

Auxiliary field transformation

- 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**

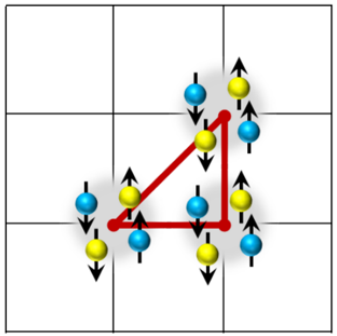


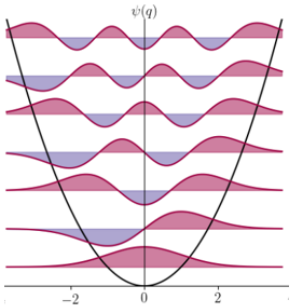
Preparation of trial states

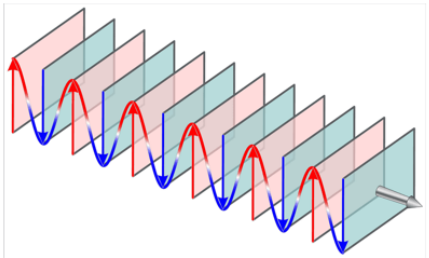
- Trial state can be choosen arbitarily as long as its overlap with real ground state is large.
- A convenient choice is Slater determinant

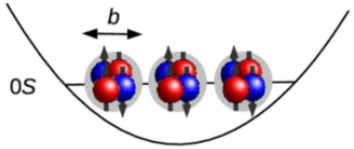
$$|\Psi\rangle = \begin{vmatrix} \psi_1(\boldsymbol{r}_1) & \psi_1(\boldsymbol{r}_2) & \cdots & \psi_1(\boldsymbol{r}_A) \\ \psi_2(\boldsymbol{r}_1) & \psi_2(\boldsymbol{r}_2) & \cdots & \psi_2(\boldsymbol{r}_A) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_A(\boldsymbol{r}_1) & \psi_A(\boldsymbol{r}_2) & \cdots & \psi_A(\boldsymbol{r}_A) \end{vmatrix}$$

- The single-particle wave functions can be either
  - Gaussian wave packets
  - Shell model wave functions
  - Plane waves
  - Alpha cluster wave functions









Evolution of Slater determinants

In imaginary time evolution, each s.p. wave function evolves independently

$$M(s_{n_t})(\psi_1 \wedge \psi_2 \wedge \cdots \wedge \psi_A) = M(s_{n_t})\psi_1 \wedge M(s_{n_t})\psi_2 \wedge \cdots \wedge M(s_{n_t})\psi_A,$$

because there is no direct interactions between nucleons.

Monte Caro integration technique

- We are interested in the ratio

$$\langle O\rangle = \lim_{\tau\to\infty} \frac{\int \mathscr{D}s \langle \Psi_T | M(s_{L_t}) \cdots M(s_{L_t/2+1}) O M(s_{L_t/2}) \cdots M(s_1) | \Psi_T \rangle}{\int \mathscr{D}s \langle \Psi_T | M(s_{L_t}) \cdots M(s_1) | \Psi_T \rangle} = \lim_{\tau\to\infty} \frac{\int \mathscr{D}s \mathscr{M}_O(s)}{\int \mathscr{D}s \mathscr{M}(s)}$$

$$= \lim_{\tau\to\infty} \frac{\int \mathscr{D}s |\mathscr{M}(s)| \frac{\mathscr{M}_O(s)}{|\mathscr{M}(s)|}}{\int \mathscr{D}s |\mathscr{M}(s)| \frac{\mathscr{M}(s)}{|\mathscr{M}(s)|}} = \lim_{\tau\to\infty} \frac{\langle \frac{\mathscr{M}_O(s)}{|\mathscr{M}(s)|} \rangle}{\langle \frac{\mathscr{M}(s)}{|\mathscr{M}(s)|} \rangle}$$

  In last step we rewrite the integral into an expectation value in a ensamle of s fields with probability distribution $P(s) \propto |\mathscr{M}(s)|$. Note that the overall normalization factors are always canceled.

- We need to generate the s fields with probability $P(s)$, this can be achieved with the Metropolis algorithm
  - For any fixe s, generate a random new configuration s'
  - Compute the ratio $\eta_{s\to s'} = \frac{P(s')}{P(s)} = \frac{|\mathscr{M}(s')|}{|\mathscr{M}(s)|}$
  - Choose a random number $r \in U(0,1)$
  - If $\eta_{s\to s'} > r$, accept; otherwise reject.
- Wait until the s-ensamle converge to the desired distribution $P(s) \propto |\mathscr{M}(s)|$.
- Choose N samples s_1, s_2, $\cdots$, s_N in the s-ensamle, calculate $\mathscr{M}(s_k)$ and $\mathscr{M}_O(s_k)$ seperately. Then the expectation value can be estimated unbiasly as

$$\langle O\rangle = \lim_{\tau\to\infty} \frac{\sum_k \mathscr{M}_O(s_k)/|\mathscr{M}(s_k)|}{\sum_k \mathscr{M}(s_k)/|\mathscr{M}(s_k)|},$$

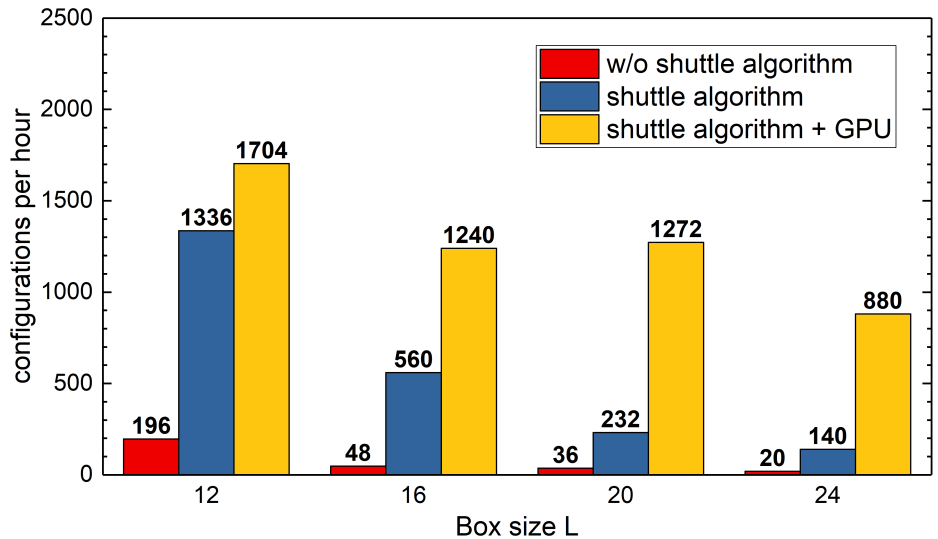
  with a statistical error scales as $\mathscr{O}(1/\sqrt{N})$.

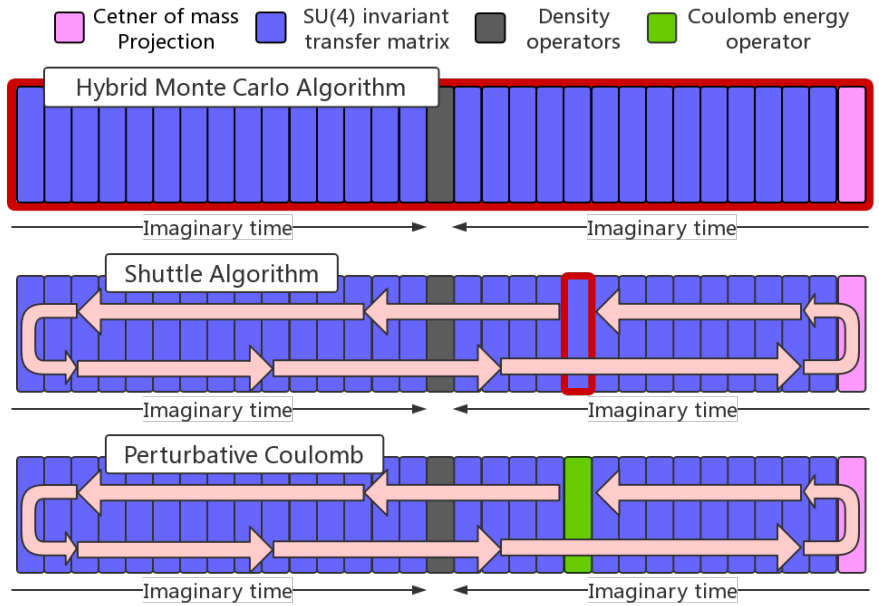
All $L_t \times L^3$ auxiliary fields $s_{\boldsymbol{n},\boldsymbol{n}_t}$ need to be updated. Two algorithms:

- **Update all fields once every iteration: Hybrid Monte Carlo**
- **Update a single time slice every iteration: Shuttle Algorithm**

B.L., et. al.,PLB 797, 134863 (2019)

SA 5∼10 times faster than HMC





- Can be implemented for GPU
- **Algorithm & Hardware** combined give a 40∼50 times speed-up

Large lattices are accessible

Essential elements of the nuclear force

We use a zeroth order lattice Hamiltonian that respects the Wigner-SU(4) symmetry

$$H_0 = K + \frac{1}{2} C_{\mathrm{SU4}} \sum_{\boldsymbol{n}} : \tilde{\rho}^2(\boldsymbol{n}) :$$

The smeared density operator $\tilde{\rho}(\boldsymbol{n})$ is defined as

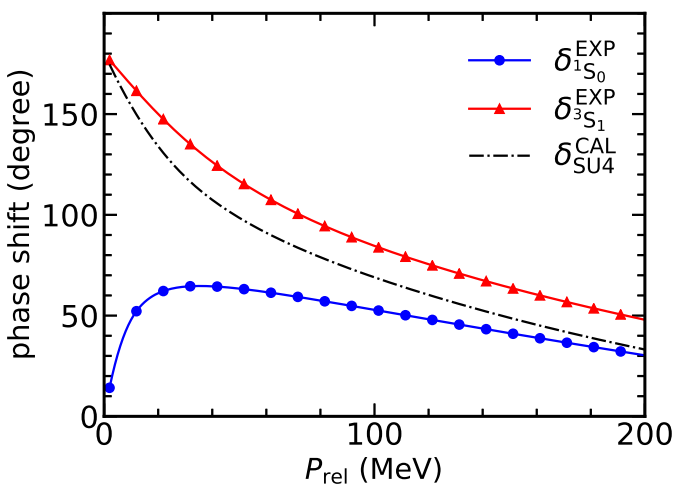
$$\tilde{\rho}(\boldsymbol{n}) = \sum_i \tilde{a}_i^\dagger(\boldsymbol{n}) \tilde{a}_i(\boldsymbol{n}) + s_L \sum_{|\boldsymbol{n}'-\boldsymbol{n}|=1} \sum_i \tilde{a}_i^\dagger(\boldsymbol{n}') \tilde{a}_i(\boldsymbol{n}'), \tag{1}$$

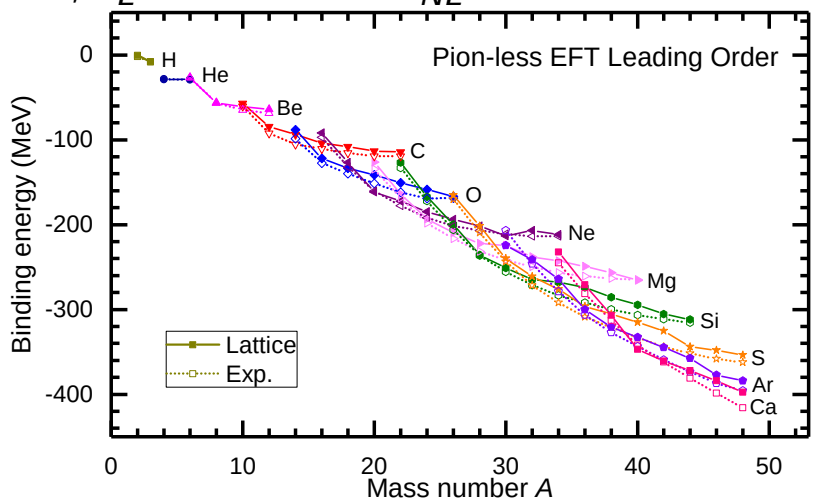
where i is the joint spin-isospin index

$$\tilde{a}_i(\boldsymbol{n}) = a_i(\boldsymbol{n}) + s_{NL} \sum_{|\boldsymbol{n}'-\boldsymbol{n}|=1} a_i(\boldsymbol{n}'). \tag{2}$$

In this work we use a lattice spacing $a = 1.32$ fm and the parameter set

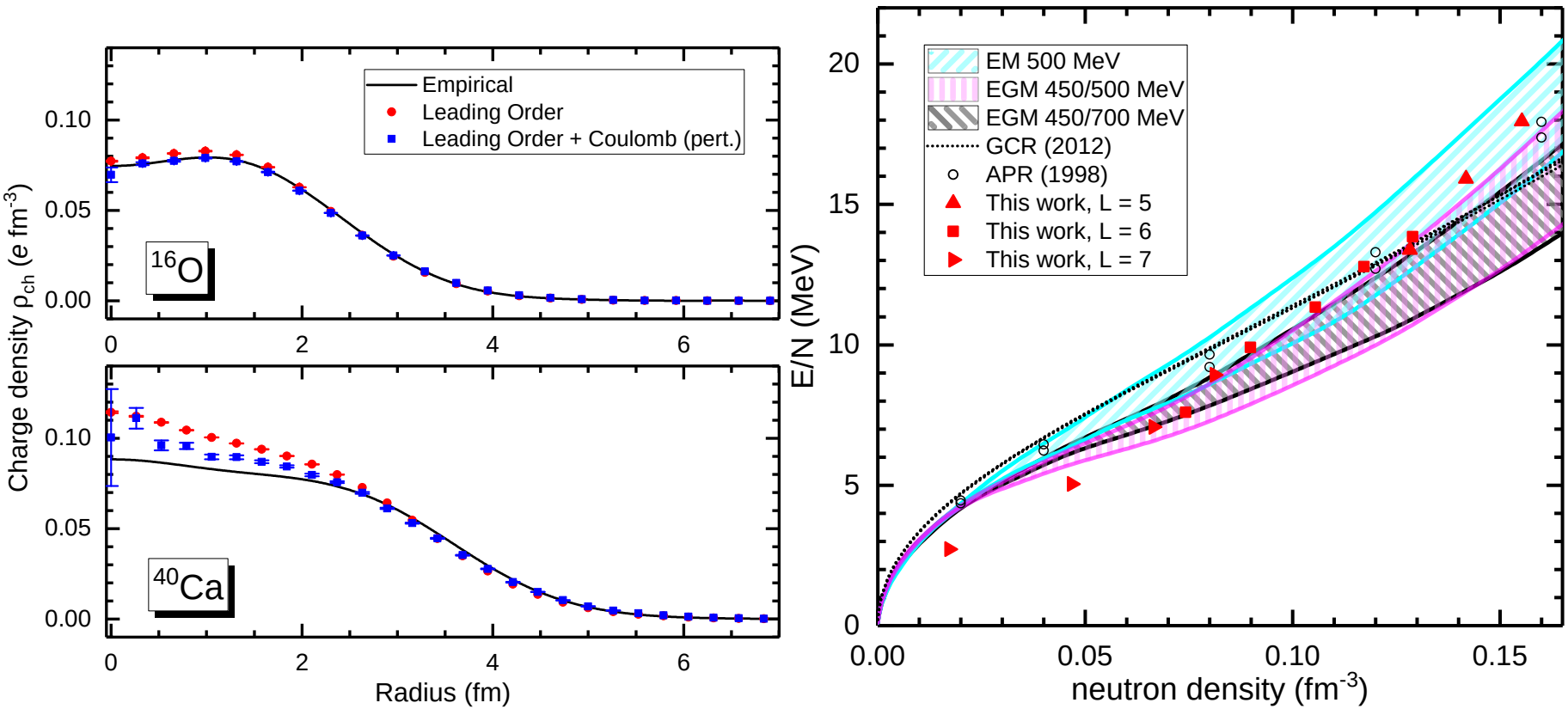
$C_{\mathrm{SU4}} = -3.41 \times 10^{-7}$ MeV^{-2}, $s_L = 0.061$ and $s_{NL} = 0.5$.





Essential elements for nuclear binding

Charge density and neutron matter equation of state
are impotant in element creation, neutron star merger, etc.



Lu *et al.*, PLB 797, 134863 (2019)

Perturbative quantum Monte Carlo method

Table: The nuclear binding energies at different orders calculated with the ptQMC. $E_{\rm exp}$ is the experimental value. All energies are in MeV. We only show statistical errors from the MC simulations.

	E_0	δE_1	E_1	δE_2	E_2	$E_{\rm exp}$
^{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

Realistic N^{2}LO chiral Hamiltonian fixed by few-body data + perturbative quantum MC simulation = nice agreement with the experiments

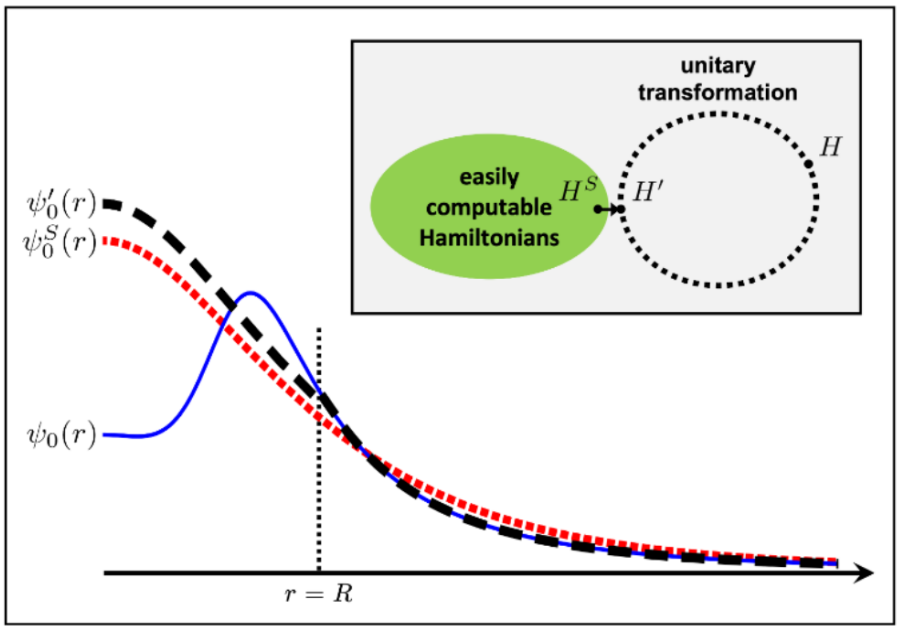
Excellent agreement $\Longrightarrow$ Demonstration of **nuclear force** & **many-body algorithm**

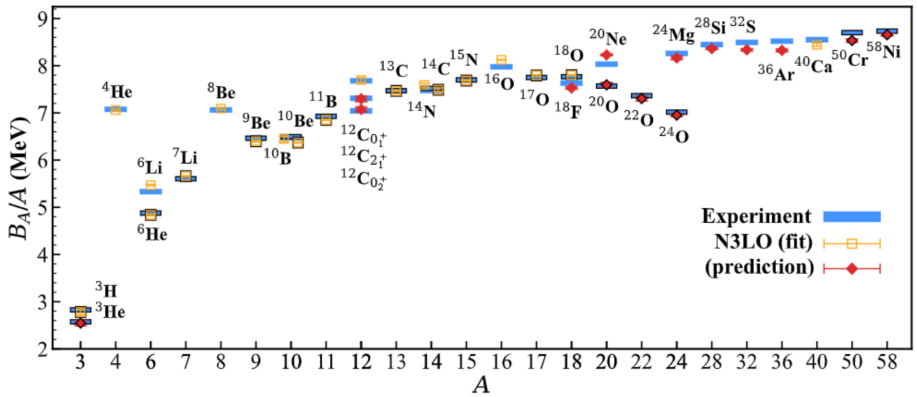
Also applicable for densities & matrix elements
Lu *et al.*, PRL 128, 242501 (2022)

Wave function matching method

Unitarily transformed Hamiltonian $H \to H' = UHU^\dagger$ reproduce the same **low-energy** (large-scale) physics

$\Longrightarrow$Design an operator U that H' is much easier to handle than H (e.g., H' with weaker sign problem in Monte Carlo)



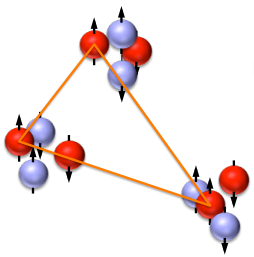


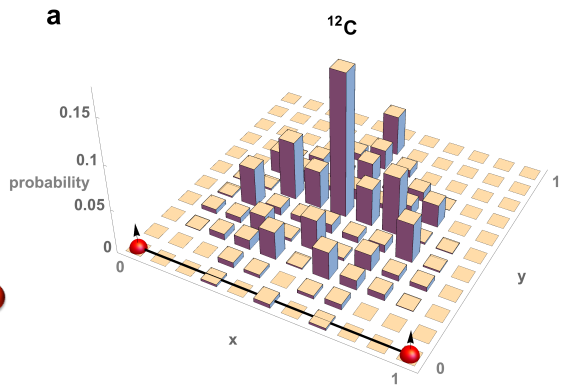
S. Elhatisari *et al.*, arXiv:2210.17488, accepted by Nature

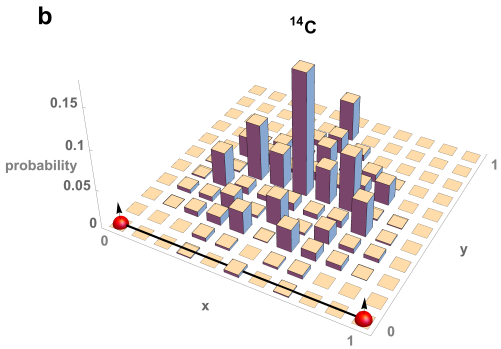
Many-body correlations: α-cluster geometry in C isotopes

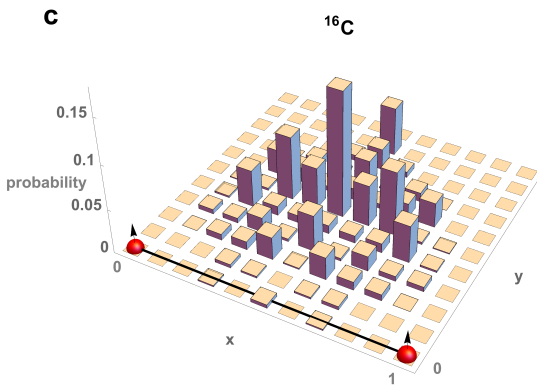
We always align the longest edge with the x-axis
and keep the triangle in the x-y plane.

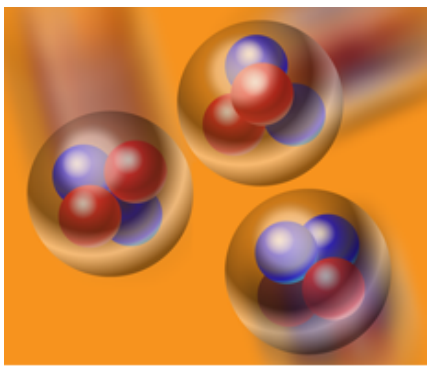
$$\rho(d_1,d_2,d_3) = \sum_{j_1,j_2,j_3} \sum_{\boldsymbol{n}_1,\boldsymbol{n}_2,\boldsymbol{n}_3} |\Phi_{\uparrow,j_1,\uparrow,j_2,\uparrow,j_3}(\boldsymbol{n}_1,\boldsymbol{n}_2,\boldsymbol{n}_3)|^2 \times \sum_{P(123)} \delta(|\boldsymbol{n}_1-\boldsymbol{n}_2|-d_3)\delta(|\boldsymbol{n}_1-\boldsymbol{n}_3|-d_2)\delta(|\boldsymbol{n}_2-\boldsymbol{n}_3|-d_1),$$







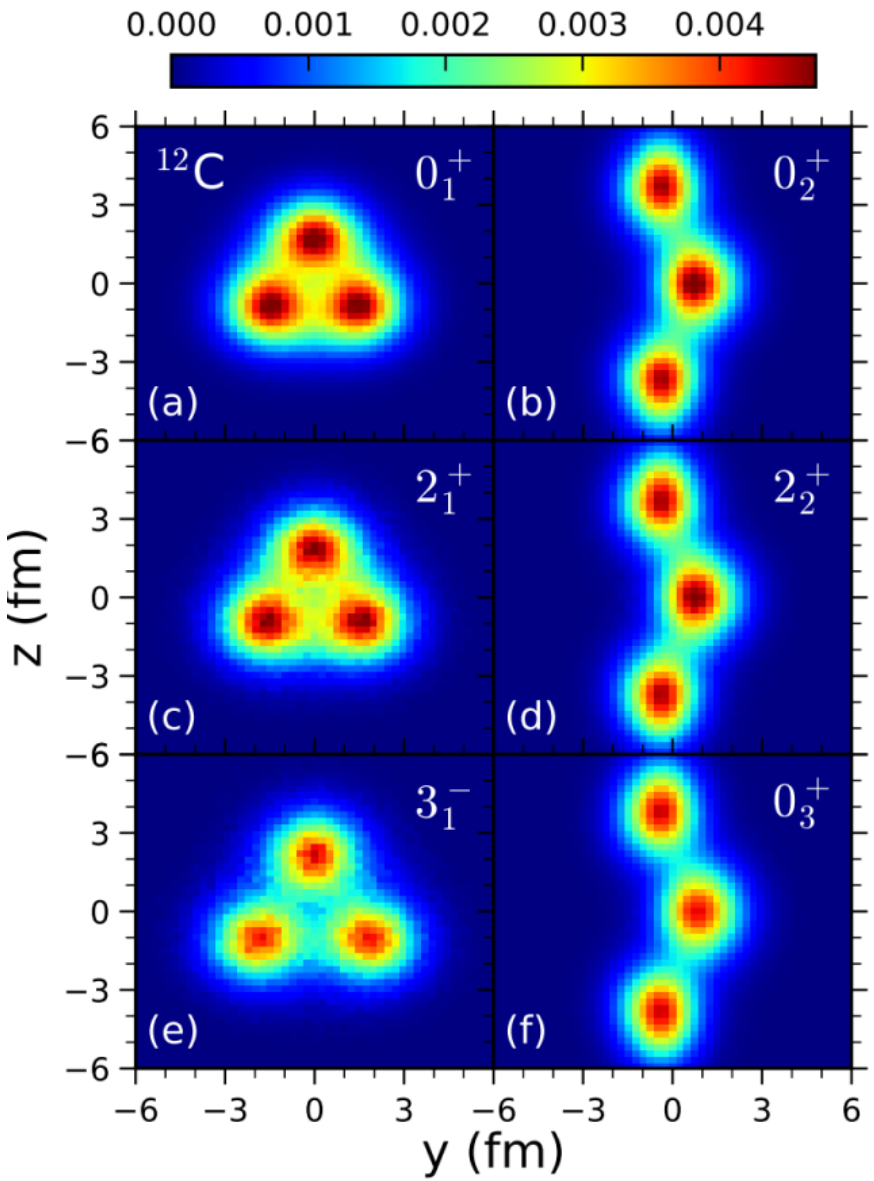




- **Hoyle state**: Triple-α resonance, essential for creating ^{12}C in stars (Hoyle, 1954). *Fine-tuning for life?*

  Epelbaum et al., PRL 106, 192501 (2011)
  Elhatisari et al., PRL 119, 222505 (2017)

Clustering from first principle: Tomographic scan of ^{12}C

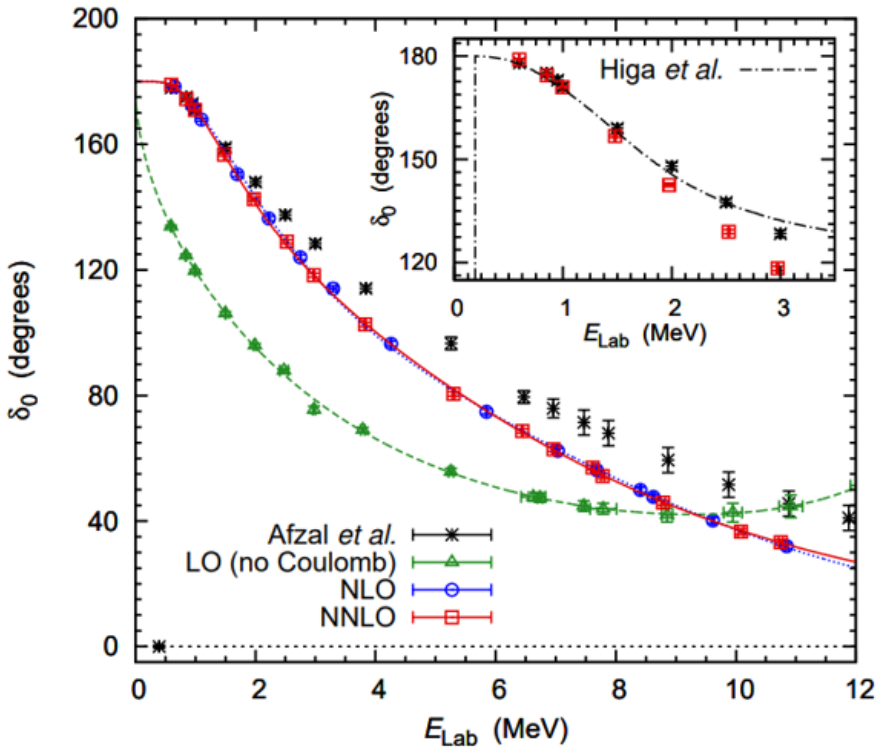


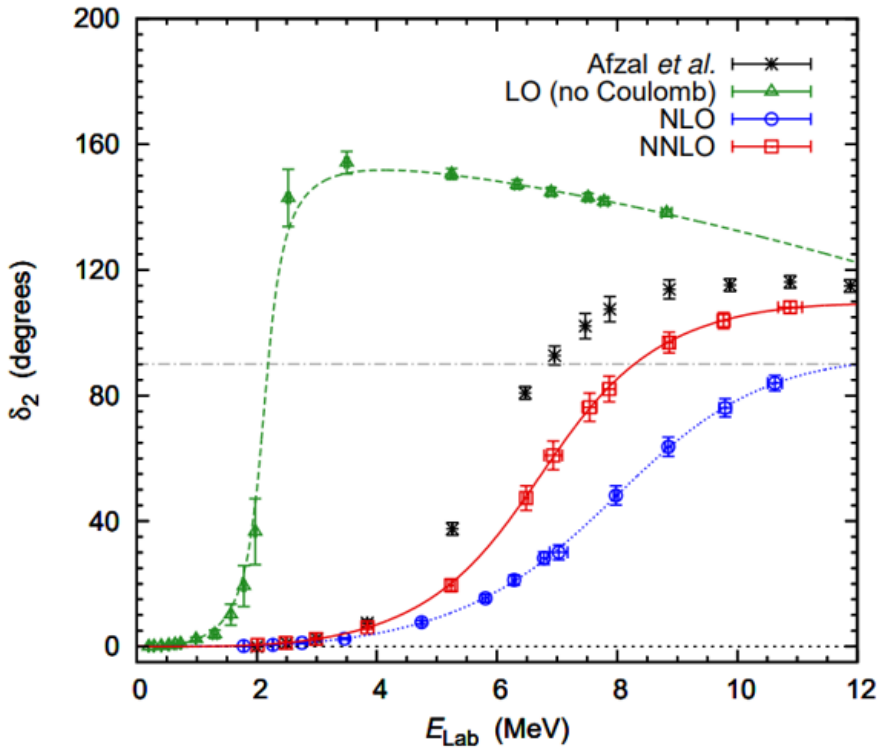
- Structure of ^{12}C states are full of complexity and duality (clustering v.s. mean-field)
- we provide the first model-independent tomographic scan of the three-dimensional geometry of the nuclear states of 12C using the ab initio framework of nuclear lattice EFT.
- 0_1^+: ground state, 0_2^+: Hoyle state

Shihang Shen et al., Nat. Comm. 14, 2777 (2023)

α-α scattering from lattice EFT

Ab-initio alpha-alpha scattering N2LO





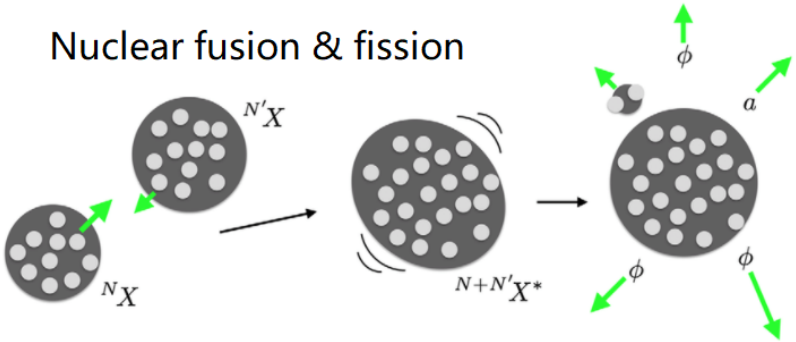
Afzal, Ahmad, Ali, *Rev. Mod. Phys.* 41, 247, (1969).

Higa, Hammer, van Kolck, *Nucl.Phys.* A809, 171 (2008), 0802.3426.

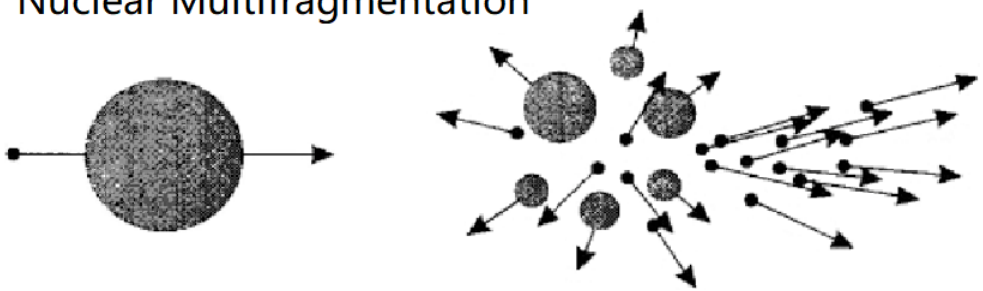
S.E., Lee, Rupak, Epelbaum, Krebs, Lähde, Luu, & Meißner. *Nature* 528, 111-114 (2015).

Hot nucleus with pinhole trace algorithm

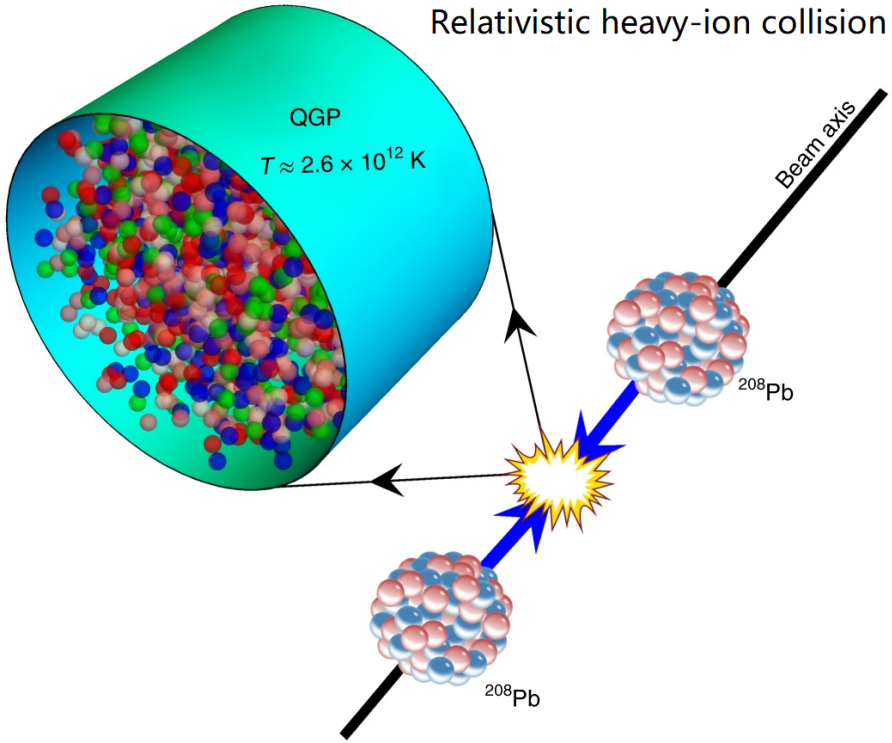
Nuclear fusion & fission

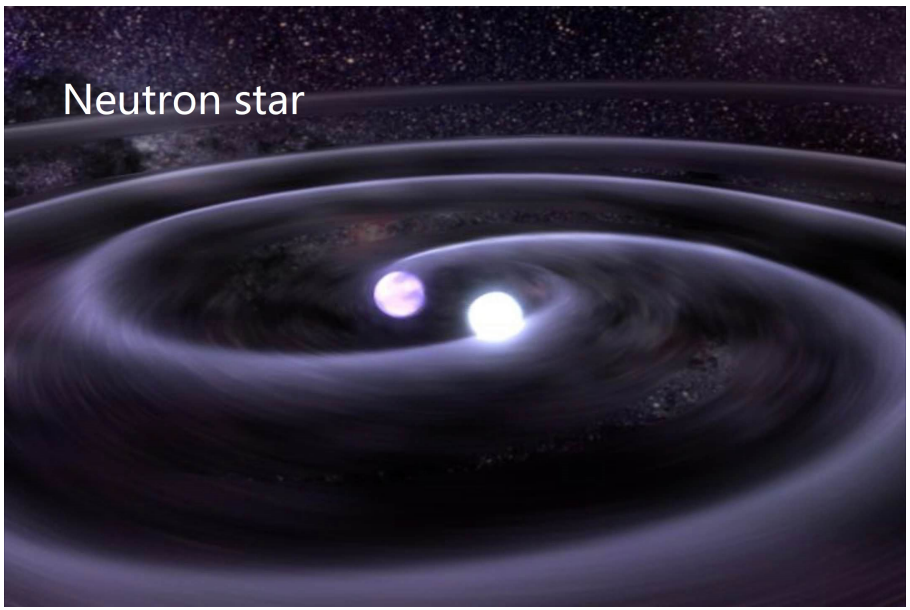


Nuclear Multifragmentation



Relativistic heavy-ion collision



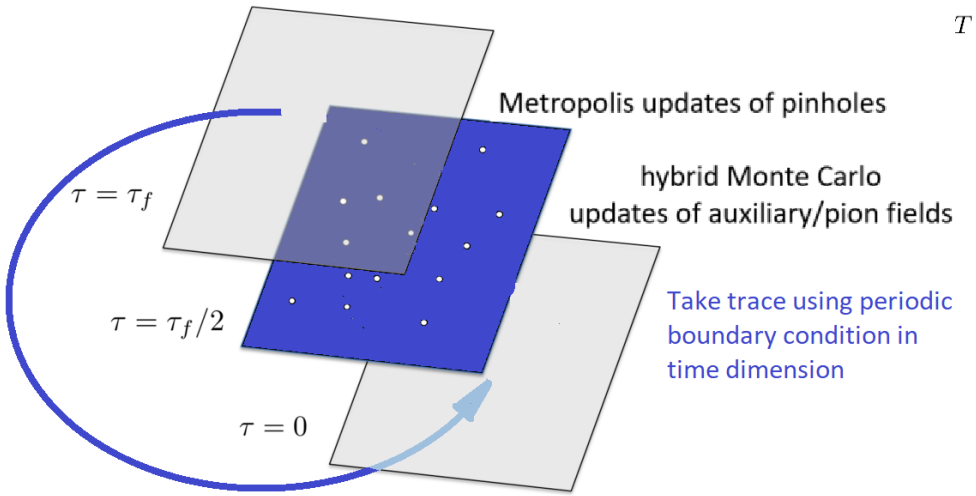


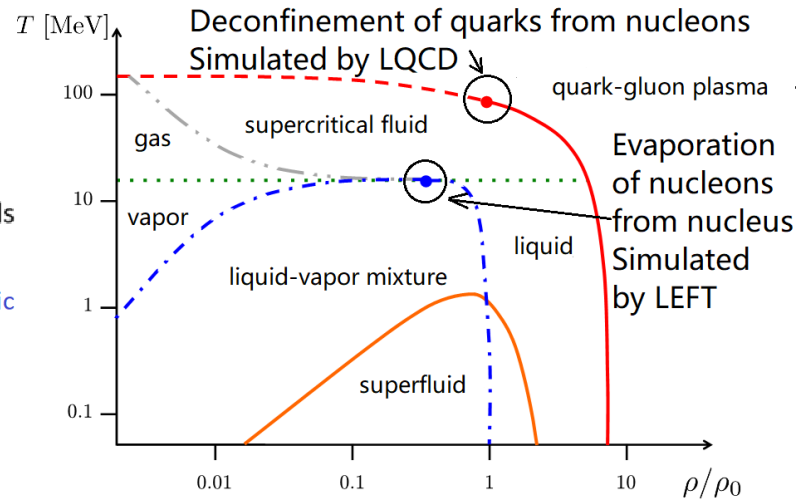
Simulate canonical ensemble with pinhole trace algorithm

- 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:

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

- **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.

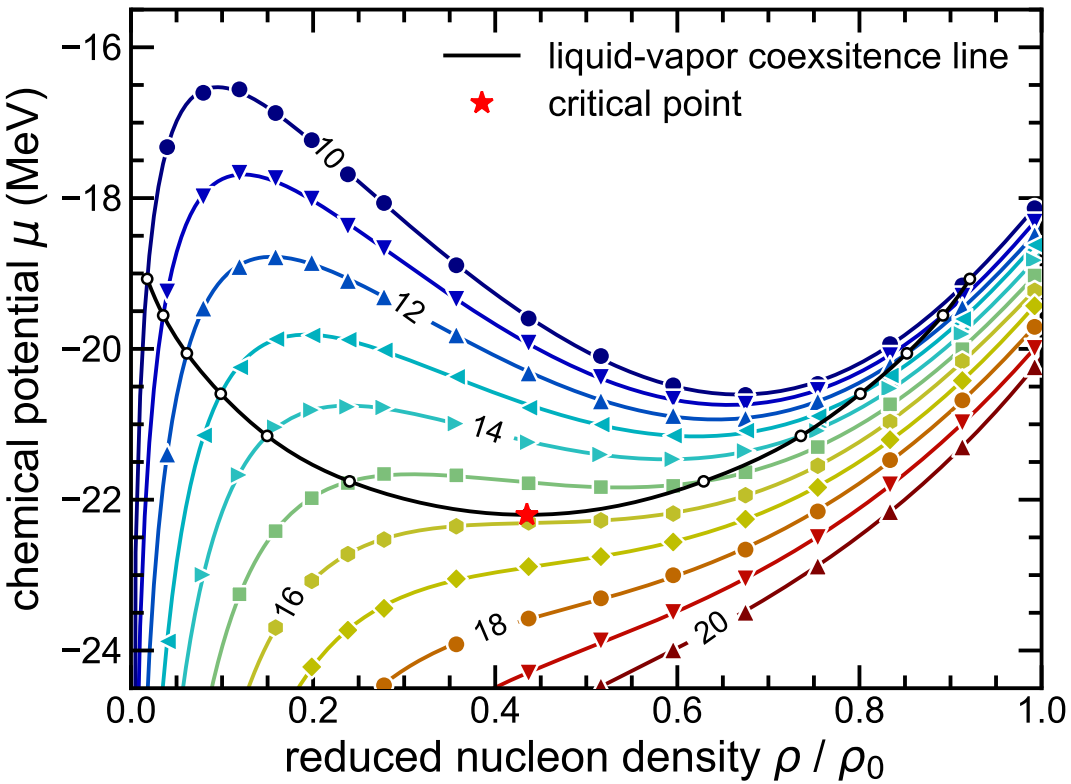


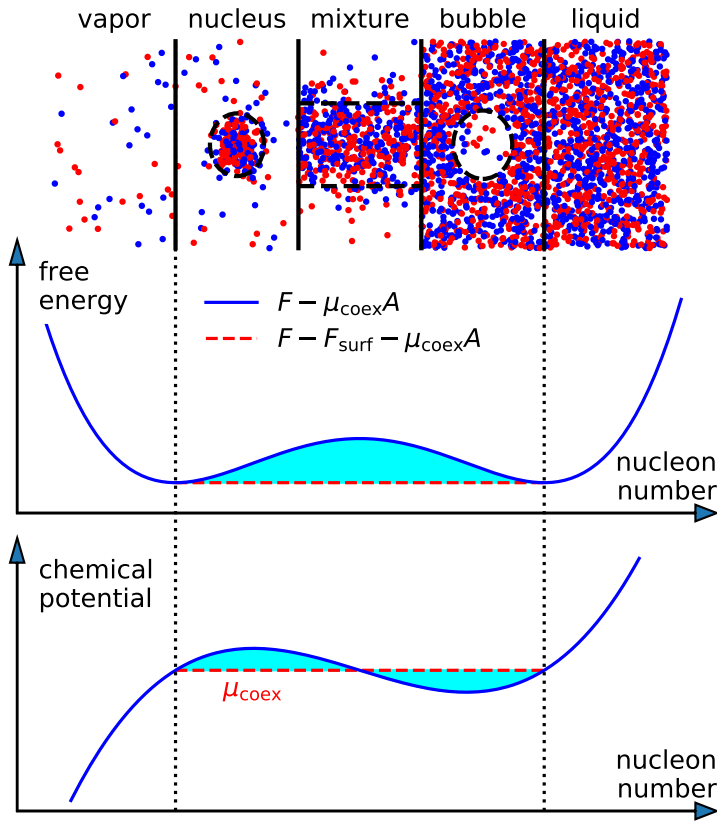


Lu et al., PRL 125, 192502 (2020)

Finite nuclear systems: Liquid-vapor coexistence line

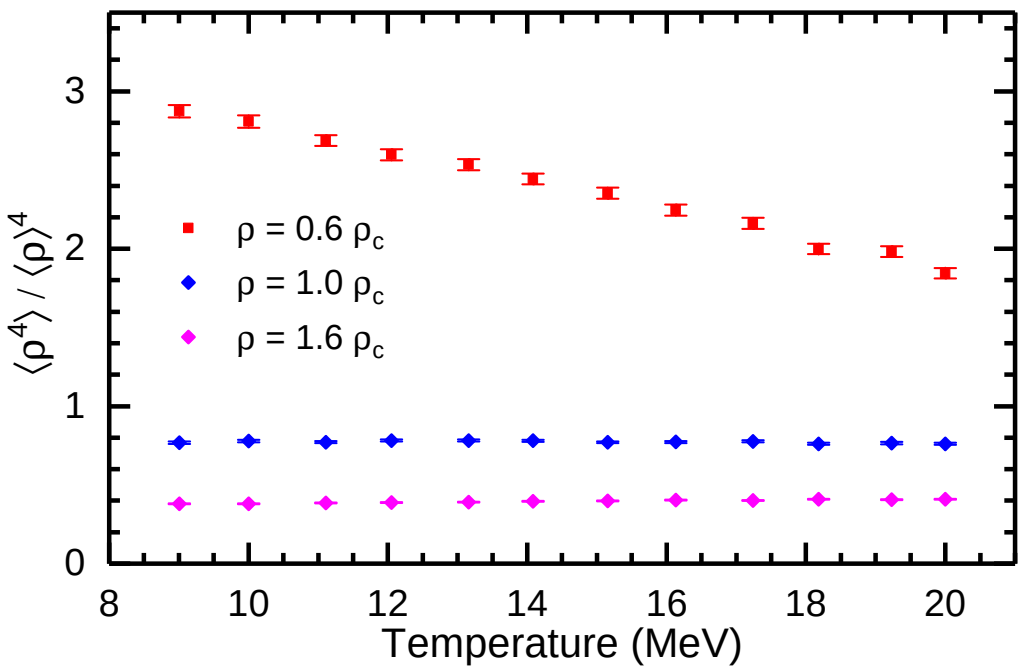
- First ***ab initio* calculation** of **nuclear liquid-gas phase transition**.
- Symmetric nuclear matter $N = Z$, lattice spacing $a = 1.32$ fm, volume $V = (6a)^3$, nucleon number $4 \leq A \leq 132$.
- Temperature 10 MeV$\leq T \leq$ 20 MeV, temporal step $\Delta\beta = 1/2000$ MeV^{-1}.
- 288000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





Other observables: Clustering in hot nuclear matter

- Mean field models can yield **bulk properties**. However, microscopic observables like **clustering** play important role in experiments.
- **Fisher's droplet model** see hot nucleus as a mixture of small droplets, F = volume term + surface terms, **not microscopic**.
- ***Ab initio*** calculation unifies all calculations in a **single framework** with **microscopic foundations**.
- Test: Ratio $\langle :\rho^4: \rangle / \langle \rho \rangle^4$ signifies the clustering correlation.

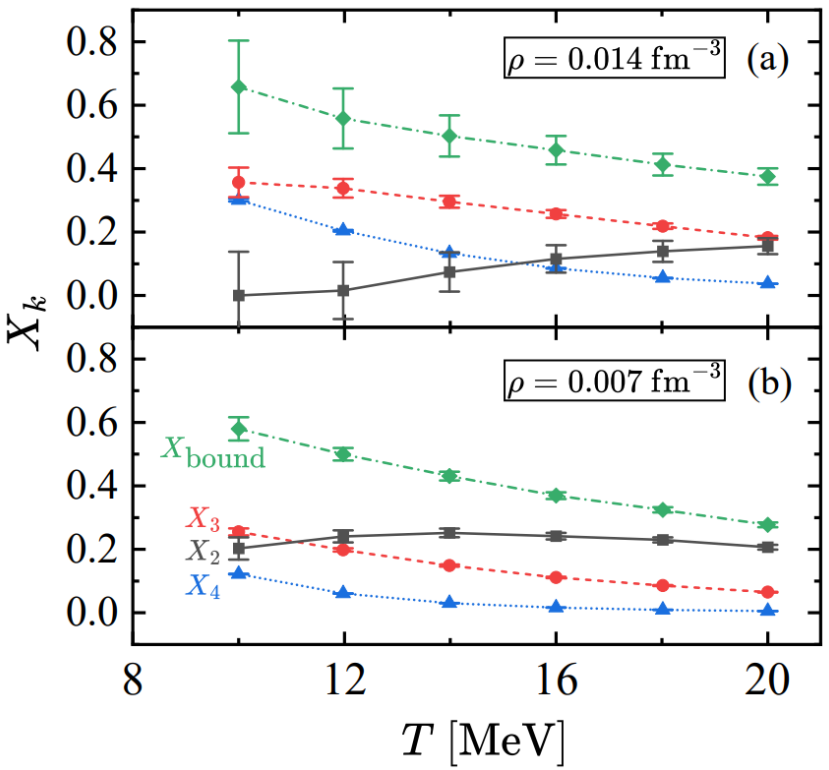


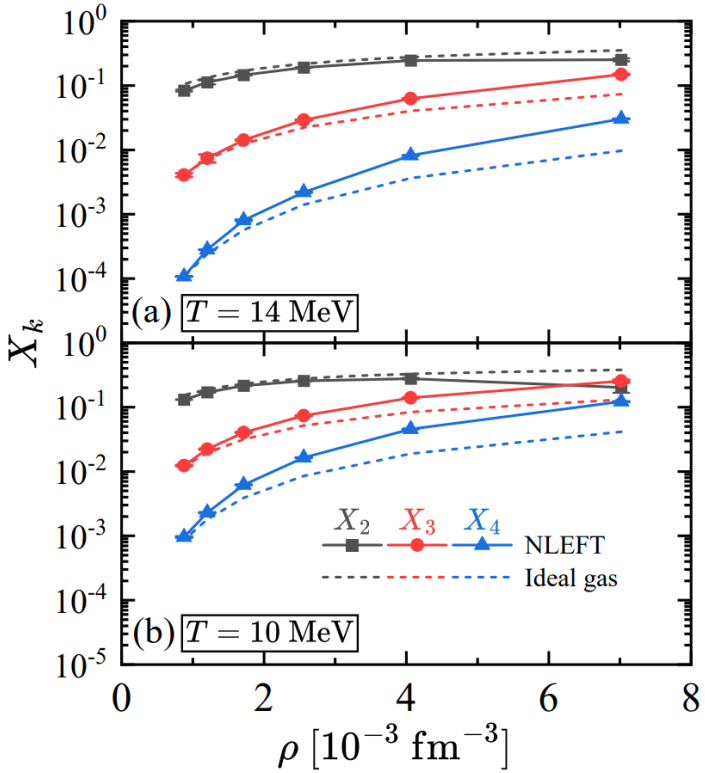
Lu et al., PRL 125, 192502 (2020)

Count clusters in hot nuclear matter

- By expanding the correlation functions on a basis of cluster correlation functions, the probability / mass fraction of clusters can be extracted

$$\langle G_{11}(n)\rangle = \langle G^I_{11}\rangle + w_4\langle G_{11}(n)\rangle_4 + w_3\langle G_{11}(n)\rangle_3 + w_2\langle G_{11}(n)\rangle_2$$
$$\langle G_{21}(n)\rangle = \langle G^I_{21}\rangle + w_4\langle G_{21}(n)\rangle_4 + w_3\langle G_{21}(n)\rangle_3$$
$$\langle G_{31}(n)\rangle = \langle G^I_{31}\rangle + w_4\langle G_{31}(n)\rangle_4$$
$$\langle G_{22}(n)\rangle = \langle G^I_{22}\rangle + w_4\langle G_{22}(n)\rangle_4, \qquad X_k = w_k\, k/A$$





"Ab initio study of nuclear clustering in hot dilute nuclear matter"
ZhengXue Ren et al., PLB 850, 138463 (2024)

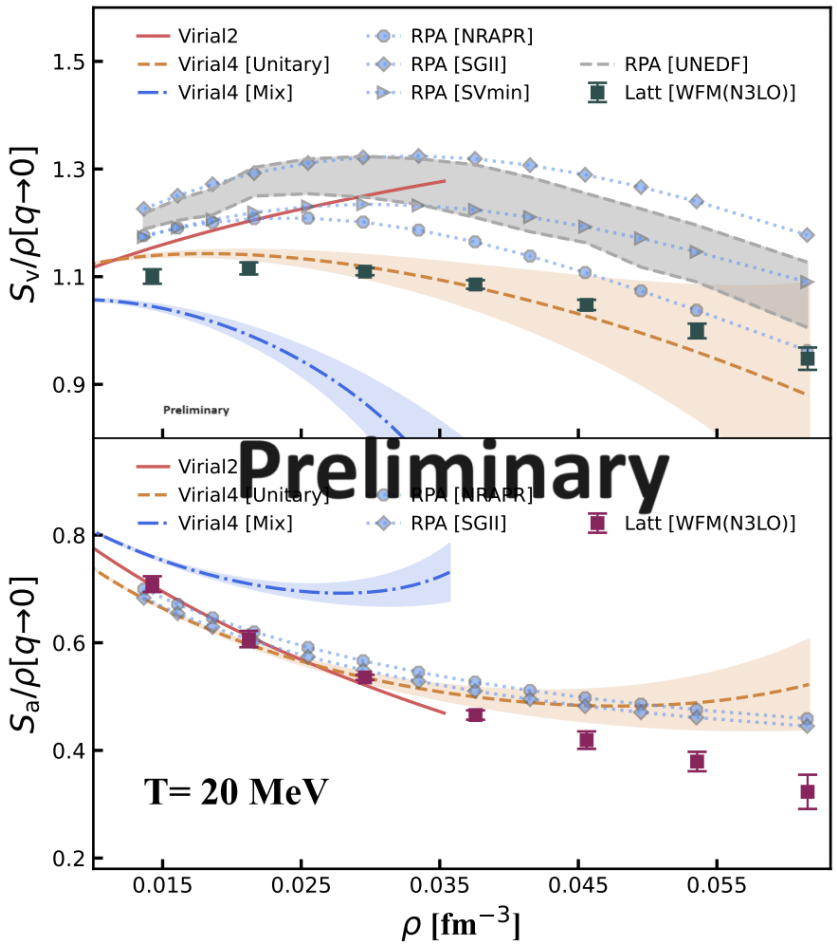
Structure factors with realistic chiral interactions

- 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
- Ab initio calculation with a N^{3}LO chiral interaction based on a rank-one operator method
  YuanZhuo Ma et al., arXiv:2306.04500, accepted by PRL

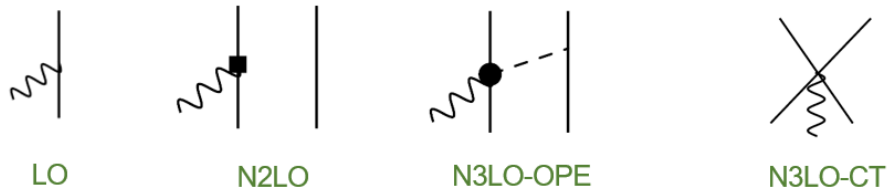


Exploring Nuclear β-decay Through NLEFT

Teng et al. in progress

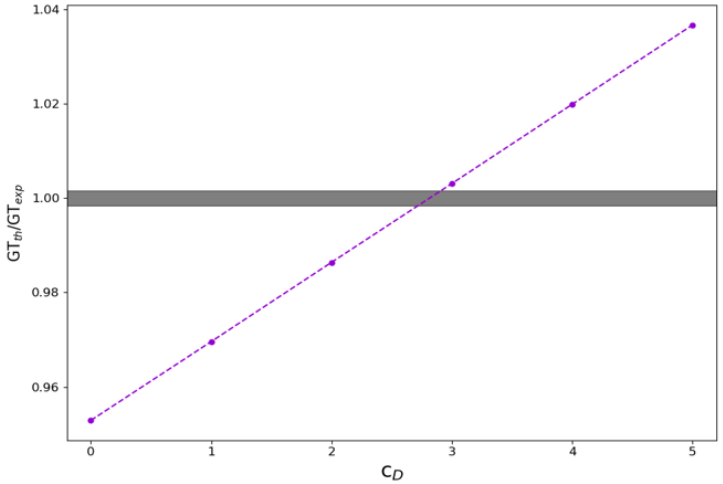
★ The first explorative study on nuclear β-decay via NLEFT.

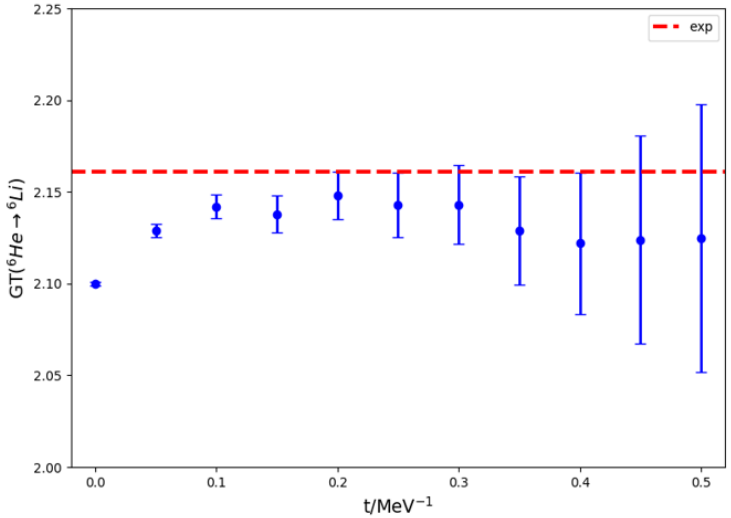
★ N2LO chiral nuclear force + chiral axial current up to N3LO.



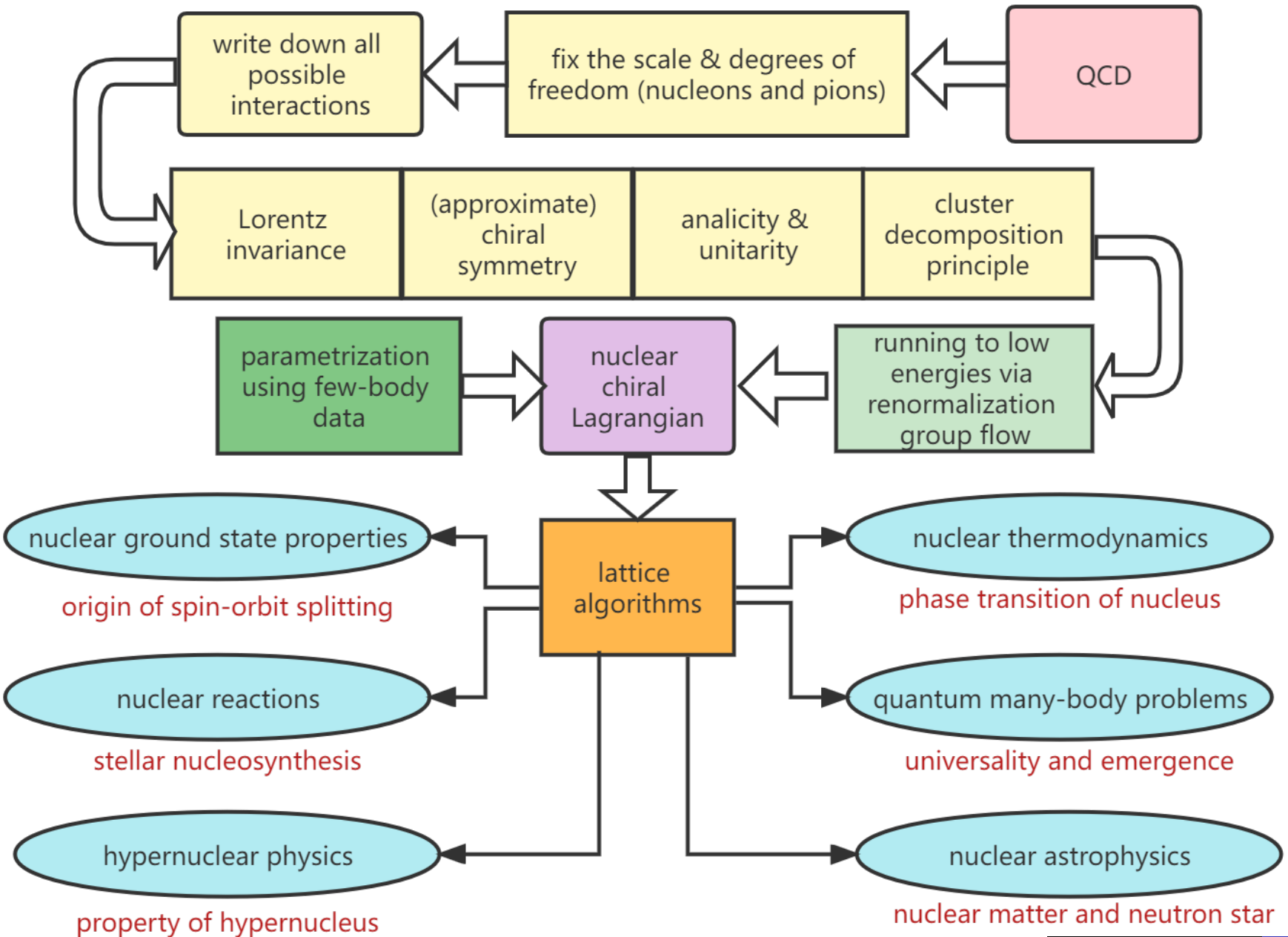
★ ^{3}H β-decay is studied to help determine 3N LECs.

★ Promising results on ^{6}He β-decay.





Summary


write down all possible interactions
fix the scale & degrees of freedom (nucleons and pions)
QCD
Lorentz invariance
(approximate) chiral symmetry
analicity & unitarity
cluster decomposition principle
parametrization using few-body data
nuclear chiral Lagrangian
running to low energies via renormalization group flow
lattice algorithms
nuclear ground state properties
origin of spin-orbit splitting
nuclear thermodynamics
phase transition of nucleus
nuclear reactions
stellar nucleosynthesis
quantum many-body problems
universality and emergence
hypernuclear physics
property of hypernucleus
nuclear astrophysics
nuclear matter and neutron star

Thank you for your attention