Nuclear clustering in ab initio nuclear theory

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Workshop on exploring nuclear physics acoss energy scales

PKU, Beijing, 2024/04/22

Nuclear physics: Seperation of scales

Lattice Quantum Chromodynamics

Chiral Effective Field Theory

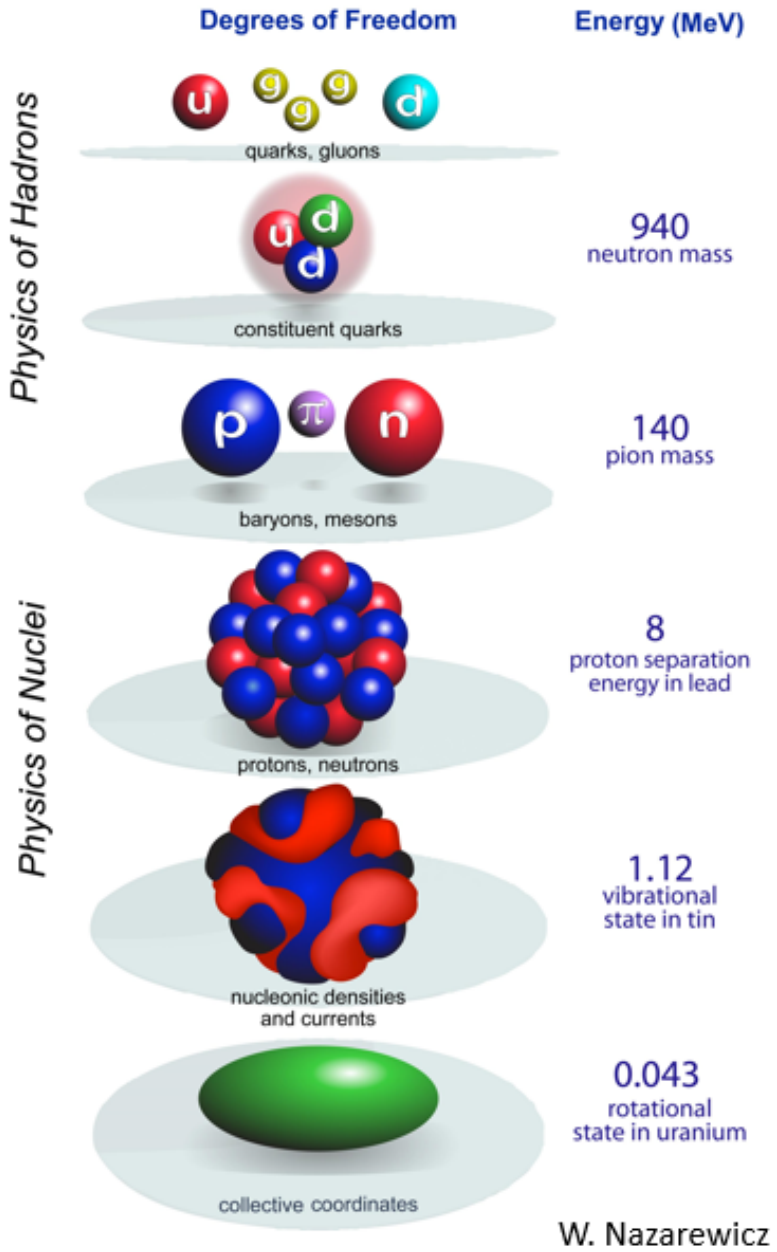
Microscopic *A*-body Methods

Configuration Interactions

Density Functional Methods

Mean Field Methods

Effective Theory of Collective Modes

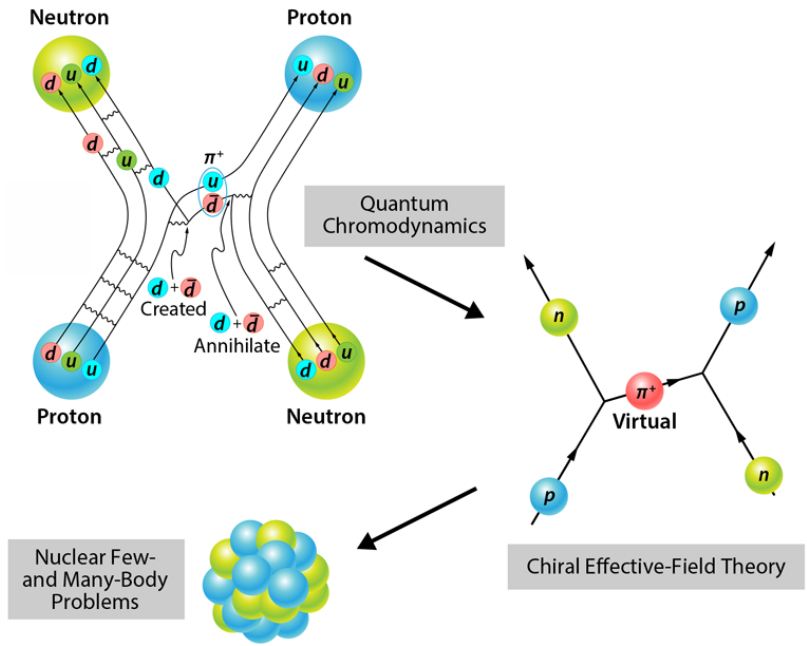


Chiral effective field theory

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 $Q \ll \Lambda_\chi$

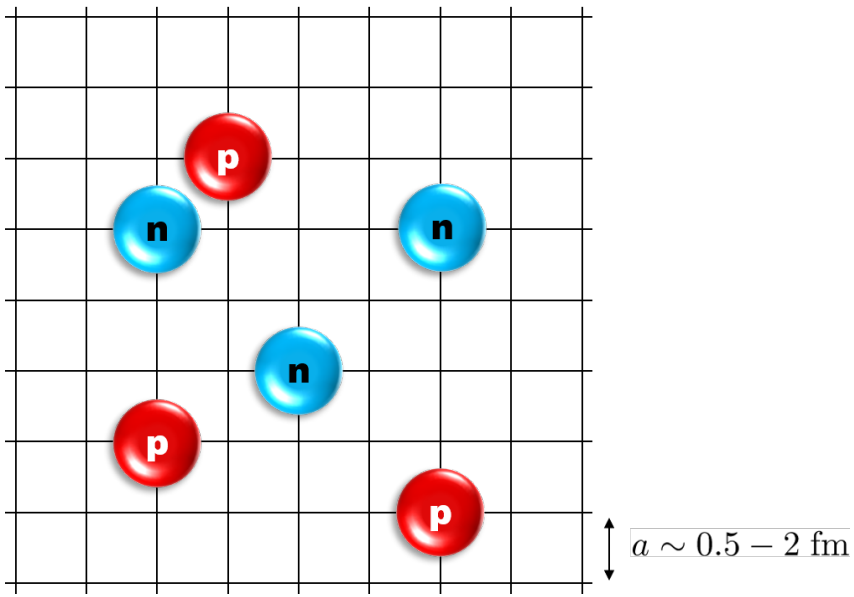


Quarks confined in nucleons and pions

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

Euclidean time projection

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

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

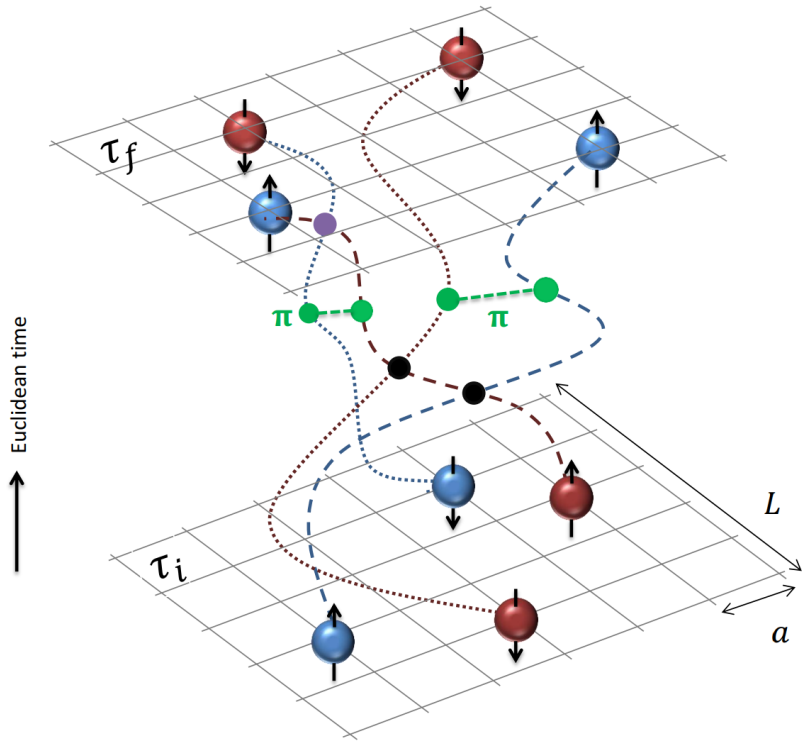
with $|\Psi_A\rangle$ representing A *free* nucleons.

- 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.

Zeroth order Hamiltonian (perturbative order)

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

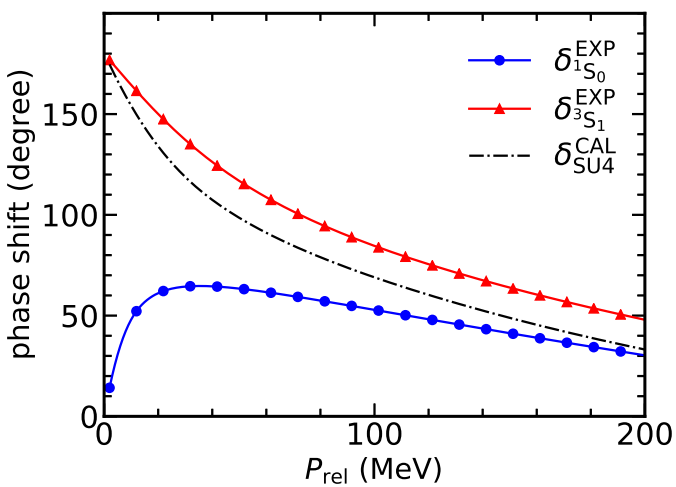
$$\tilde{\rho}(\boldsymbol{n}) = \sum_i \tilde{a}_i^\dagger(\boldsymbol{n}) \tilde{a}_i(\boldsymbol{n}) + s_L \sum_{|\boldsymbol{n}'-\boldsymbol{n}|=1} \sum_i \tilde{a}_i^\dagger(\boldsymbol{n}') \tilde{a}_i(\boldsymbol{n}'), \tag{1}$$

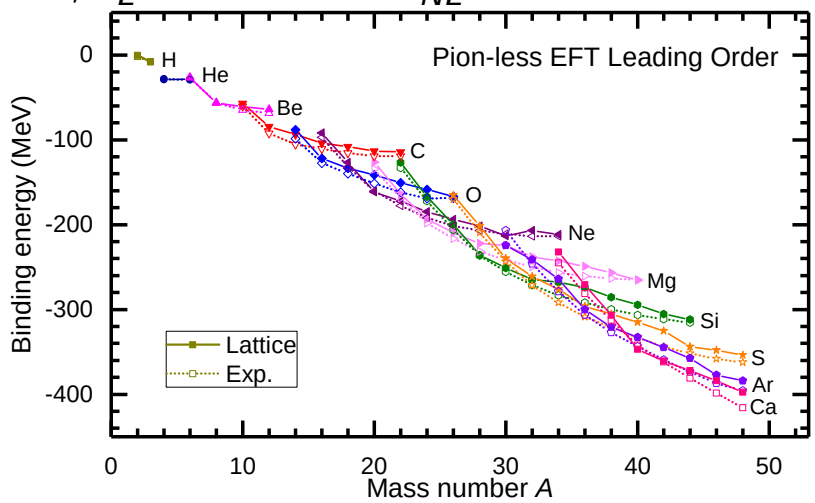
where i is the joint spin-isospin index

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

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

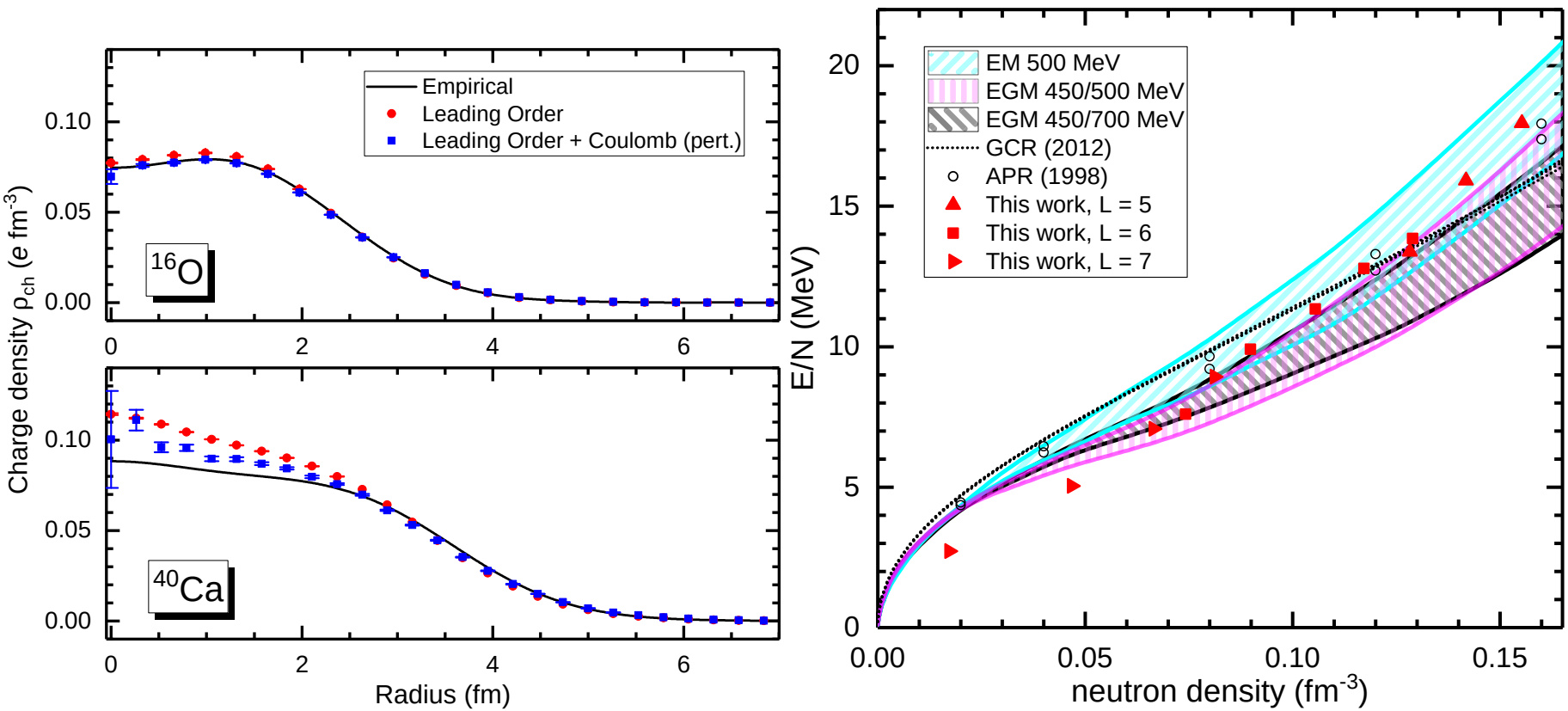
$C_{\mathrm{SU4}} = -3.41 \times 10^{-7}$ MeV^{-2}, $s_L = 0.061$ and $s_{NL} = 0.5$.





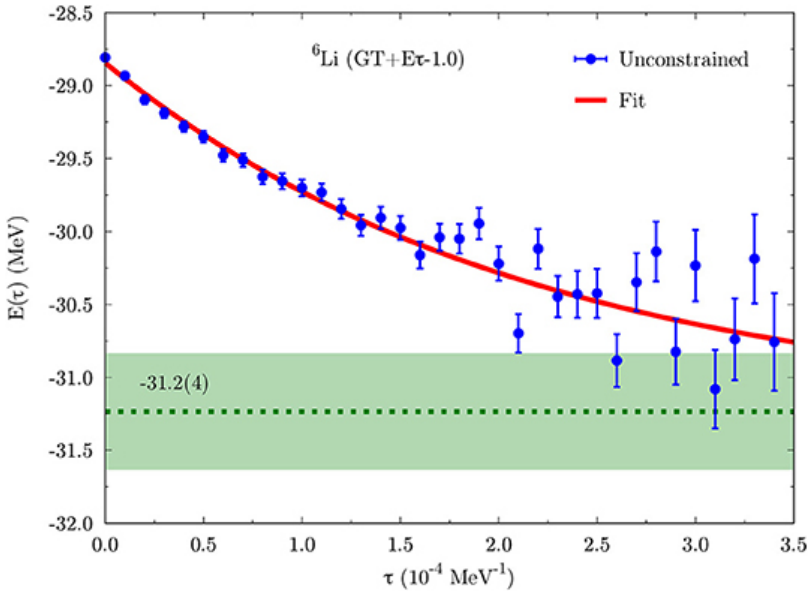
Essential elements for nuclear binding

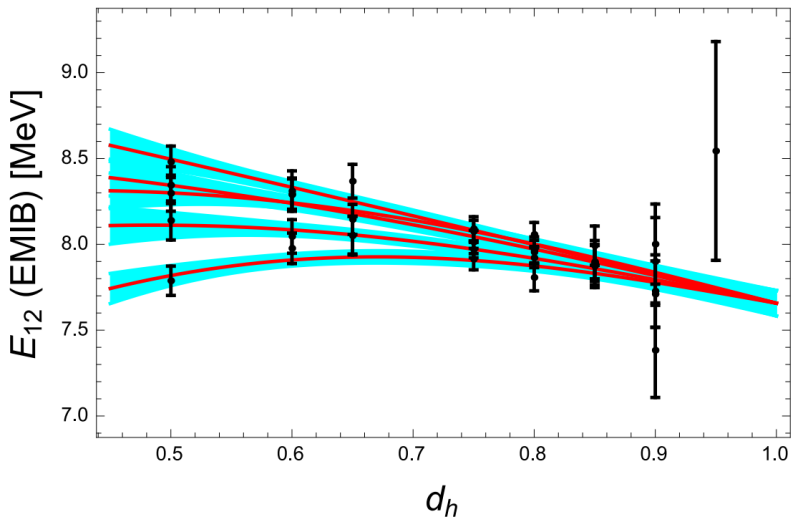
Charge density and neutron matter equation of state
are impotant in element creation, neutron star merger, etc.

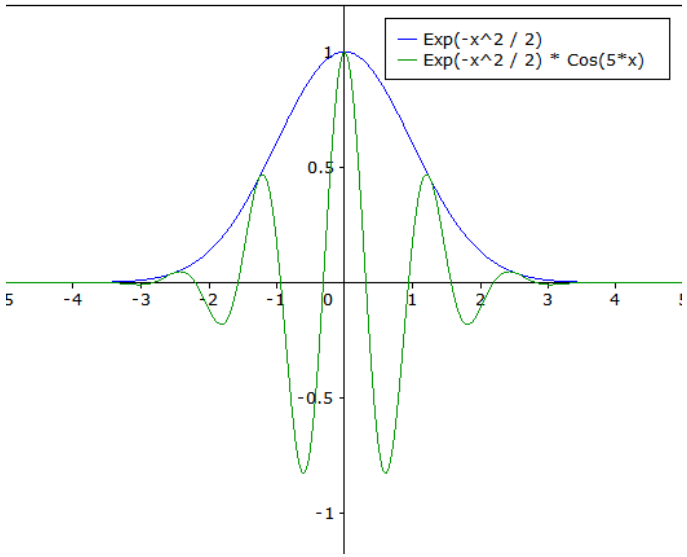


Lu *et al.*, PLB 760 (2016), 309

MC sign problem for realistic interactions

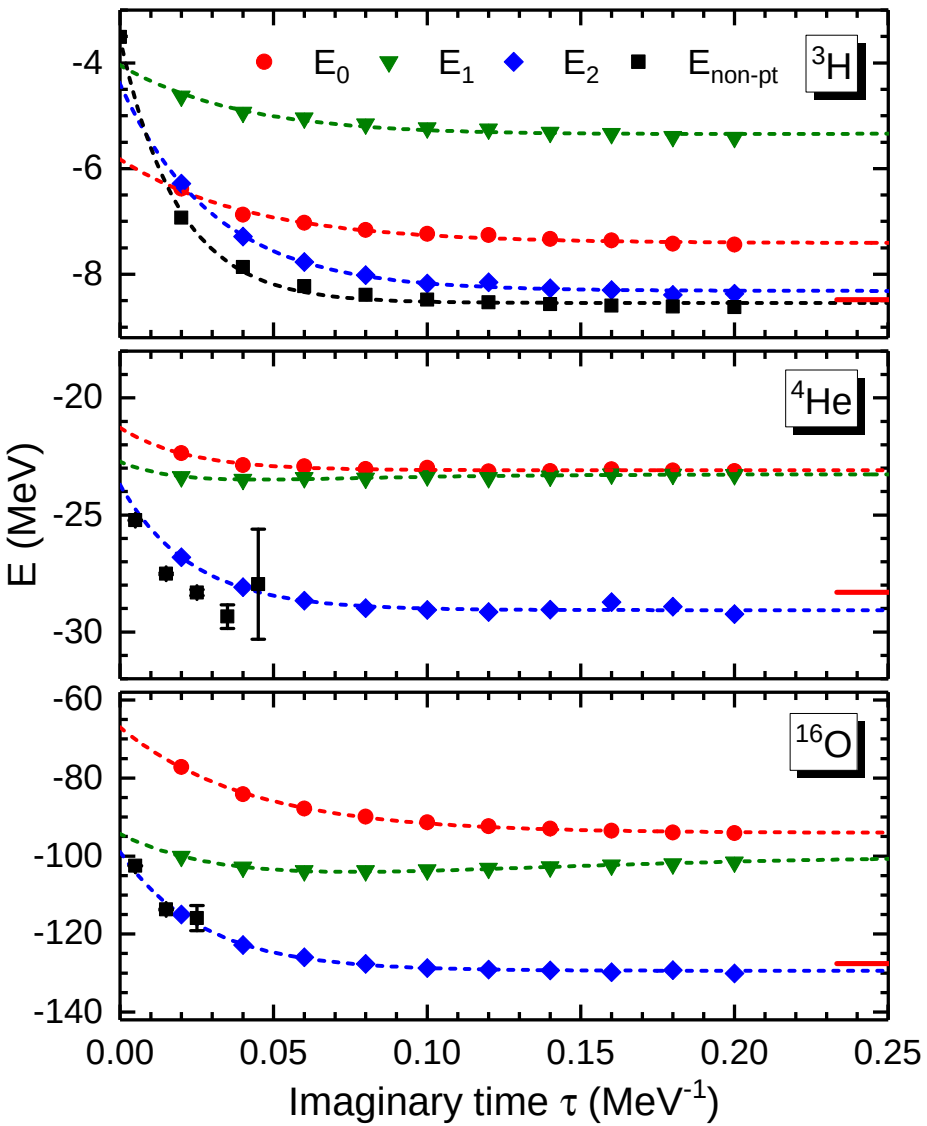






- Sign problem: Monte Carlo works well for well-behaved functions, however, sometimes the integral becomes highly oscillating.
- QMC sign problem comes from the fermion anti-symmetrization.
- Split $H = H_0 + \lambda V_C$. H_0: w/o sign problem; V_C: w/ sign problem.
- **Solution 1**: numerical extrapolation from $\lambda = 0$ to $\lambda = 1$.
- **Solution 2**: perturbative calculation near $\lambda = 0$.

Perturbative quantum Monte Carlo Method



- We split $H = H_0 + (H - H_0)$ and perform perturbative calculations
- E_0 is the ground state of H_0
- $E_1 = E_0 + \delta E_1$ is the first order corrected energy
- $E_2 = E_1 + \delta E_2$ is the second order corrected energy
- $E_{\mathrm{non-pt}}$ is the exact solution (~infinite order)

- Red bars on the right: Experiments Lu *et al.*, PRL 128, 242501 (2022)

For ^{4}He and ^{16}O, sign problem prevent us from going to large τ, resulting in large statistical errors.

Perturbative QMC theory reduce the statistical errors at a cost of perurbative truncation errors!

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)

Exploring densities with pinhole algorithm

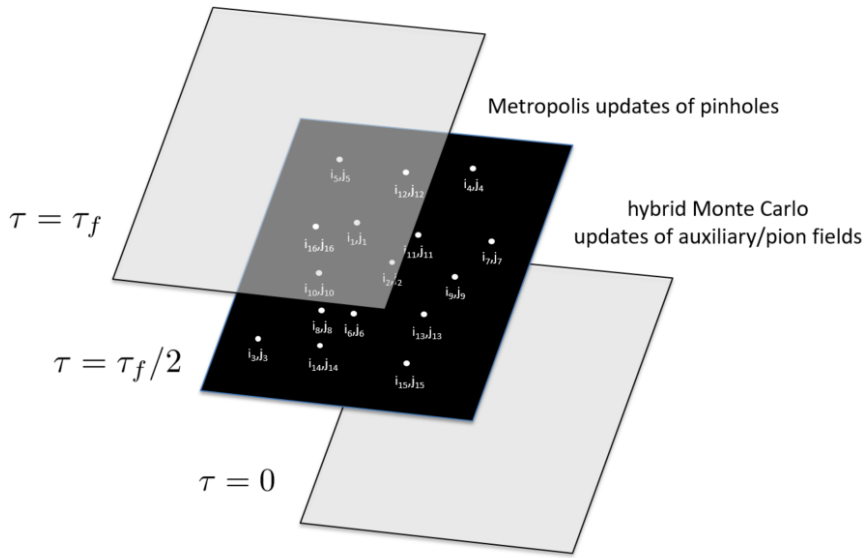
In terms of auxiliary fields, the amplitude Z can be written as a path-integral,

$$Z_{f,i}(i_1, j_1, \cdots, i_A, j_a; \boldsymbol{n}_!, \cdots \boldsymbol{n}_A; L_t)$$
$$= \int \mathscr{D}s \mathscr{D}\pi \langle \Psi_f(s,\pi) | \rho_{i_1,j_1,\cdots,i_A,j_A}(\boldsymbol{n}_1, \cdots, \boldsymbol{n}_A) | \Psi_i(s,\pi) \rangle.$$

We generate a combined probability distribution

$$P(s, \pi, i_1, j_1, \cdots, i_A, j_a; \boldsymbol{n}_!, \cdots \boldsymbol{n}_A) = |\langle \Psi_f(s,\pi) | \rho_{i_1,j_1,\cdots,i_A,j_A}(\boldsymbol{n}_1, \cdots, \boldsymbol{n}_A) | \Psi_i(s,\pi) \rangle|$$

by updating both the auxiliary fields and the pinhole quantum numbers.

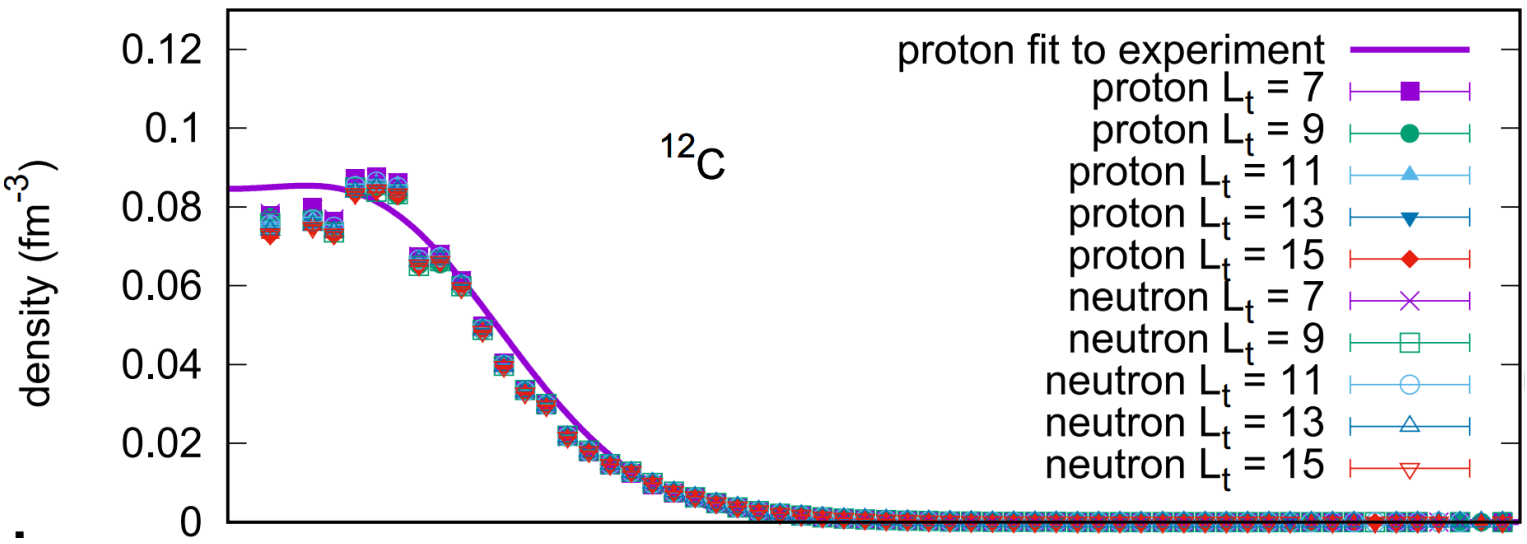


Pinhole algorithm: Intrinsic density distributions

- Densities relative to the center of mass:

$$\rho_{\text{c.m.}}(r) = \sum_{\boldsymbol{n}_1,\cdots,\boldsymbol{n}_A} |\Phi(\boldsymbol{n}_1,\cdots \boldsymbol{n}_A)|^2 \sum_{i=1}^{A} \delta\left(r - |\boldsymbol{r}_i - R_{\text{c.m.}}|\right)$$

- First LEFT calculation of **nuclear intrinsic densities**.
- **Proton radius** is included by **numerical convolution**
  $\rho(\boldsymbol{r}) = \int \rho_{\text{Point}}(\boldsymbol{r}') e^{-(\boldsymbol{r}-\boldsymbol{r}')/(2a^2)} d^3 r'$, proton radius $a \approx 0.84$ fm.

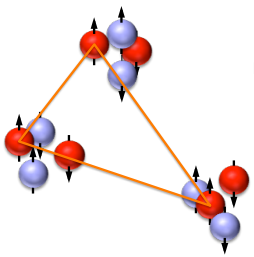


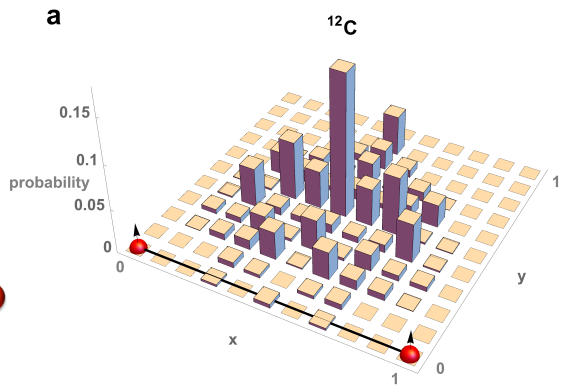
- Independent of projection time $L_t \Longleftrightarrow$ In ground state
- Sign problem suppressed $\longrightarrow$ Small errorbars
  Elhatisari et al., PRL 119, 222505 (2017)

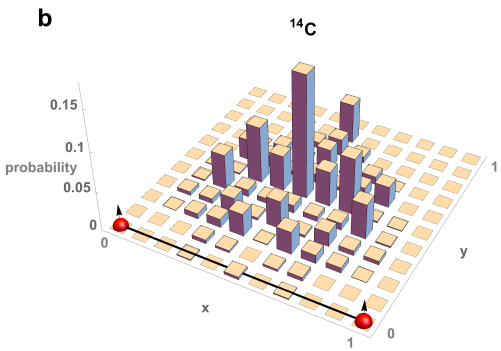
Many-body correlations: α-cluster geometry in C isotopes

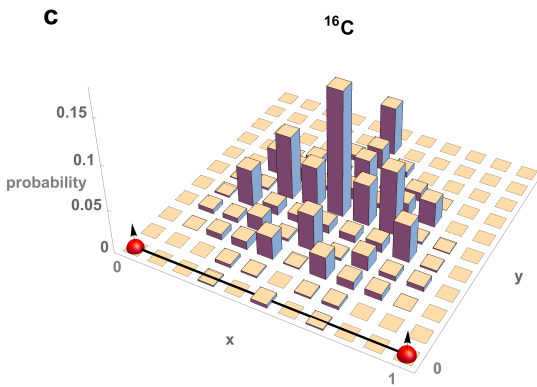
We always align the longest edge with the x-axis and keep the triangle in the x-y plane.

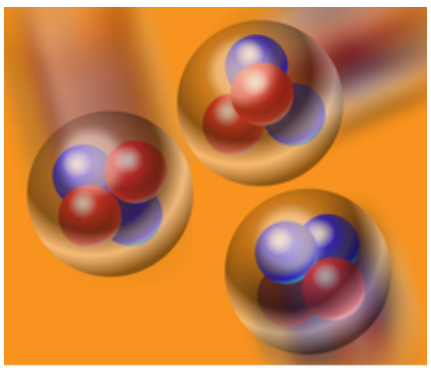
$$\rho(d_1,d_2,d_3) = \sum_{j_1,j_2,j_3} \sum_{\boldsymbol{n}_1,\boldsymbol{n}_2,\boldsymbol{n}_3} |\Phi_{\uparrow,j_1,\uparrow,j_2,\uparrow,j_3}(\boldsymbol{n}_1,\boldsymbol{n}_2,\boldsymbol{n}_3)|^2 \times \sum_{P(123)} \delta(|\boldsymbol{n}_1-\boldsymbol{n}_2|-d_3)\delta(|\boldsymbol{n}_1-\boldsymbol{n}_3|-d_2)\delta(|\boldsymbol{n}_2-\boldsymbol{n}_3|-d_1),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







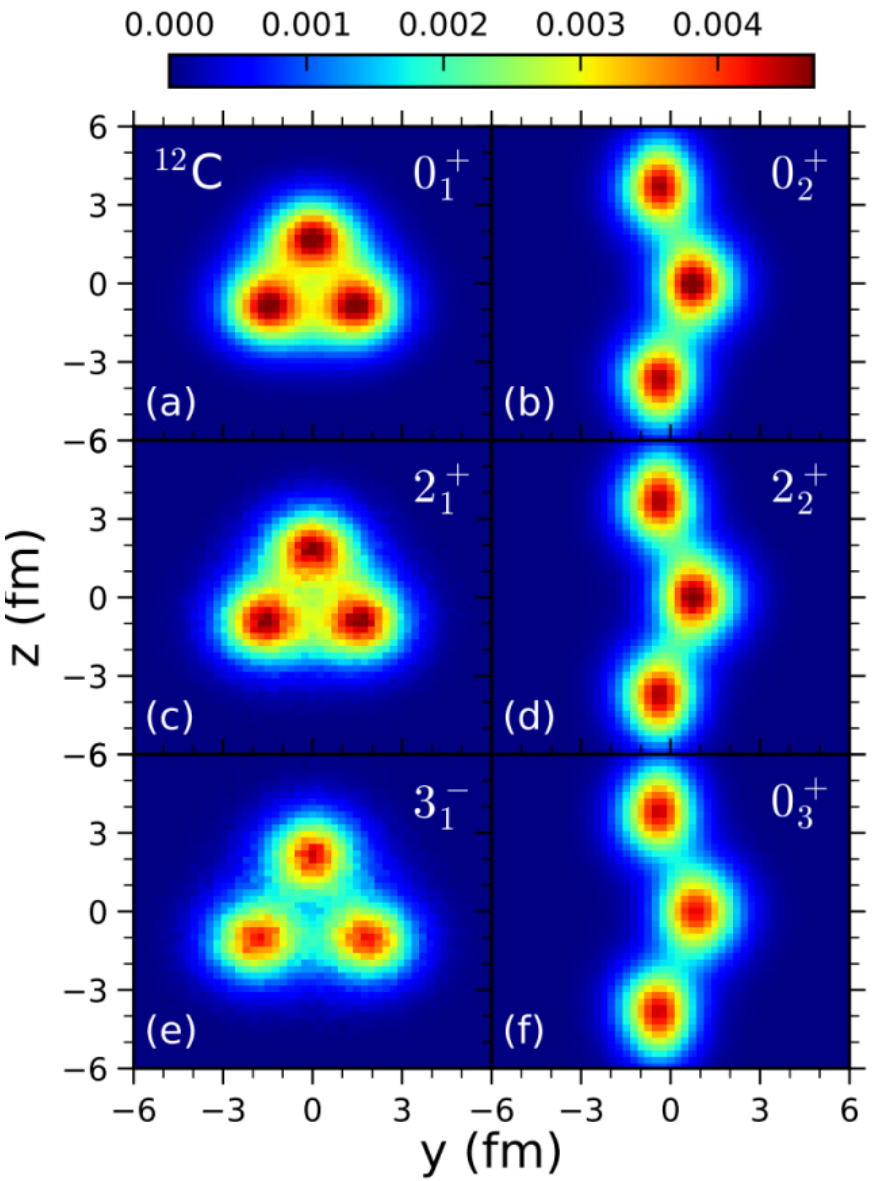




- **Hoyle state**: Triple-α resonance, essential for creating ^{12}C in stars (Hoyle, 1954). *Fine-tuning for life?*

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

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



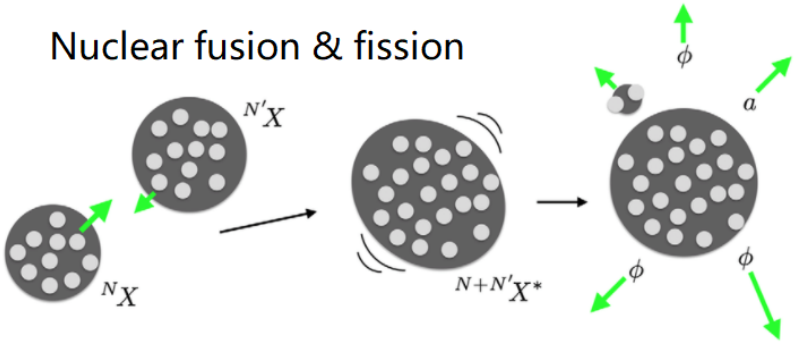
- Structure of ^{12}C states are full of complexity and duality (clustering v.s. mean-field)
- we provide the first model-independent tomographic scan of the three-dimensional geometry of the nuclear states of 12C using the ab initio framework of nuclear lattice EFT.
- 0_1^+: ground state, 0_2^+: Hoyle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

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

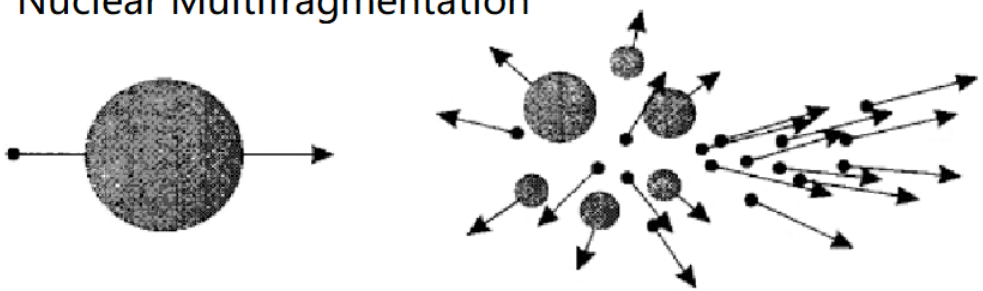
Also see Dean & Ulf's talks

Hot nucleus with pinhole trace algorithm

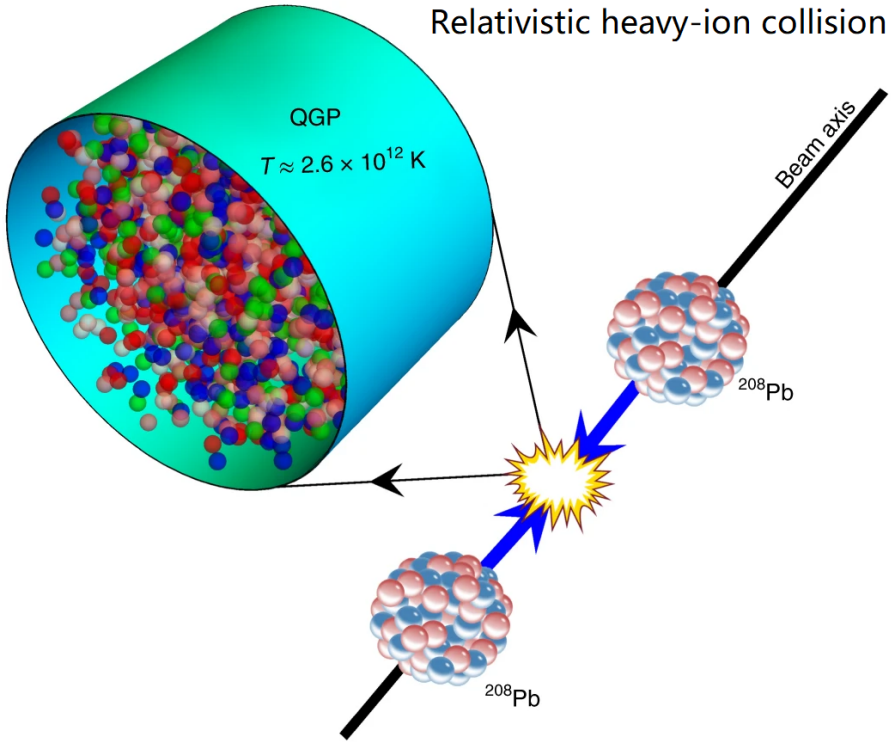
Nuclear fusion & fission

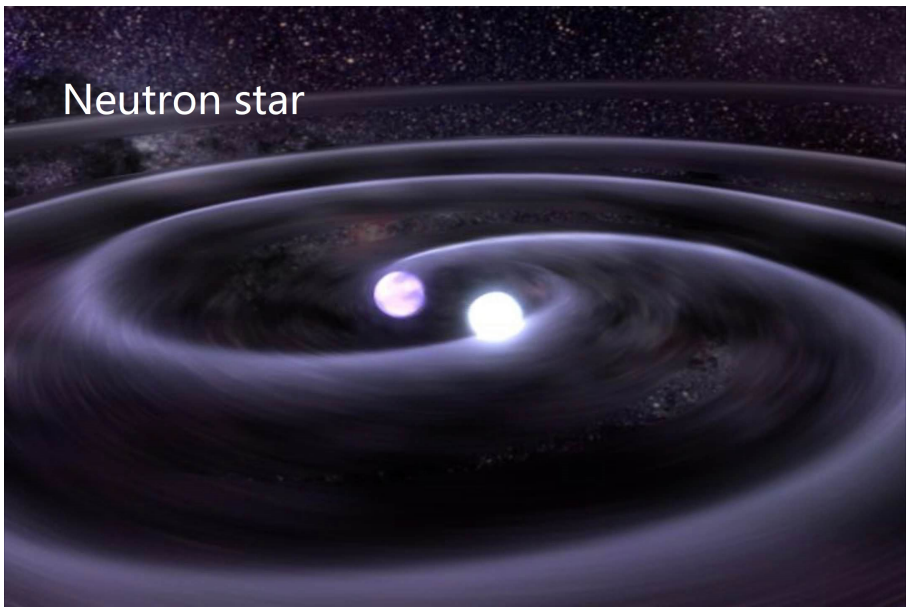


Nuclear Multifragmentation

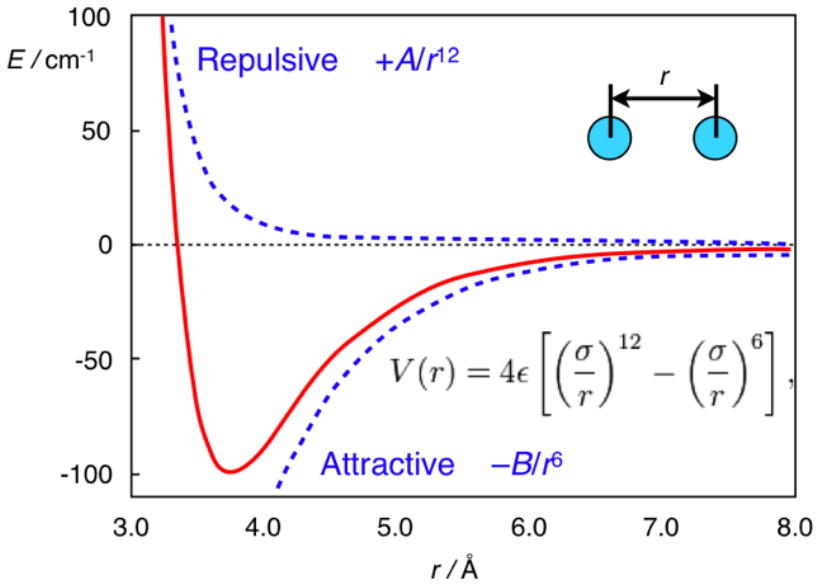


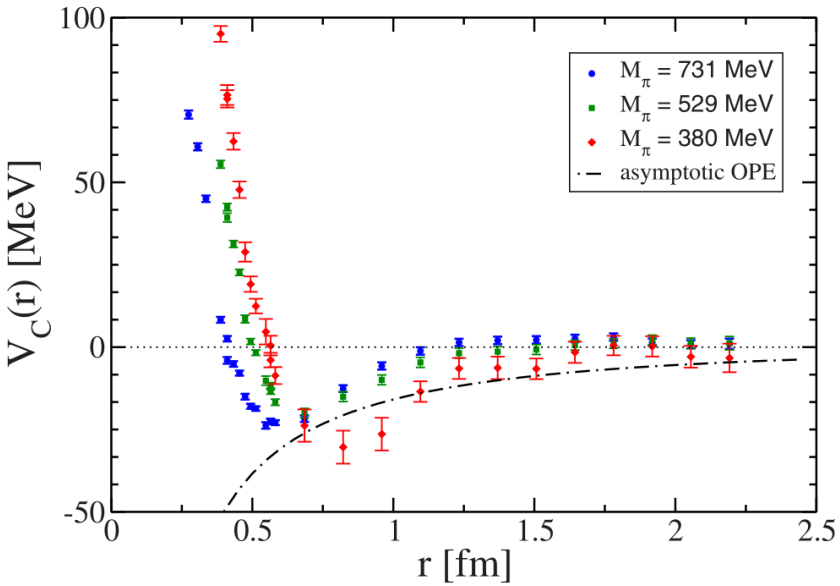
Relativistic heavy-ion collision





Water molecule versus nucleons





Ishii et al., PoS LAT2007, 146

Upper: Van-der-Waals force between water molecules

- Strength ∼0.1 eV, range ∼1 Å
- Phase transition at $T \sim 300$ K ~ 0.03 eV

Lower: Nucleon-nucleon potential from Lattice QCD

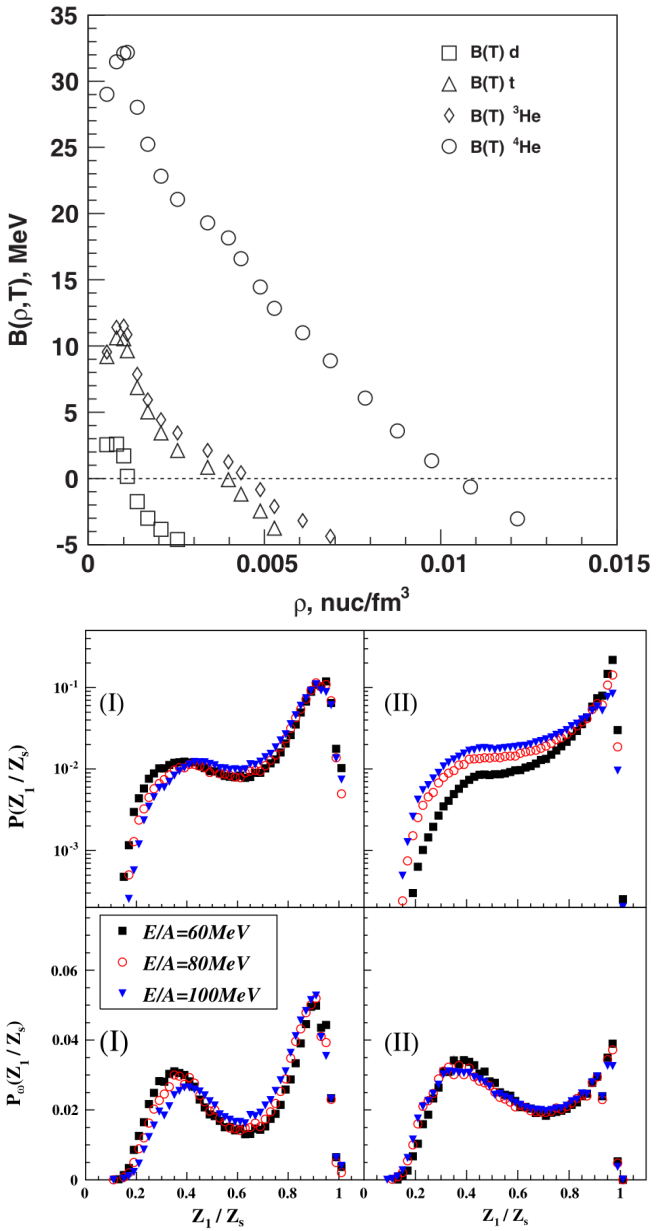
- Strength ∼10 MeV, range ∼1 fm
- What is the characteristic temperature?

Boltzmann constant

$k \approx 10^{-4}$ eV/K $= 10^{-10}$ MeV/K

$\Longrightarrow$ **Nuclear phase transition** occurs at order $T \sim 10^{11}$ **K**

Clustering in hot nucleus from experiments



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**

Fisher's droplet model

- Fisher assume an **ideal gas of clusters**

  with size A=1, 2, ..., ∞ (Classical model)
  ME Fisher, Rep. Prog. Phys. 30, 615 (1967)

- Ansatz for clusters' energy & entropy,

$$E(A) = -a_v A + c_0 A^{\sigma}$$
$$S(A) = b_v A + b_s A^{\sigma} - \tau \ln A + \ln q_0$$

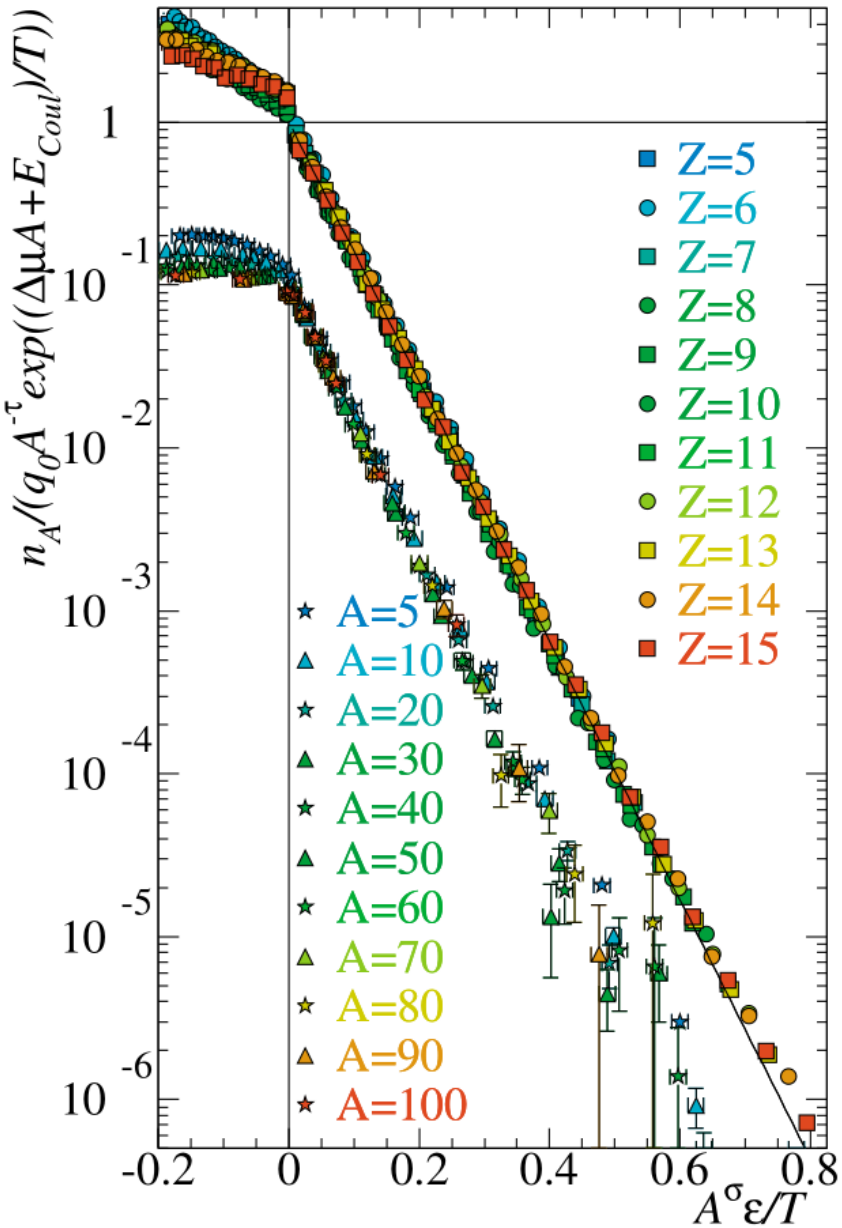
  Volume/Surface terms & phenomenological terms to account for critical scaling

- **Concentration** of mass-A cluster in thermal equilibrium:

$$n(A) = e^{-F(A)/T} = e^{-(E(A)-TS(A))/T}$$

  $F(A)$: Free energy

- Parameters fitted to **cluster yields** in multi-fragmentation experiments, T_c, ρ_c,... determined from the model parameters



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

Nuclear thermodynamic models

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

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

Review

Dynamics of clusters and fragments in heavy-ion collisions

Akira Ono

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"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**'

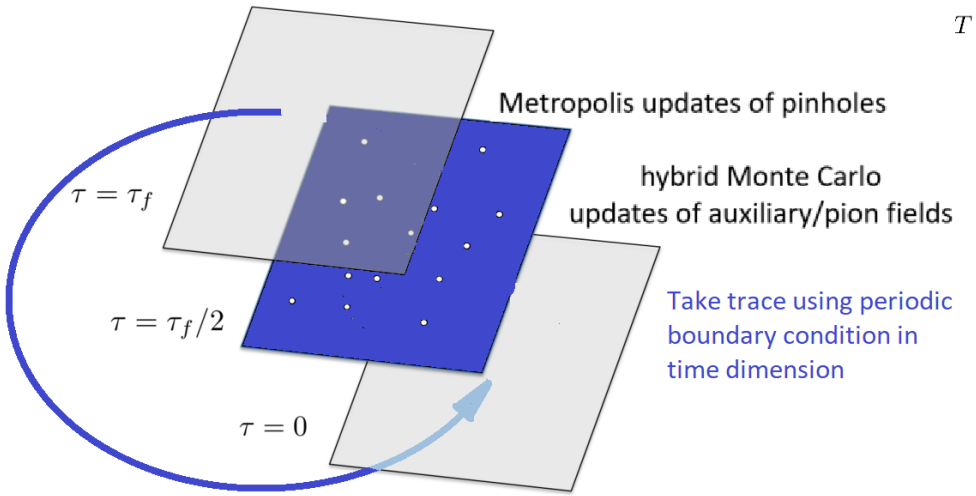
"It is **not possible** to exactly solve such quantum many-body problem **from the first principle** with computational facilities available currently or in near future"

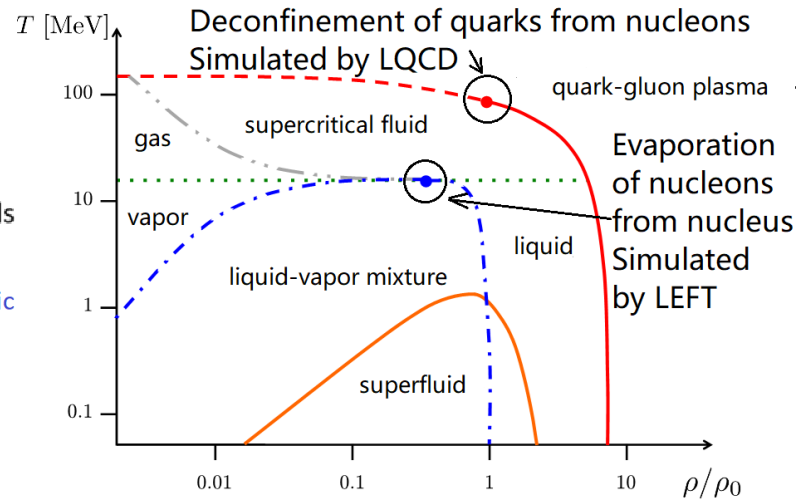
Simulate canonical ensemble with pinhole trace algorithm

- 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.





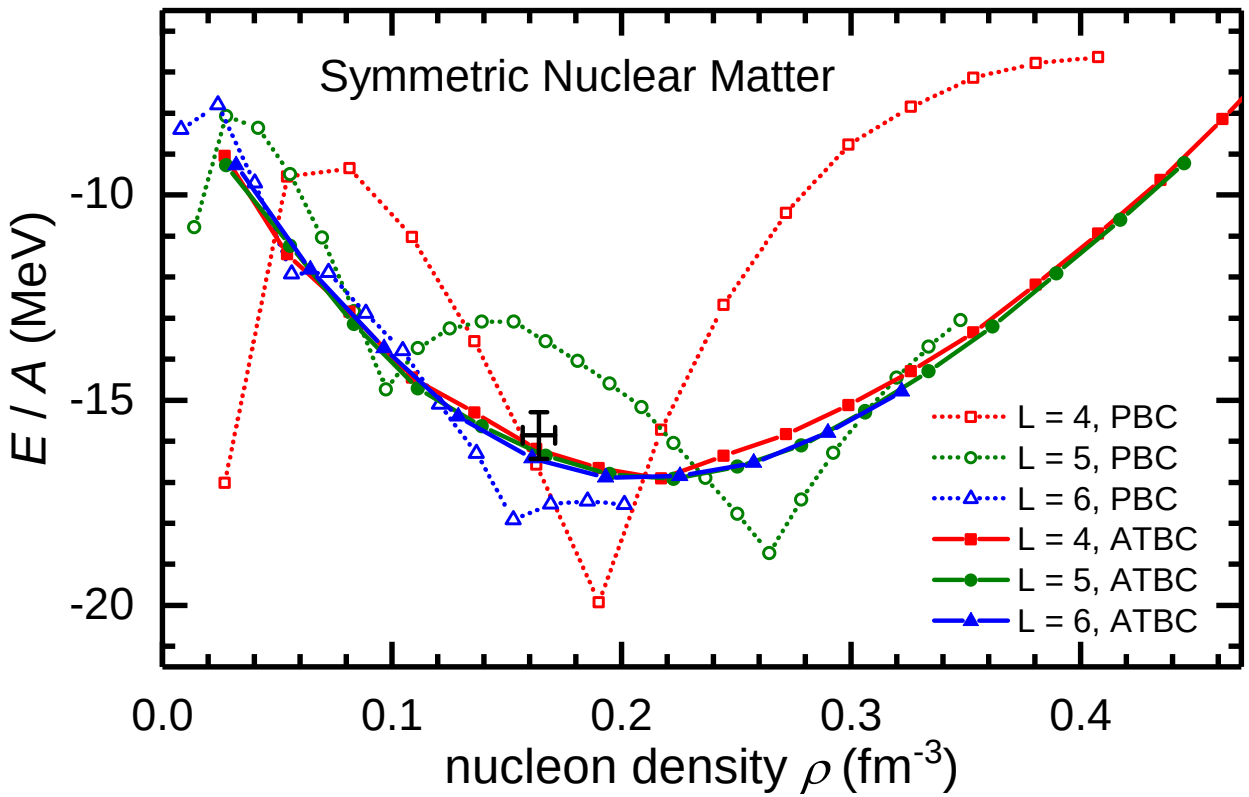
Lu et al., PRL 125, 192502 (2020)

Nuclear matter with twisted boundaries

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)

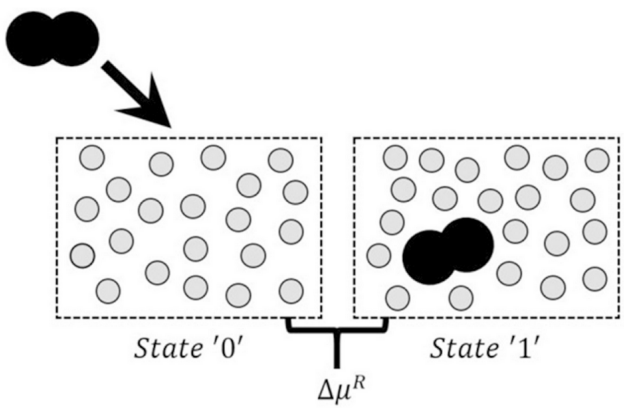
interaction from LU, *et. al.*, Phys. Lett. B 797, 134863 (2019)
"Essential elements for nuclear binding"

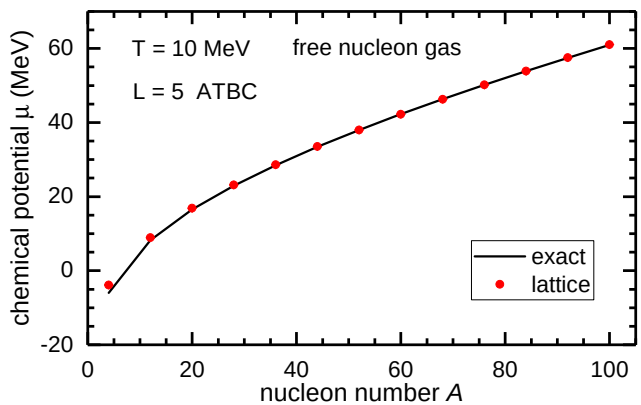
Extract intensive variables with Widom insertion method

- **Extensive variables:** Measured by operator insertion,
  - E.g., energy $E = \langle H \rangle_\Omega$, density correlation $G_{12} = \langle \rho(\boldsymbol{r}_1)\rho(\boldsymbol{r}_2) \rangle_\Omega$.
- **Intensive variables:** Measured by numerical derivatives,
  - E.g., pressure $p = -\frac{\partial F}{\partial V}$, chemical potential $\mu = -\frac{\partial F}{\partial A}$.
- Widom insertion method: Measure μ by inserting test particles (holes)
  B. Widom, J. Chem. Phys. 39, 2808 (1963)

$$\mu = \frac{1}{2}\left[F(A+1) - F(A-1)\right] = \frac{T}{2}\ln\frac{Z_{A-1}}{Z_{A+1}} = \frac{T}{2}\ln\left[\frac{\sum_{1,2}\mathrm{Tr}_A\left(\hat{a}_2^\dagger \hat{a}_1^\dagger e^{-\beta H}\hat{a}_1\hat{a}_2\right)/(A-1)!}{\sum_{1,2}\mathrm{Tr}_A\left(\hat{a}_1\hat{a}_2 e^{-\beta H}\hat{a}_2^\dagger\hat{a}_1^\dagger\right)/(A+1)!}\right]$$

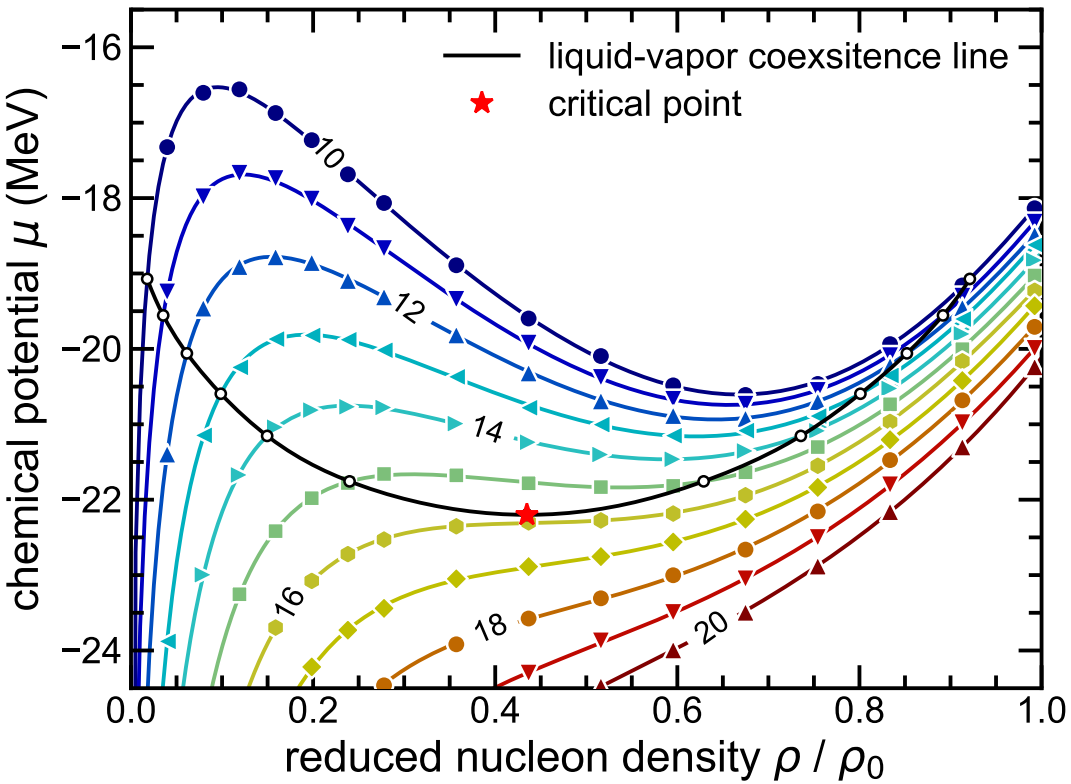
- 1, 2: $L^3 \times 2 \times 2$ lattice sites, spins and isospins, sampled with **Monte Carlo**
- $(A \pm 1)!$: **Combinatorial factors** for identical Fermions

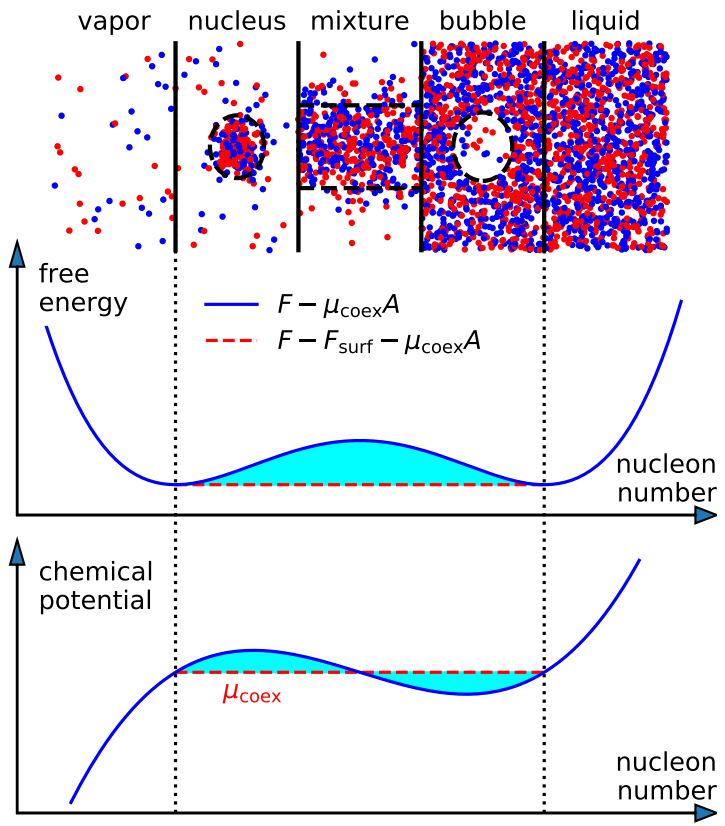




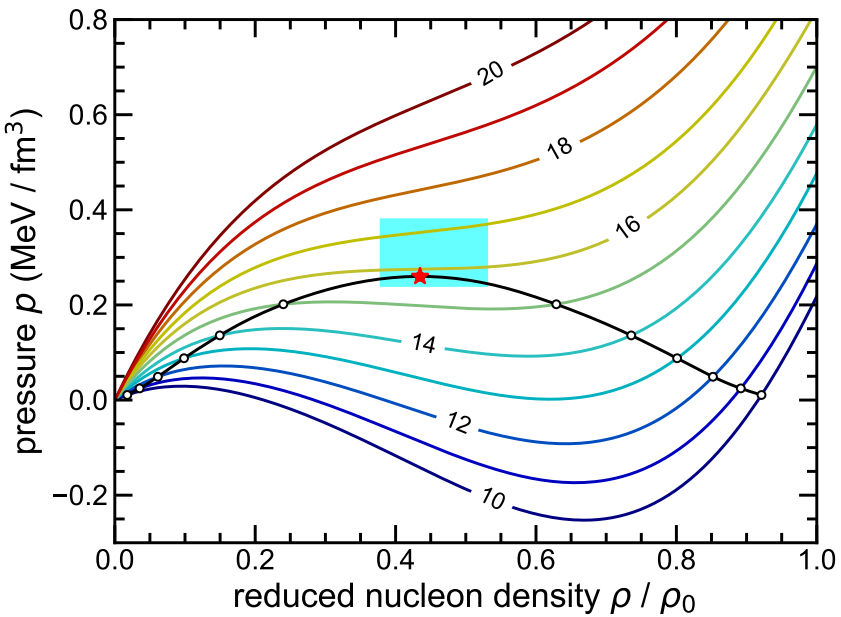
Finite nuclear systems: Liquid-vapor coexistence line

- 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)





Critical point: Compare with experiment



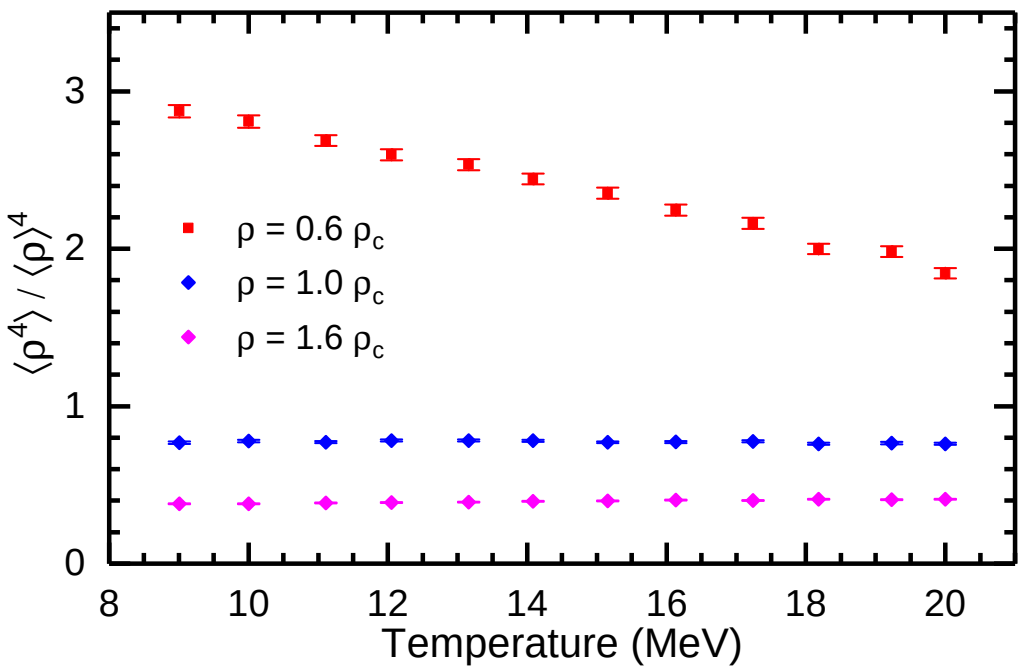
- **Pressure** $p = \int \rho d\mu$ along every isotherm (Gibbs-Duhem equation).
- Extract T_c, P_c and ρ_c of neutral symmetric nuclear matter by numerical interpolation.
- Uncertainties estimated by adding **noise** and repeat the calculation.
- **Experimental values** and **mean field** results taken from
  Elliott et al., Phys. Rev. C 87, 054622 (2013)

	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)

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.

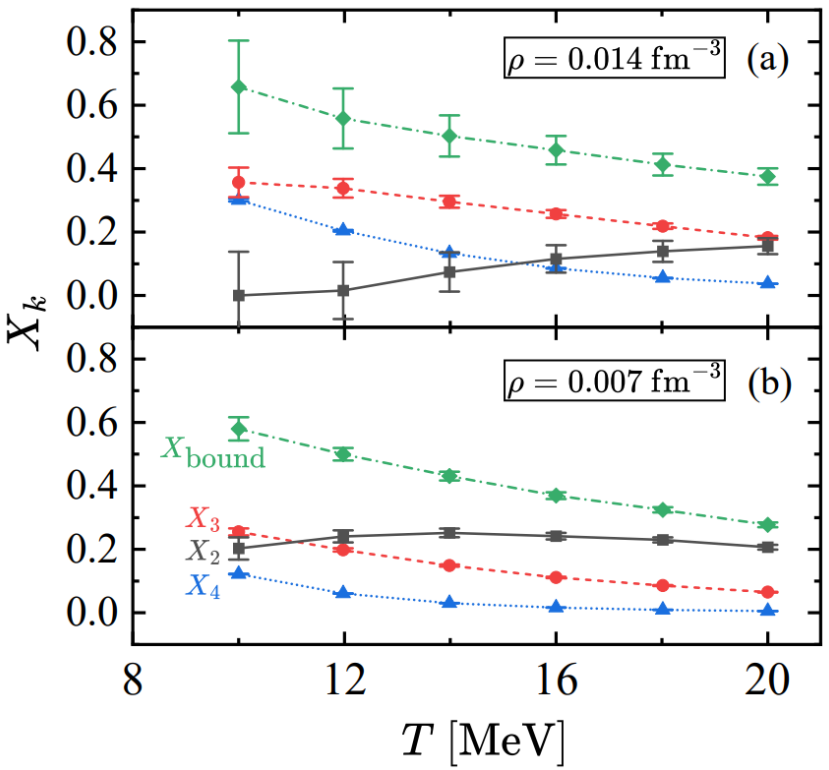


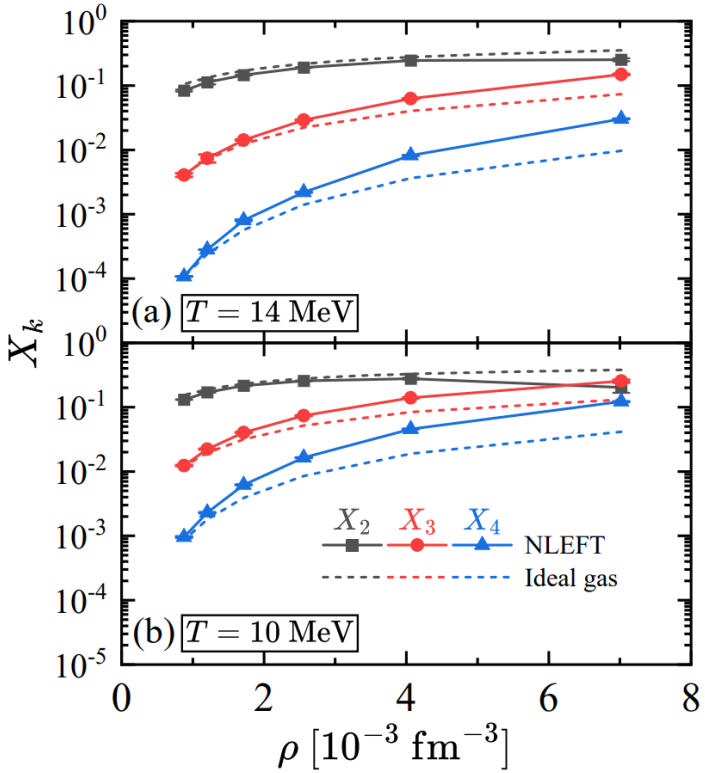
Lu et al., PRL 125, 192502 (2020)

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

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





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

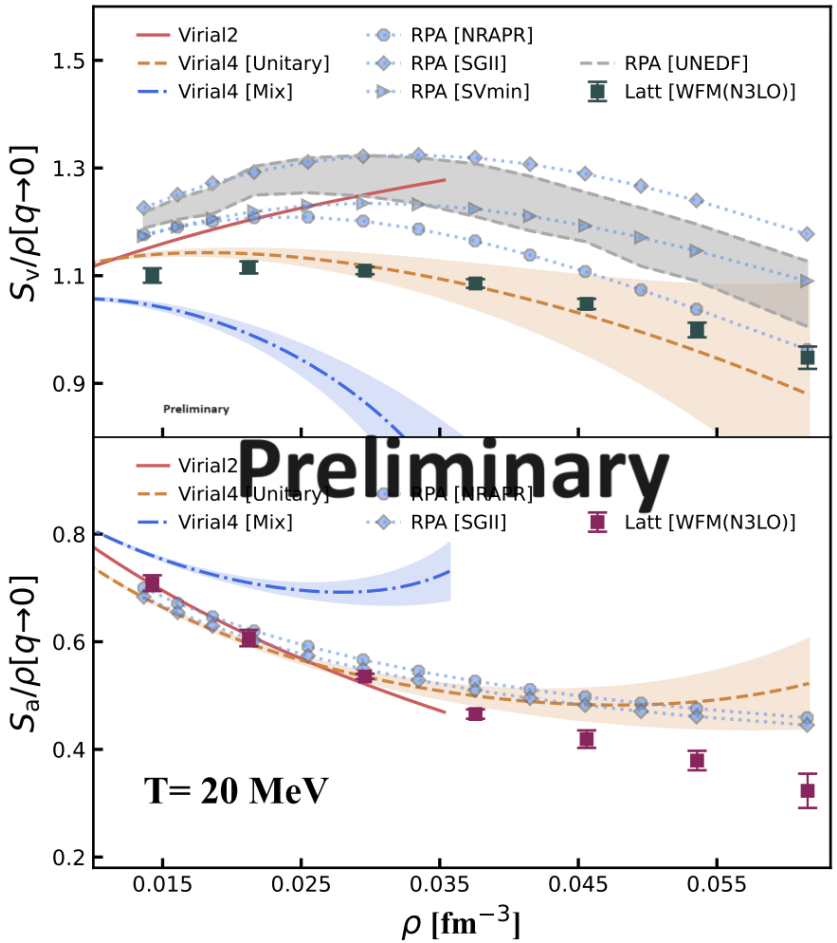
Structure factors with realistic chiral interactions

- Structure factors are Fourier transforms of correlation functions

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

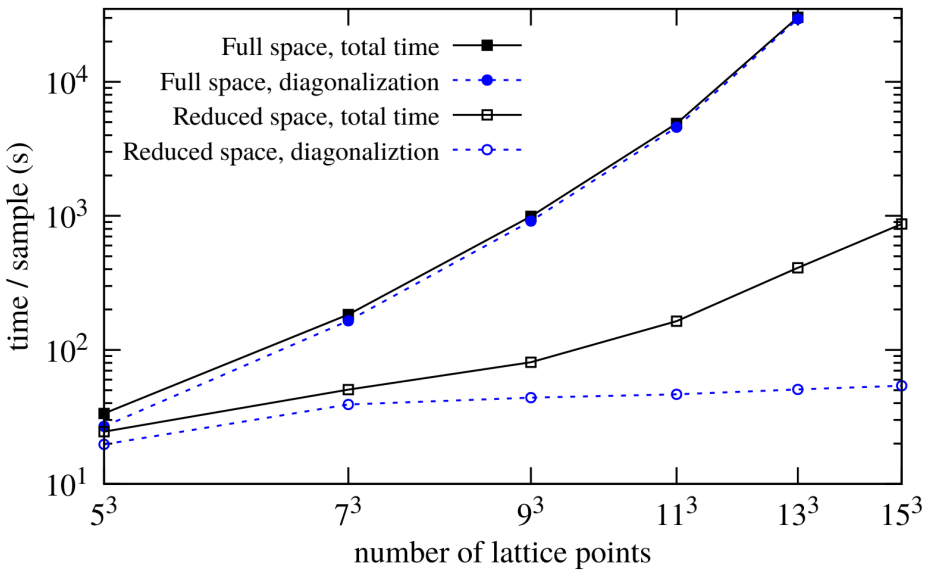
$$S_a(\boldsymbol{q}) = \int d^3r[\hat{\rho}_z(\boldsymbol{r}+\boldsymbol{r}')\hat{\rho}_z(\boldsymbol{r}')\rangle - \rho_{z0}^2]e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}$$

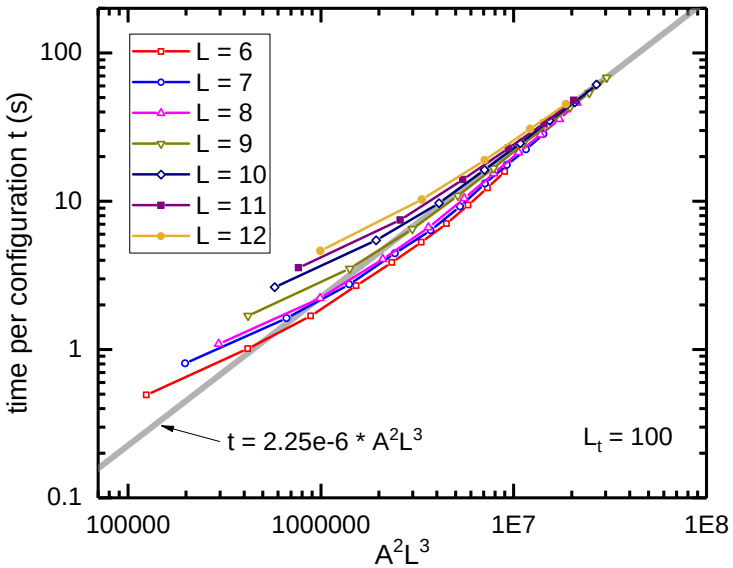
- Key for modeling Core-collapse supernovae explosions via neutrino-nucleon scattering
- Ab initio calculation with a N^{3}LO chiral interaction based on a rank-one operator method
  YuanZhuo Ma et al., arXiv:2306.04500



Performance of Pinhole Trace Algorithm

- Direct diagonalization scales exponentially $\sim \mathcal{O}(e^{\lambda L^3})$.
- Conventional grand-canonical ensemble MC method scales as $\mathcal{O}(L^9)$.
- **Left:** Recently finite-T auxiliary field MC accelerated by removing unoccupied states. Complexity$\sim \mathcal{O}(L^3 N_{\rm occ}^2)$, $N_{\rm occ} \sim A$ at low T.
  Gilbreth, Jensen, Alhassid, arXiv:1907.10596 (2019)
- **Right:** Pinhole trace algorithm complexity $\sim \mathcal{O}(L^3 A^2)$ for any T.
  Lu et al., PRL 125, 192502 (2020)





New methods can be thousands of times faster for $A \ll L$

Summary

- Lattice simulations are able to incoorporate all essential **many-body correlations**, reproducing the nuclear **clustering** based on a fully **microscopic universal Hamiltonian**
  - Ground state
  - Excited state
  - Finite temperature
  - Reaction
  - Hyper nucleus
  - ...
- Interactions with Wigner SU(4) symmetry works well with MC
- Precision interactions (e.g, chiral EFT) are more challenging (sign problem...), new algorithms required
  - Perturbative Quantum MC method
  - Rank-One operator method
  - ...

Thank you for your attention