

# Recent Progress on Lattice Effective Field Theory

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Nuclear Lattice EFT Collaboration



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FACILITY



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# Nuclear physics: Separation 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

Physics of Hadrons

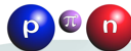
Degrees of Freedom



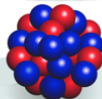
quarks, gluons



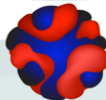
constituent quarks



baryons, mesons



protons, neutrons



nucleonic densities  
and currents



collective coordinates

Energy (MeV)

940  
neutron mass

140  
pion mass

8  
proton separation  
energy in lead

1.12  
vibrational  
state in tin

0.043  
rotational  
state in uranium

W. Nazarewicz

# Write down an interaction (fundamentally/effectively)



C. N. Yang, non-Abelian gauge field

"Symmetry dictates interaction"



K. G. Wilson, renormalization group

"Interaction flows with the scale"

We can write a most general Lagrangian for quarks and gluons containing all possible terms  
Most of them are excluded by **symmetries** and **renormalizability**

Renormalizable interactions survive when running to low-energies

Non-renormalizable interactions are suppressed when running to low-energies

$$\mathcal{L}_{\text{QCD}} = \sum_{\text{flavors}} \bar{\psi}(i\gamma^\mu \partial_\mu - M)\psi - gA_\mu^i \bar{\psi}\gamma^\mu t_i \psi - \frac{1}{4} G_i^{\mu\nu} G_{\mu\nu}^i$$
$$+ \frac{1}{2} m_g^2 A_\mu^i A_i^\mu + \frac{1}{2} c \bar{\psi} \sigma^{\mu\nu} t_i \psi G_{\mu\nu}^i + \dots$$

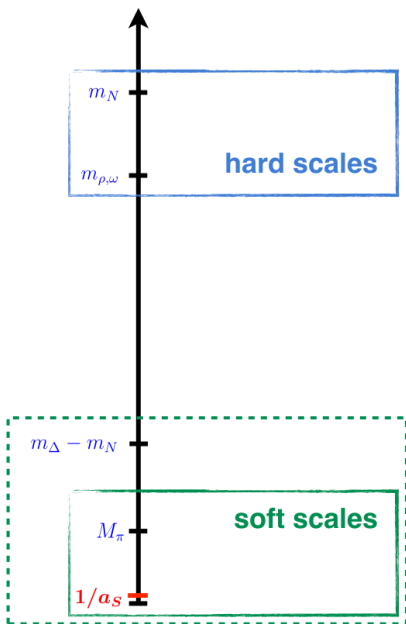
Suppressed by  
gauge symmetry

Suppressed by  
renormalizability

Given the **degrees of freedom**, **symmetries** and **energy scales**, we can always construct an effective field theory with the same philosophy.

All theories are EFT. Standard model is an EFT of a quantum gravity theory (string theory?)

# Scales in chiral EFT



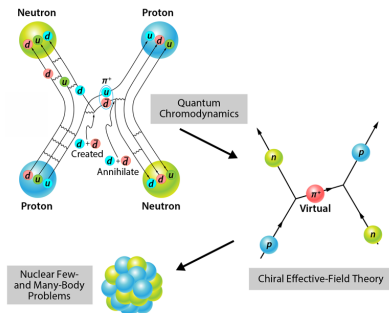
- Chiral EFT: Perturbative expansion of the  $N$ - $N$  and  $\pi$ - $N$  potentials in powers of

$$Q \in \left\{ \frac{M_\pi}{\Lambda}, \frac{|\vec{p}|}{\Lambda} \right\}, \Lambda \sim m_\rho \sim 4\pi F_\pi \sim 1\text{GeV}$$

- QCD has an approximate chiral symmetry
  - Explicitly broken by non-zero quark mass ( $m_q \sim 3$  MeV)
  - Spontaneously broken,  $SU(2) \times SU(2) \rightarrow SU(2)$
- SB exact symmetry  $\rightarrow$  massless Goldstone bosons
- SB approx. symm.  $\rightarrow$  very light bosons  $\rightarrow$  pions ( $M_\pi \sim 140$  MeV)
- In nucleus, Fermi momentum  $p_F \sim 200$  MeV

**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:**  
 $SU(2)_L \times SU(2)_R \rightarrow SU(2)_V$
- Goldstone theorem implies a light pion:  
Long-range part of the nuclear force
- Contact terms:  
Short-range part of the nuclear force
- **Hard scale:**  $\Lambda_\chi \sim 1 \text{ GeV}$ : Chiral EFT works for momentum  $Q \ll \Lambda_\chi$


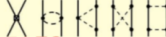

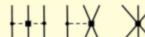
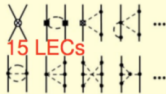
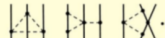
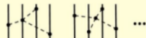


Quarks confined  
in nucleons and pions

# $N$ - $N$ interaction in nuclear chiral EFT

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

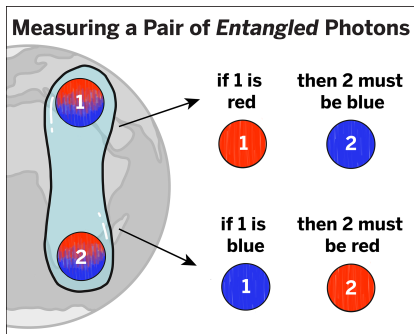
$\mathbf{q} = \mathbf{p}'_1 - \mathbf{p}_1, \mathbf{k} = \mathbf{p}'_1 - \mathbf{p}_2, \boldsymbol{\sigma}_{1,2}$  for spins,  $\boldsymbol{\tau}_{1,2}$  for isospins,  $C_{1-7}, g_A$ , etc. are Low Energy Constants fitted to  $N$ - $N$  scattering data

		Two-nucleon force	Three-nucleon force	Four-nucleon force
$\mathcal{O}((Q/\Lambda_\chi)^0)$	LO	 2 LECs	—	—
$\mathcal{O}((Q/\Lambda_\chi)^2)$	NLO	 7 LECs	—	—
$\mathcal{O}((Q/\Lambda_\chi)^3)$	$N^2$ LO		 2 LECs	—
$\mathcal{O}((Q/\Lambda_\chi)^4)$	$N^3$ LO	 15 LECs		

# Why need nuclear ab initio methods

Mean field models are useful  
but **quantum correlations** not included

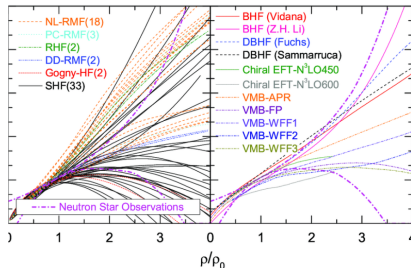
$$|\Psi\rangle = 1/\sqrt{2}[|0\rangle|1\rangle + |1\rangle|0\rangle]$$



In mean field models, motion of particle 1  
is independent of other particles  
 $P(1,2) = P(1) \times P(2)$

Predictions are **model-dependent**

Example: symmetry energy

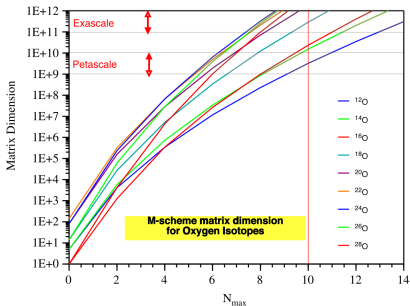
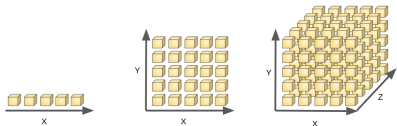


N.-B. Zhang and B.-A. Li, EPJA 55, 39 (2019)

**Problem 1:** Lack of quantum correlations  
**Problem 2:** Imprecise nuclear forces  
**Recipe:** **Exactly** solve many-body  
Schrödinger equation with **precise** nuclear  
force  $\implies$  **nuclear ab initio methods**

# Dimensionality curse in nuclear many-body problems

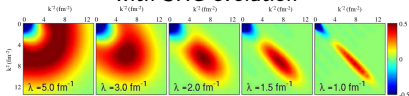
## Exponential increase of resources



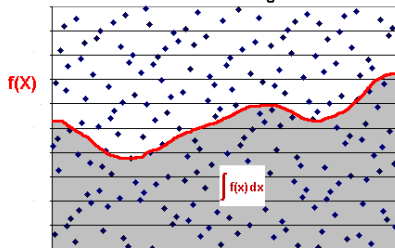
PRC 101, 014318 (2020)

## Solution 1: Reduce effective Hilbert space

with SRG evolution



## Solution 2: Monte Carlo algorithms The Monte Carlo Integral



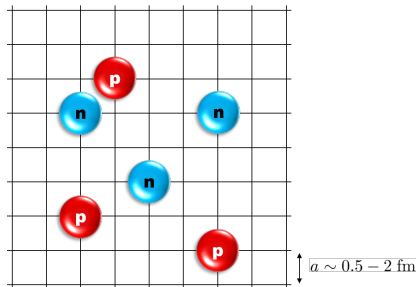


# Introduction to Lattice Effective Field Theory

**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)

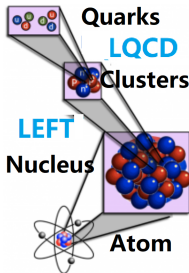
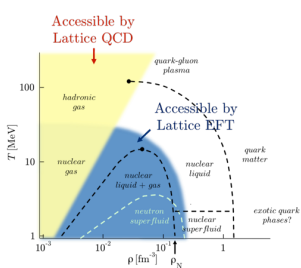
- Discretized **chiral nuclear force**
- Lattice spacing  $a \approx 1 \text{ fm} = 620 \text{ MeV}$   
( $\sim$ chiral symmetry breaking scale)
- Protons & neutrons interacting via **short-range,  $\delta$ -like** and **long-range, pion-exchange** interactions
- Exact method, **polynomial scaling**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



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 $\rho$	low $T$ / $\rho_{\text{sat}}$
sign problem	severe for $\mu > 0$	moderate



# Euclidean time projection

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

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

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

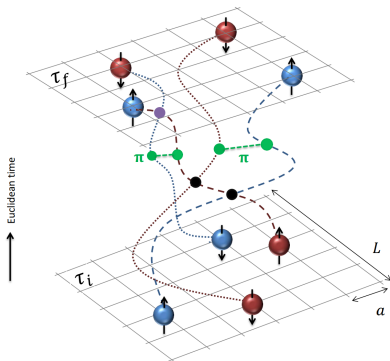
- Expectation value of any operator  $\mathcal{O}$ :

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

- $\tau$  is discretized into time slices:

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

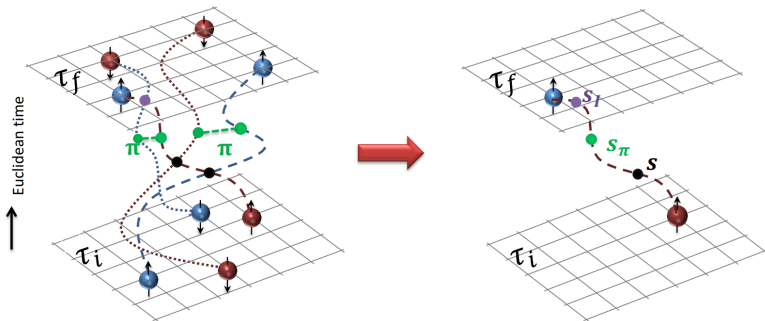
All possible configurations in  $\tau \in [\tau_i, \tau_f]$  are sampled.  
Complex structures like nucleon clustering emerges naturally.



# Auxiliary field transformation

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

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



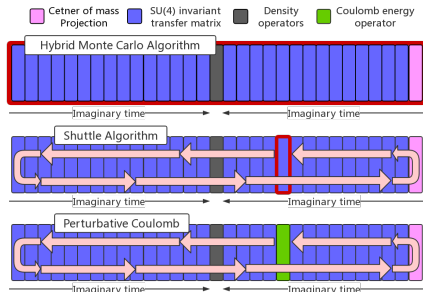
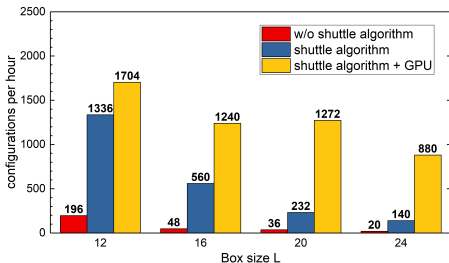
# Advanced algorithm and programming paradigm

All  $L_t \times L^3$  auxiliary fields  $s_{n,n_t}$  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**



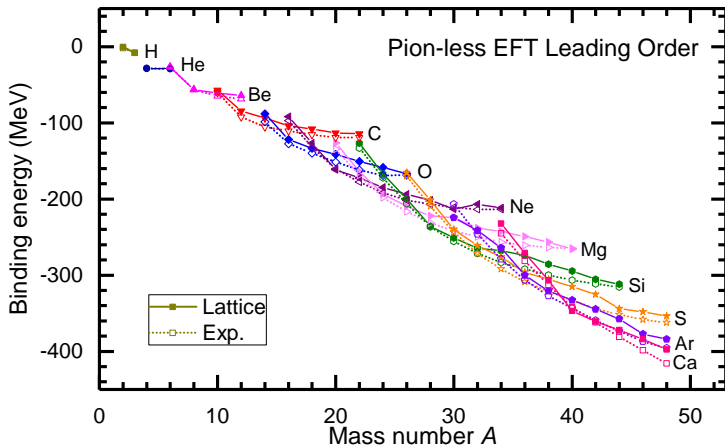
- Can be implemented for **GPU**
- **Algorithm & Hardware** combined give a **40~50 times** speed-up

**Large lattices are accessible**

# Essential elements for nuclear binding

How many free parameters are essential for a proper nuclear force?

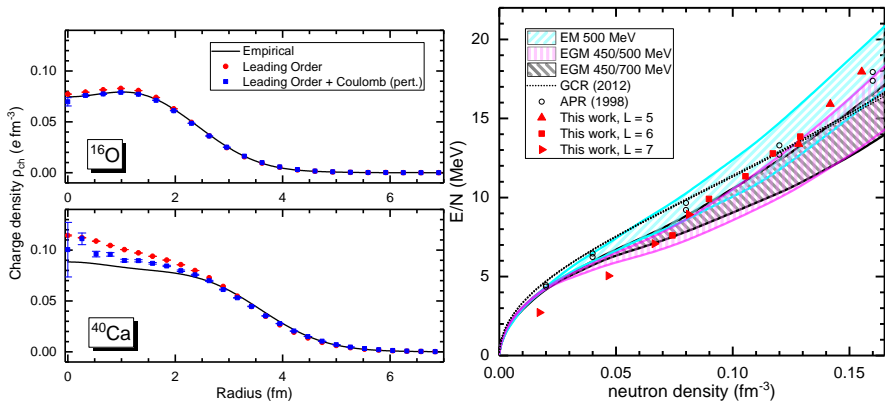
**Answer:** 4, Strength, Range, Three-body, Locality



Lu, Li, Elhatisari, Lee, Epelbaum, Meißner, [Phys. Lett. B 760 \(2016\), 309](#)

# Essential elements for nuclear binding

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



Lu, Li, Elhatisari, Lee, Epelbaum, Meißner, [Phys. Lett. B 760 \(2016\), 309](#)

# Perturbative quantum Monte Carlo method

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

	$E_0$	$\delta E_1$	$E_1$	$\delta E_2$	$E_2$	$E_{\text{exp}}$
$^3\text{H}$	-7.41(3)	+2.08	-5.33(3)	-2.99	-8.32(3)	-8.48
$^4\text{He}$	-23.1(0)	-0.2	-23.3(0)	-5.8	-29.1(1)	-28.3
$^8\text{Be}$	-44.9(4)	-1.7	-46.6(4)	-11.1	-57.7(4)	-56.5
$^{12}\text{C}$	-68.3(4)	-1.8	-70.1(4)	-18.8	-88.9(3)	-92.2
$^{16}\text{O}$	-94.1(2)	-5.6	-99.7(2)	-29.7	-129.4(2)	-127.6
$^{16}\text{O}^\dagger$	-127.6(4)	+24.2	-103.4(4)	-24.3	-127.7(2)	-127.6
$^{16}\text{O}^\ddagger$	-161.5(1)	+56.8	-104.7(2)	-22.3	-127.0(2)	-127.6

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

Excellent predictive power  $\implies$  Demonstration of both **nuclear force model** and

**many-body algorithm**

Lu *et al.*, PRL 128, 242501 (2022)



# Pinhole algorithm: Schematic

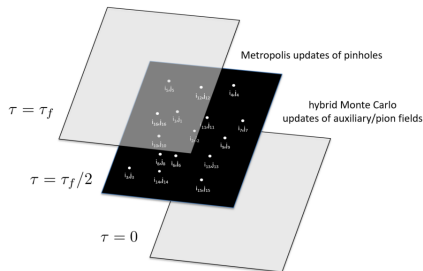
In terms of auxiliary fields, the amplitude  $Z$  can be written as a path-integral,

$$Z_{f,i}(i_1, j_1, \dots, i_A, j_A; \mathbf{n}_1, \dots, \mathbf{n}_A; L_t) \\ = \int \mathcal{D}s \mathcal{D}\pi \langle \Psi_f(s, \pi) | \rho_{i_1, j_1, \dots, i_A, j_A}(\mathbf{n}_1, \dots, \mathbf{n}_A) | \Psi_i(s, \pi) \rangle.$$

We generate a combined probability distribution

$$P(s, \pi, i_1, j_1, \dots, i_A, j_A; \mathbf{n}_1, \dots, \mathbf{n}_A) = |\langle \Psi_f(s, \pi) | \rho_{i_1, j_1, \dots, i_A, j_A}(\mathbf{n}_1, \dots, \mathbf{n}_A) | \Psi_i(s, \pi) \rangle|$$

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



# Pinhole algorithm: Intrinsic density distributions

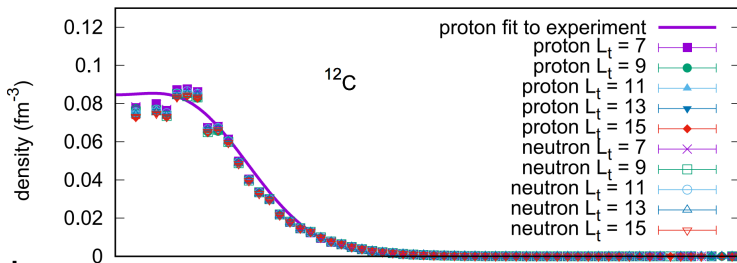
- Densities relative to the **center of mass**:

$$\rho_{\text{c.m.}}(r) = \sum_{n_1, \dots, n_A} |\Phi(n_1, \dots, n_A)|^2 \sum_{i=1}^A \delta(r - |r_i - R_{\text{c.m.}}|)$$

- First LEFT calculation of **nuclear intrinsic densities**.

- Proton radius** is included by **numerical convolution**

$$\rho(r) = \int \rho_{\text{Point}}(r') e^{-(r-r')/(2a^2)} d^3r', \quad \text{proton radius } a \approx 0.84 \text{ fm.}$$



- Independent of projection time  $L_t \iff$  In **ground state**

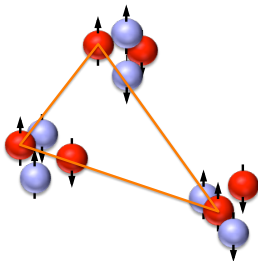
- Sign problem** suppressed  $\rightarrow$  Small errorbars

Elhatisari et al., Phys. Rev. Lett. 119, 222505 (2017)

# Triangles in carbon isotopes

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

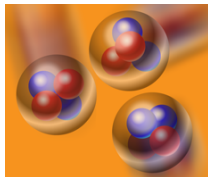
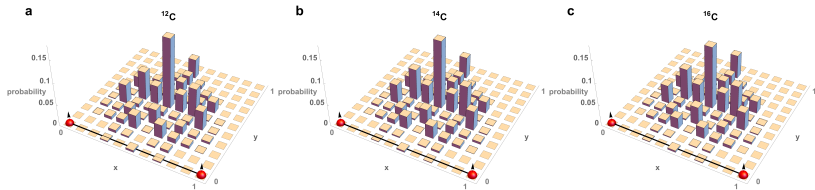
$$\rho(d_1, d_2, d_3) = \sum_{j_1 j_2 j_3} \sum_{\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3} |\Phi_{\uparrow j_1, \uparrow j_2, \uparrow j_3}(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3)|^2 \\ \times \sum_{P(123)} \delta(|\mathbf{n}_1 - \mathbf{n}_2| - d_3) \delta(|\mathbf{n}_1 - \mathbf{n}_3| - d_2) \delta(|\mathbf{n}_2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



Elhatisari, Epelbaum, Krebs, Lahde, Lee, Li, BNL, Meissner, Rupak, PRL 119, 222505 (2017)

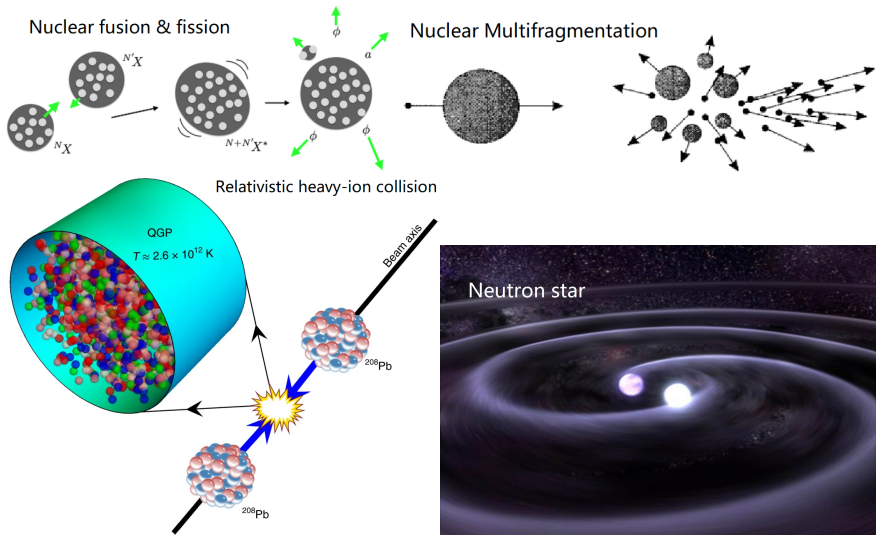
# Pinhole algorithm: $\alpha$ -cluster geometry in carbon isotopes

Positions of 3rd **proton** relative to the other two in  $^{12,14,16}\text{C}$



- **Hoyle state:** Triple- $\alpha$  resonance, essential for creating  $^{12}\text{C}$  in stars (Hoyle, 1954). *Fine-tuning for life?* Epelbaum et al., Phys. Rev. Lett. 106, 192501 (2011)
- **Perspective:** important many-body correlations, understand **internal structures** of ground and excited states by *ab initio calculations*.
- **Next step:** high-precision chiral interaction  $\rightarrow$  EM form factors, shape coexistence, clustering, ... Elhatisari et al., Phys. Rev. Lett. 119, 222505 (2017)

# How to heat up a nucleus



# Microscopic picture of a hot nucleus

- **Low excitation energies**

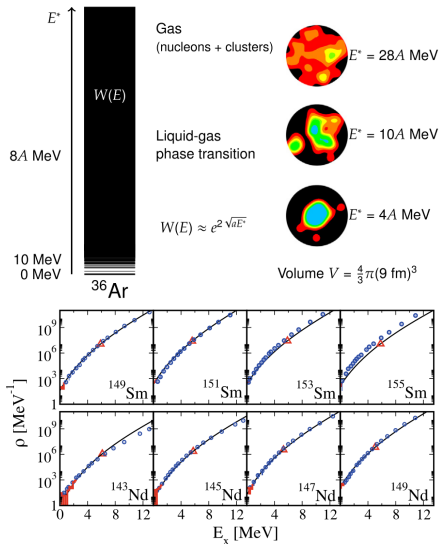
- Ground state, High spin, rotation, vibration, single particle motion, pairing, clustering...

- **High excitation energies**

- Individual energy levels indistinguishable
- Level densities, temperature, pressure, chemical potential,...
- Evaporation, liquid-gas phase transition, multifragmentation,...

- **Extremely high energies**

- Hadron & quark degrees of freedom
- Quark-gluon plasma, quark deconfinement, ...

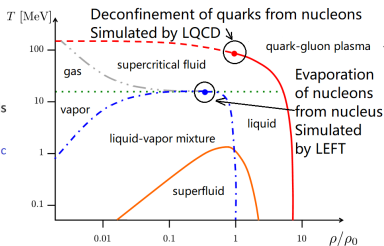
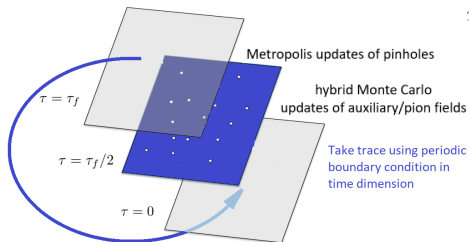


# Simulate canonical ensemble with pinhole trace algorithm

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

$$Z_A = \text{Tr}_A [\exp(-\beta H)] = \sum_{\mathbf{n}_1, \dots, \mathbf{n}_A} \int \mathcal{D}s \mathcal{D}\pi \langle \mathbf{n}_1, \dots, \mathbf{n}_A | \exp[-\beta H(s, \pi)] | \mathbf{n}_1, \dots, \mathbf{n}_A \rangle$$

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



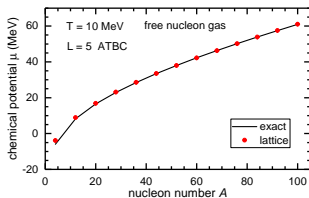
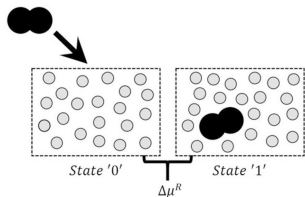
PRL 125, 192502 (2020)

# Extract intensive variables with Widom insertion method

- **Extensive variables:** Measured by operator insertion,
  - E.g., energy  $E = \langle H \rangle_{\Omega}$ , density correlation  $G_{12} = \langle \rho(r_1)\rho(r_2) \rangle_{\Omega}$ .
- **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  $\mu$  by inserting test particles (holes)  
B. Widom, J. Chem. Phys. 39, 2808 (1963)

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

- 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



PRL 125, 192502 (2020)

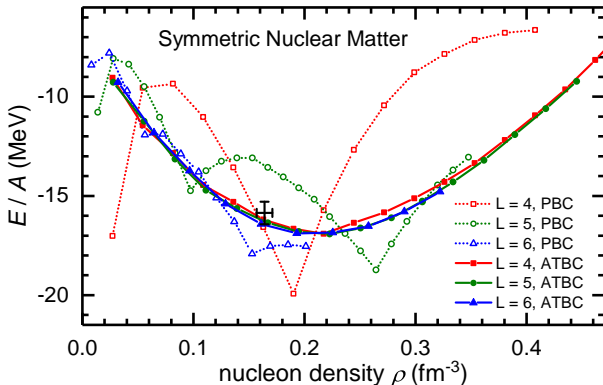


# Lattice interaction: Nuclear matter

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

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

Averaging over  $\theta$ 's to remove fictitious shell effects

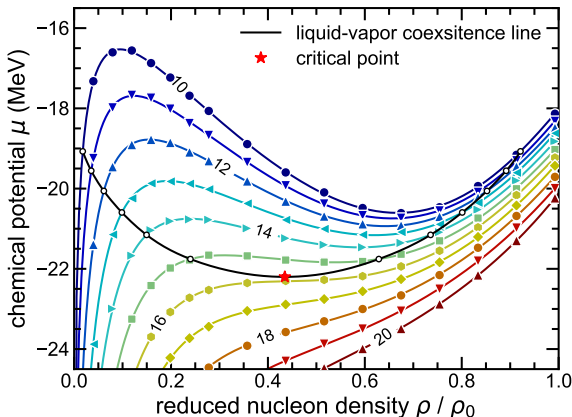


interaction from LU, *et. al.*, [Phys. Lett. B 797, 134863 \(2019\)](#)  
["Essential elements for nuclear binding"](#)

# Finite nuclear systems: Liquid-vapor coexistence line

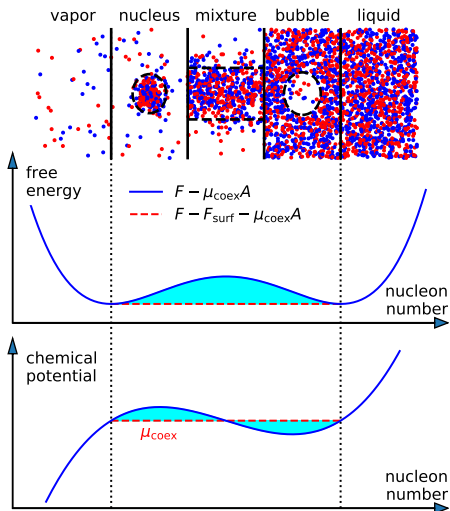
- First *ab initio* calculation of **nuclear liquid-gas phase transition**.
- Symmetric nuclear matter  $N = Z$ , lattice spacing  $a = 1.32$  fm, volume  $V = (6a)^3$ , nucleon number  $4 \leq A \leq 132$ .
- Temperature  $10 \text{ MeV} \leq T \leq 20 \text{ MeV}$ , temporal step  $\Delta\beta = 1/2000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

Lu et al., *Phys. Rev. Lett.* 125, 192502 (2020)

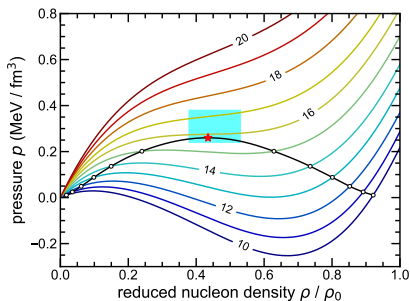


# Finite nuclear systems: Surface effect

- The **backbending** in  $\mu$ - $\rho$  curves comes from the **surface effects**.
- **Thermodynamic limit** ( $A \rightarrow \infty$ ,  $N \rightarrow \infty$ ),  $\mu_{\text{liquid}} = \mu_{\text{vapor}} = \text{const.}$  at coexistence;
- **Finite systems**: extra contribution of the **surface** to free energy  $F$ ;
- **Surface area** maximized at intermediate densities;
- $\mu = \partial F / \partial A$  exhibits a **backbending** at coexistence.



# Critical point: Compare with experiment



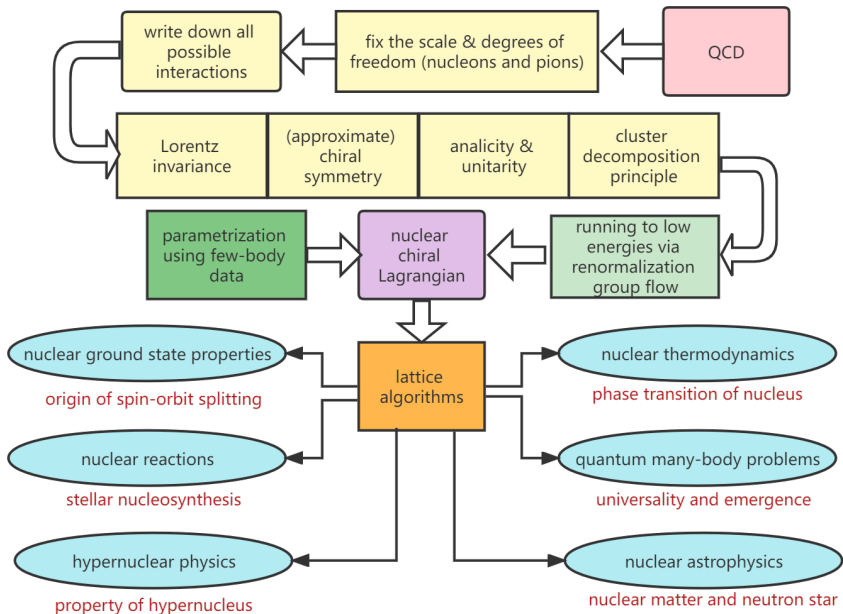
Lu et al., Phys. Rev. Lett. 125, 192502 (2020)

- **Pressure**  $p = \int \rho d\mu$  along every isotherm (Gibbs-Duhem equation).
- Extract  $T_c$ ,  $P_c$  and  $\rho_c$  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 <sup>3</sup> )	0.260(3)	0.31(7)	0.26	0.2020
$\rho_c$ (fm <sup>-3</sup> )	0.089(1)	0.06(1)	0.0526	0.0463
$\rho_0$ (fm <sup>-3</sup> )	0.205(0)	0.132		
$\rho_c/\rho_0$	0.43	0.45		

Lu et al., Phys. Rev. Lett. 125, 192502 (2020)

# Summary



THANK YOU FOR YOUR  
ATTENTION