Nuclear *ab initio* calculation on the lattice

Bing-Nan Lü
吕炳楠
Nuclear Lattice EFT Collaboration

中国工程物理研究院研究生院
GRADUATE SCHOOL OF CHINA ACADEMY OF ENGINEERING PHYSICS
FRIB
MICHIGAN STATE UNIVERSITY
中山大學
SUN YAT-SEN UNIVERSITY
JÜLICH FORSCHUNGSZENTRUM
OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY
UNIVERSITÄT BONN

Sun Yat-Sen university, Zhu-Hai, March-16-2024

Nuclear physics: Seperation of scales

Lattice Quantum Chromodynamics

Chiral Effective Field Theory

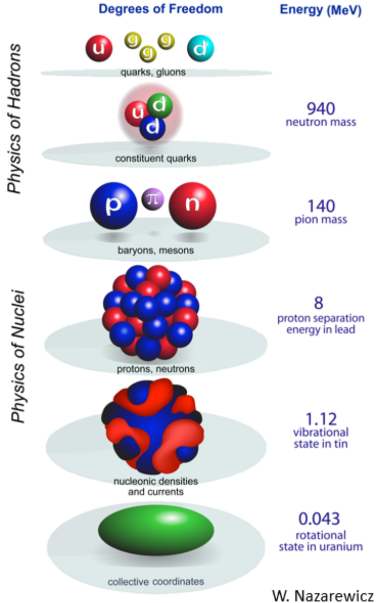
Microscopic *A*-body Methods

Configuration Interactions

Density Functional Methods

Mean Field Methods

Effective Theory of Collective Modes



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

$$\mathscr{L}_{\mathrm{QCD}} = \sum_{\text{flavors}} \bar{\psi}(i\gamma^\mu \partial_\mu - M)\psi - gA^i_\mu \bar{\psi}\gamma^\mu t_i \psi - \frac{1}{4} G^{\mu\nu}_i G^i_{\mu\nu}$$

$$+ \frac{1}{2}\cancel{m_g^2 A^i_\mu A^\mu_i} + \frac{1}{2}\cancel{c\bar{\psi}\sigma^{\mu\nu} t_i \psi G^i_{\mu\nu}} + \cdots$$

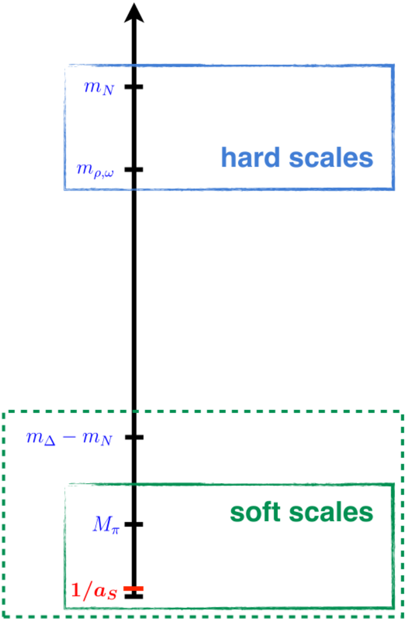
Suppressed by gauge symmetry

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 π-N potentials in powers of

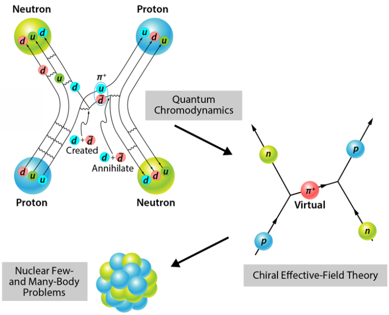
$$Q \in \left\{ \frac{M_\pi}{\Lambda}, \frac{|\vec{p}|}{\Lambda} \right\}, \Lambda \sim m_\rho \sim 4\pi F_\pi \sim 1\mathrm{GeV}$$

- QCD has an approximate chiral symmetry
  - Explicitly broken by non-zero quark mass (m_q~3 MeV)
  - Spontaneously broken, SU(2)×SU(2)→SU(2)
- SB exact symmetry → massless Goldstone bosons
- SB approx. symm. → very light bosons → pions ($M_\pi \sim 140$ MeV)
- In nucleus, Fermi momentum p_F~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: $\mathrm{SU}(2)_L \times \mathrm{SU}(2)_R \to \mathrm{SU}(2)_V$
- 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 $Q \ll \Lambda_\chi$

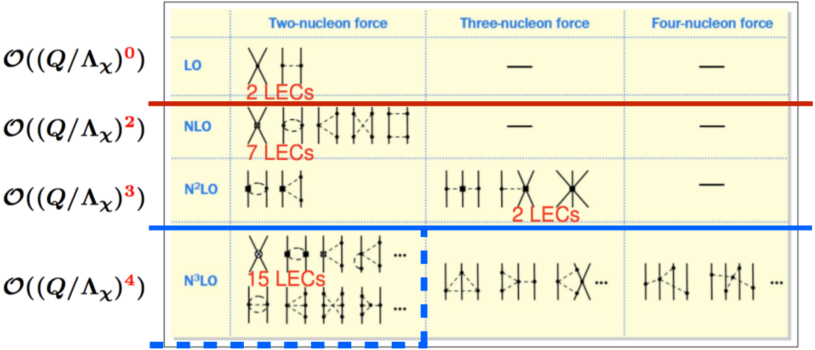


Quarks confined in nucleons and pions

N-N interaction in nuclear chiral EFT

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

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

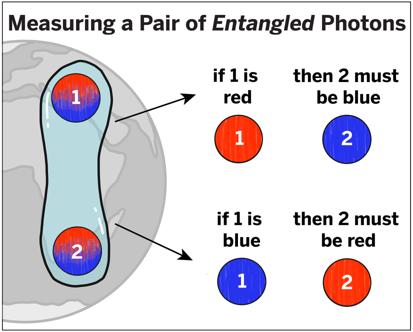


Why need nuclear ab initio methods

Mean field models are useful

but **quantum correlations** not included

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



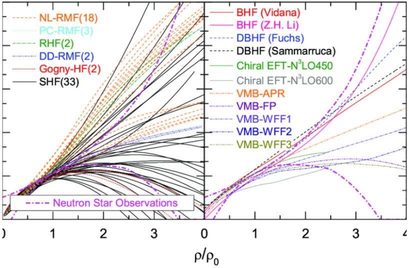
In mean field models, motion of particle 1

is independent of other particles

$$P(1,2) = P(1) \times P(2)$$

Predictions are model-dependent

Example: symmetry energy

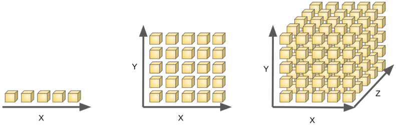


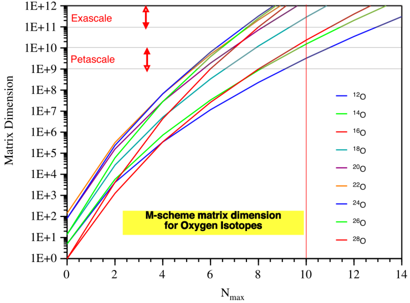
N.-B. Zhang and B.-A. Li, EPJA 55, 39 (2019)

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

Dimensionality curse in nuclear many-body problems

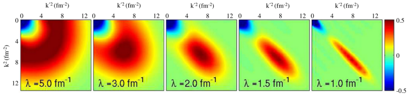
Exponential increase of resources



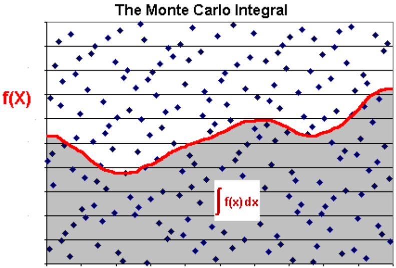


PRC 101, 014318 (2020)

Solution 1: Reduce effective Hilbert space with SRG evolution



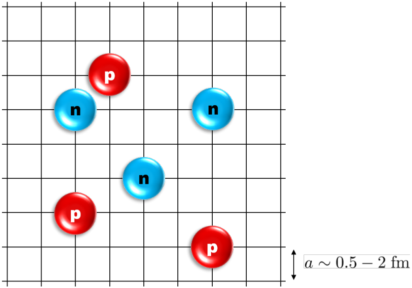
Solution 2: Monte Carlo algorithms



Lattice EFT = **Chiral EFT** + **Lattice** + **Monte Carlo**

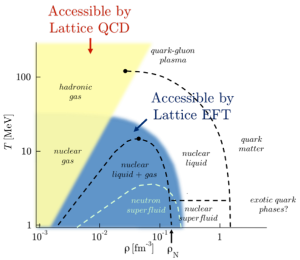
Review: Dean Lee, Prog. Part. Nucl. Phys. 63, 117 (2009),
Lähde, Meißner, "Nuclear Lattice Effective Field Theory", Springer (2019)

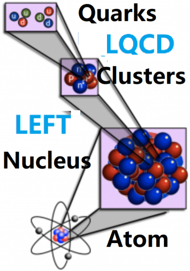
- Discretized chiral nuclear force
- Lattice spacing $a \approx 1$ fm = 620 MeV (∼chiral symmetry breaking scale)
- Protons & neutrons interacting via **short-range, δ-like** and **long-range, pion-exchange** interactions
- Exact method, polynomial scaling ($\sim A^2$)



Lattice adapted for nucleus

	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





Euclidean time projection

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

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

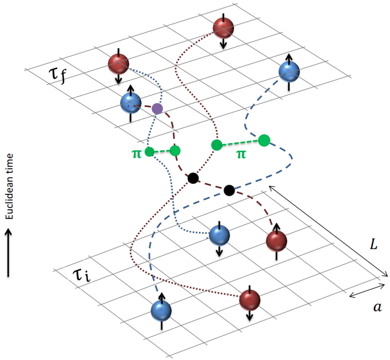
with $|\Psi_A\rangle$ representing A *free* nucleons.

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

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

- τ is discretized into time slices:

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

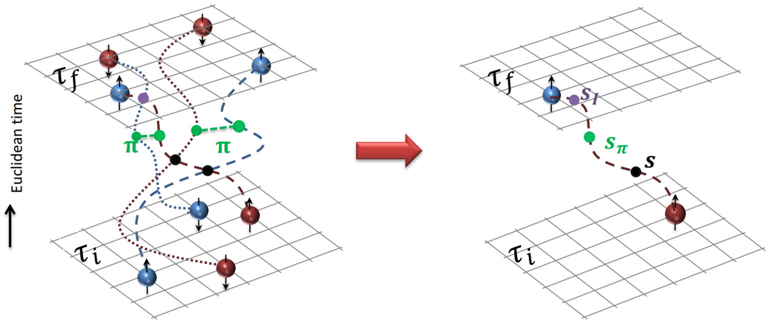


All possible configurations in $\tau \in [\tau_i, \quad \tau_f]$ are sampled.
Complex structures like nucleon clustering emerges naturally.

Auxiliary field transformation

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

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



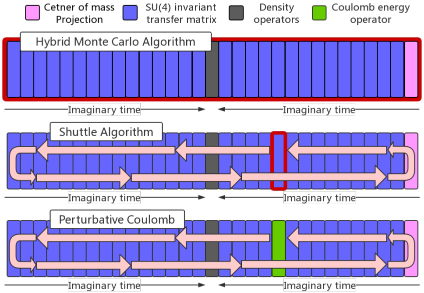
Advanced algorithm and programming paradigm

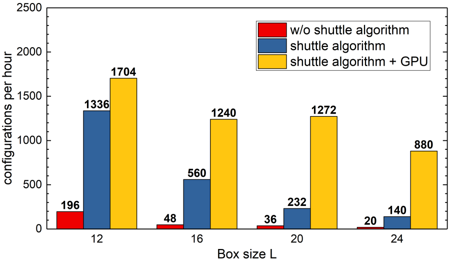
All $L_t \times L^3$ auxiliary fields $s_{\boldsymbol{n},n_t}$ need to be updated. Two algorithms:

- **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





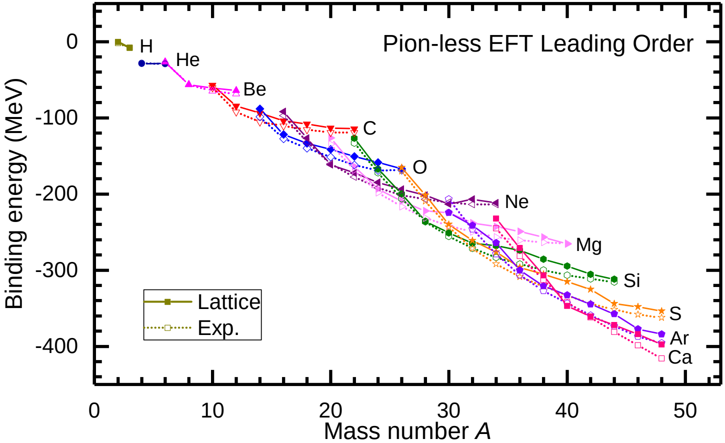
- Can be implemented for GPU
- **Algorithm & Hardware** combined give a 40∼50 times speed-up

Large lattices are accessible

Essential elements for nuclear binding

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

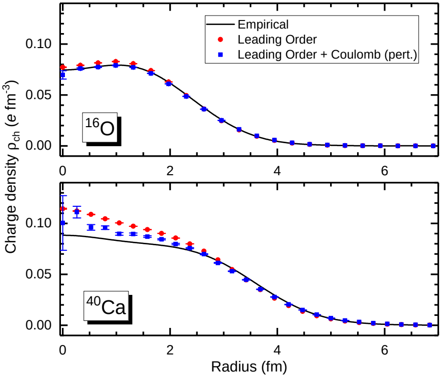
Answer: 4, Strength, Range, Three-body, Locality

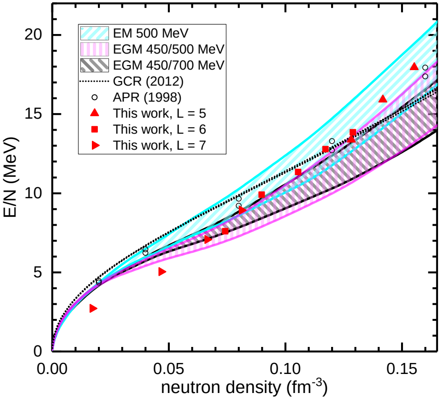


Lu, Li, Elhatisari, Lee, Epelbaum, Meißner, Phys. Lett. B 760 (2016), 309

Essential elements for nuclear binding

Charge density and neutron matter equation of state are impotant 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_{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_{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 predicative power $\Longrightarrow$ Demonstration of both **nuclear force model** and **many-body algorithm**

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

Pinhole algorithm: Schematic

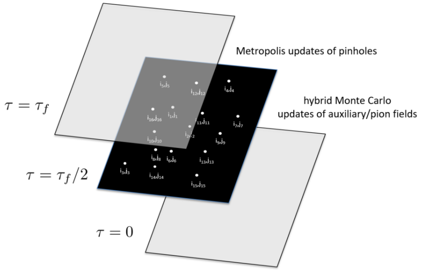
In terms of auxiliary fields, the amplitude Z can be written as a path-integral,

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

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.

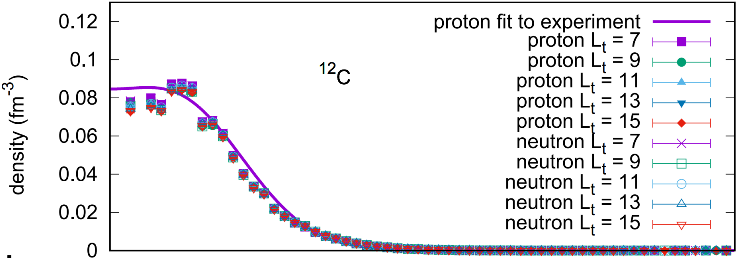


Pinhole algorithm: Intrinsic density distributions

- Densities relative to the center of mass:

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

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

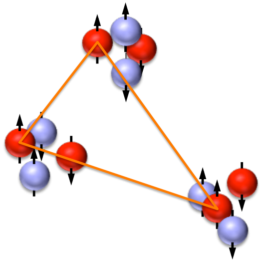


- Independent of projection time $L_t \Longleftrightarrow$ In ground state
- Sign problem suppressed $\longrightarrow$ Small errorbars
  Elhatisari et al., Phys. Rev. Lett. 119, 222505 (2017)

Triangles in carbon isotopes

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

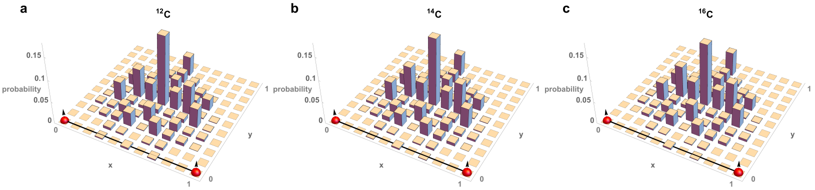
$$\rho(d_1, d_2, d_3) = \sum_{j_1,j_2,j_3} \sum_{\boldsymbol{n}_1,\boldsymbol{n}_2,\boldsymbol{n}_3} |\Phi_{\uparrow,j_1,\uparrow,j_2,\uparrow,j_3}(\boldsymbol{n}_1, \boldsymbol{n}_2, \boldsymbol{n}_3)|^2 \times \sum_{P(123)} \delta(|\boldsymbol{n}_1 - \boldsymbol{n}_2| - d_3)\delta(|\boldsymbol{n}_1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

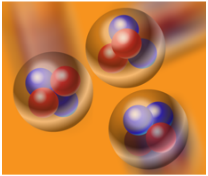


Elhatisari, Epelbaum, Krebs, Lahde, Lee, Li, BNL, Meissner, Rupak, PRL 119, 222505 (2017)

Pinhole algorithm: α-cluster geometry in carbon isotopes

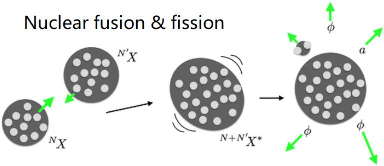
Positions of 3rd proton relative to the other two in ^{12,14,16}C



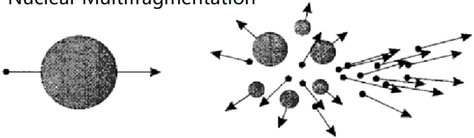


- **Hoyle state**: Triple-α resonance, essential for creating ^{12}C in stars (Hoyle, 1954). *Fine-tuning for life?*
  Epelbaum et al., Phys. Rev. Lett. 106, 192501 (2011)
- **Perspective:** important many-body correlations, understand **internal structures** of ground and excited states by ***ab initio*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

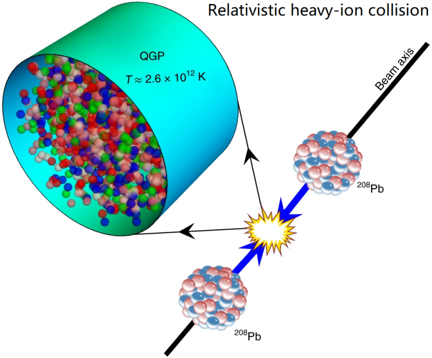
Nuclear fusion & fission

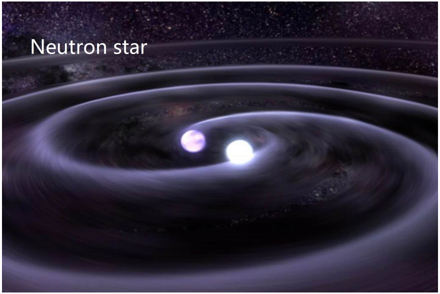


Nuclear Multifragmentation



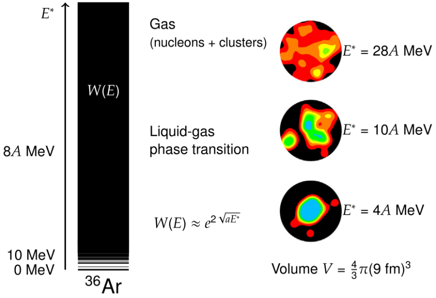
Relativistic heavy-ion collision

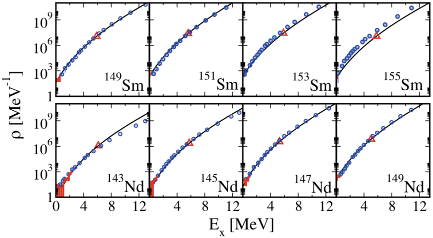




Microscopic picture of a hot nucleus

- **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, ...



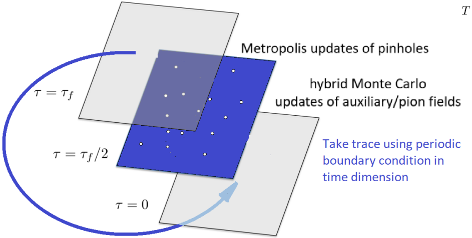


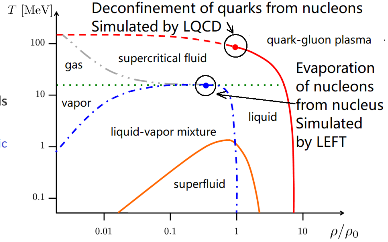
Simulate canonical ensemble with pinhole trace algorithm

- All we need: **partition function** $Z(T,V,A) = \sum_k \langle \exp(-\beta H) \rangle_k$, sum over all 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:

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

- **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.





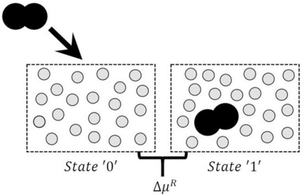
PRL 125, 192502 (2020)

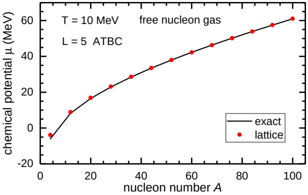
Extract intensive variables with Widom insertion method

- **Extensive variables:** Measured by operator insertion,
  - E.g., energy $E = \langle H \rangle_\Omega$, density correlation $G_{12} = \langle \rho(\boldsymbol{r}_1)\rho(\boldsymbol{r}_2)\rangle_\Omega$.
- **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)

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

- 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





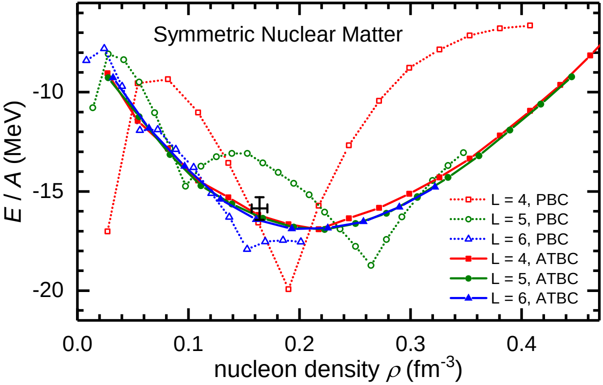
PRL 125, 192502 (2020)

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 θs' to remove fictitious shell effects

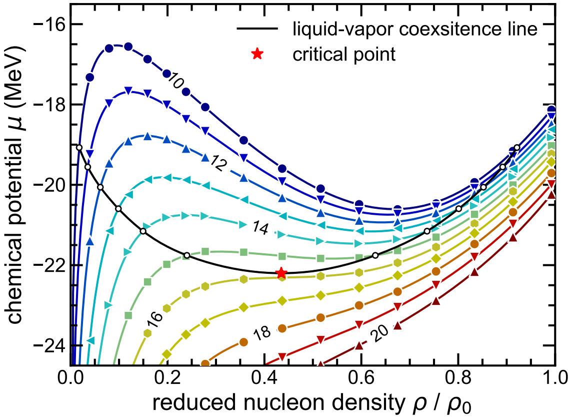


interaction from LU, *et. al.*, Phys. Lett. B 797, 134863 (2019)
"Essential elements for nuclear binding"

Finite nuclear systems: Liquid-vapor coexistence line

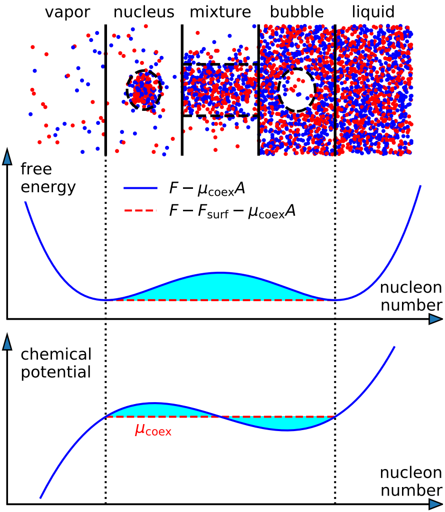
- First ***ab initio* calculation** of **nuclear liquid-gas phase transition**.
- Symmetric nuclear matter $N = Z$, lattice spacing $a = 1.32$ fm, volume $V = (6a)^3$, nucleon number $4 \leq A \leq 132$.
- Temperature 10 MeV$\leq T \leq$ 20 MeV, temporal step $\Delta\beta = 1/2000$ MeV^{-1}.
- 288000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

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

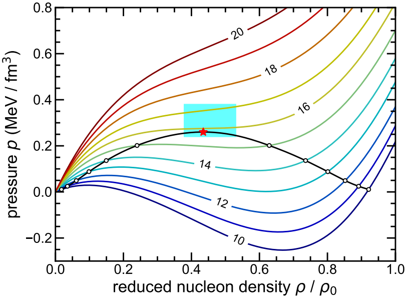


Finite nuclear systems: Surface effect

- The **backbending** in μ-ρ curves comes from the surface effects.
- **Thermodynamic limit** ($A \to \infty$, $N \to \infty$), $\mu_{\text{liquid}} = \mu_{\text{vapor}}$ =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



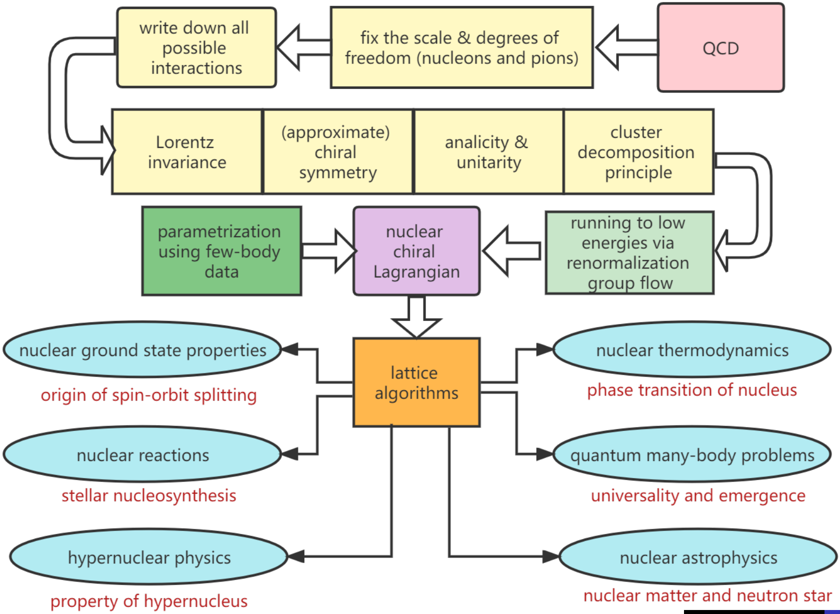
Lu et al., Phys. Rev. Lett. 125, 192502 (2020)

- **Pressure** $p = \int \rho\, d\mu$ along every isotherm (Gibbs-Duhem equation).
- Extract T_c, P_c and 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., Phys. Rev. Lett. 125, 192502 (2020)

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 reactions
stellar nucleosynthesis
hypernuclear physics
property of hypernucleus
nuclear thermodynamics
phase transition of nucleus
quantum many-body problems
universality and emergence
nuclear astrophysics
nuclear matter and neutron star

Thank you for your attention