Ab initio Nuclear Physics on the Lattice

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Collaborate with
Nuclear Lattice EFT Collaboration

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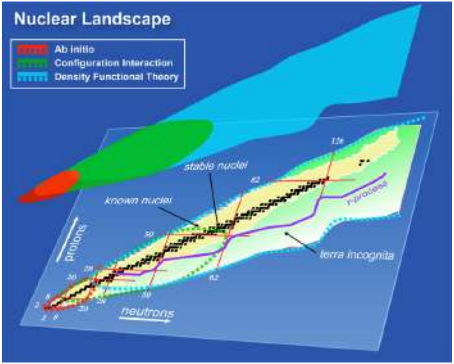
Road map - Towards a comprehensive description of the nucleus

- ***Ab initio* methods**:
  Microscopic interactions
  full many-body correlations

- **Configuration-interaction theories**:
  Phenomenological interactions
  full many-body correlations

- **Density functional theories**:
  Phenomenological interactions
  mean field approximation



A calculation is said to be ***"ab initio"***
if it relies on ***basic and established laws of nature***
without additional ***assumptions or special models***

Introduction: Why *ab initio* nuclear physics?

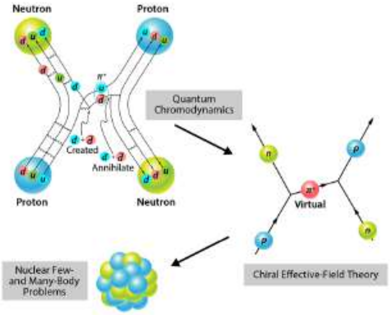
- Simulate **nucleus** from **bare nucleus-nucleus force**
- **Not** brute force! Also requires deep physical insights and clever algorithms

  Memory for N classical particles $\sim \mathcal{O}(N)$
  Memory for N quantum particles $\sim \mathcal{O}(\exp(N))$
- Solutions: Renormalization group, **Monte Carlo**, Quantum computing...

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 $Q \ll \Lambda_\chi$

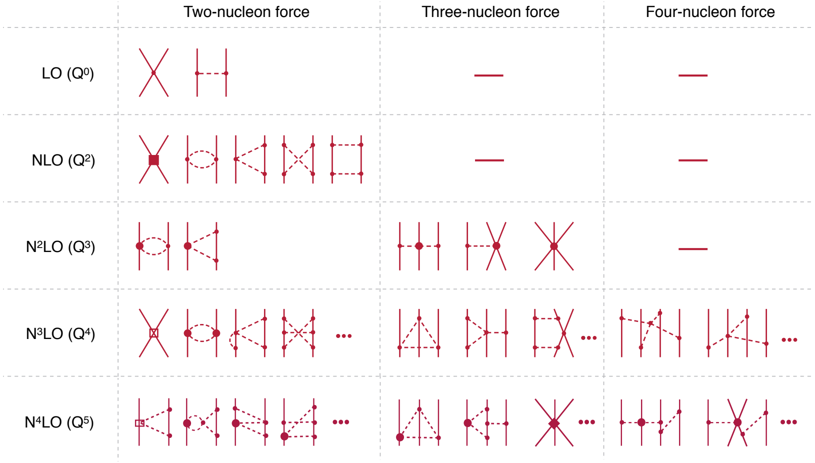


Quarks confined in nucleons and pions

Introduction: Chiral effective field theory

A systematic expansion of the nuclear force

Available up to the Next-to-Next-to-Next-to-Leading Order (N^3LO)

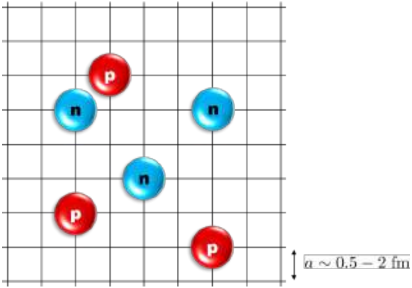


Quantum many-body problem can be solved on a lattice

Lattice QCD, Hubbard model, Cold atoms...

Lattice EFT = Chiral EFT + Lattice + Monte Carlo

- Discretized chiral EFT
- Lattice spacing $a \sim 1$ fm
- Lattice imposes a momentum cutoff $\Lambda = \pi\hbar/a \sim 600$ MeV
- Exact method, polynomial scaling ($\sim A^2$)



Lattice adapted for nucleus

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

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

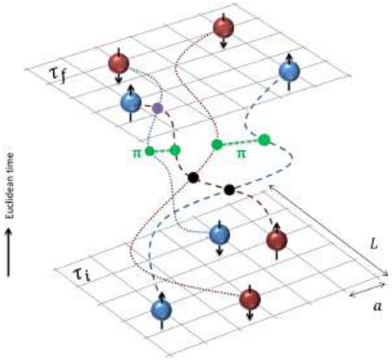
with $|\Psi_A\rangle$ representing A *free* nucleons.

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

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

- τ is discretized into time slices:

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



Complex structures like nucleon clustering emerges naturally.

Lattice EFT: Auxiliary field transformation

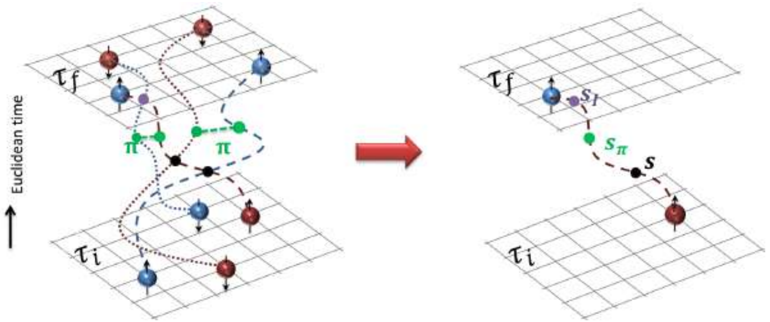
For a two-body $\delta-$ function interaction on the lattice

$$H = \sum_{nn'} -\psi_n^\dagger \frac{\nabla^2_{nn'}}{2M} \psi_{n'} + C \sum_n : (\psi_n^\dagger \psi_n)^2 :$$

$\psi_n^\dagger(\psi_n)$ create (annihilate) a partice at mesh point n

Hubbard–Stratonovich transformation:

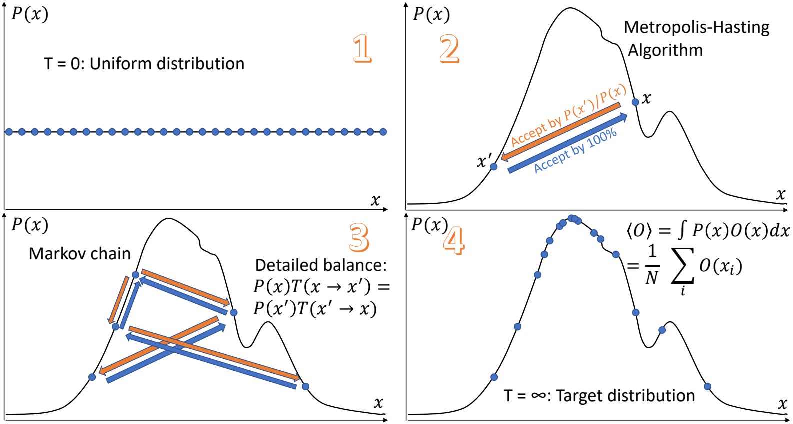
$$: \exp(-a_t H) := \int \prod_n ds_n : \exp\left[\sum_n \left(-\frac{s_n^2}{2} + a_t \psi_n^\dagger \sum_{n'} \frac{\nabla^2_{nn'}}{2M} \psi_{n'} + \sqrt{-a_t C}\, s_n \psi_n^\dagger \psi_n\right)\right] :$$

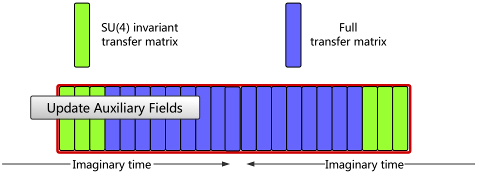


Integrating over a continuous domain

$\Longrightarrow$ Arithmetic averaging over an ensamble

Central limit theorem: Statistical error $\propto 1/\sqrt{N}$





Samples are generated by **Markov Chain Monte Carlo**

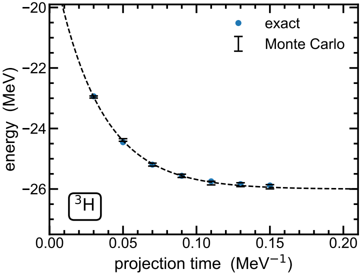
Total energies at large t follow

$$E_A(t) = E_A(\infty) + c \exp[-\Delta E \tau].$$

For any inserted operator $\mathscr{O}$,

$$\mathscr{O}_A(\tau) = \mathscr{O}_A(\infty) + c' \exp[-\Delta E \tau/2],$$

c, c', ΔE are fitting parameters.



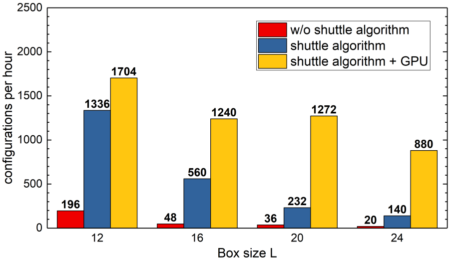
Advanced algorithm and programming paradigm

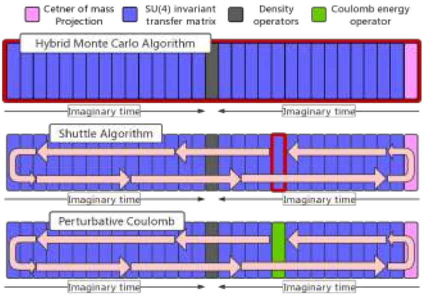
All $L_t \times L^3$ auxiliary fields s_{n,n_t} need to be updated. Two algorithms:

- **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

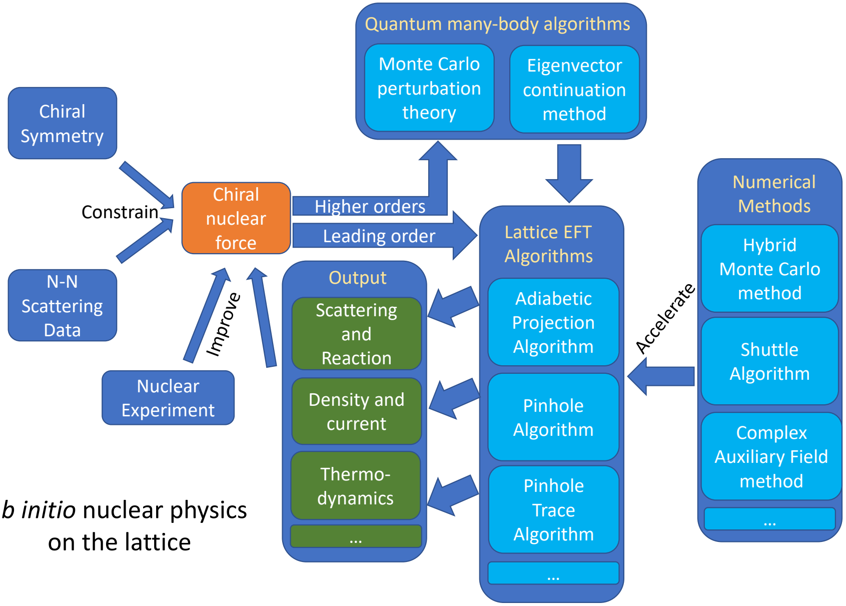




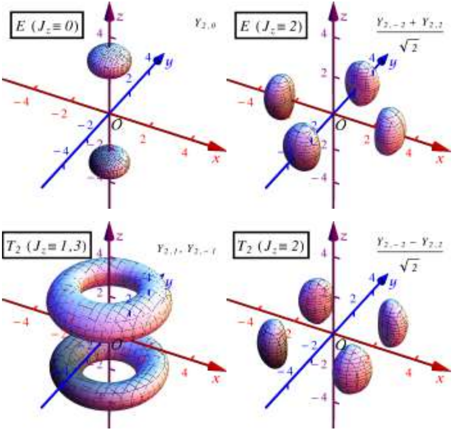
- Can be implemented for GPU
- **Algorithm & Hardware** combined give a 40∼50 times speed-up

Large lattices are accessible

Lattice EFT: A unified framework for *ab initio* calculations



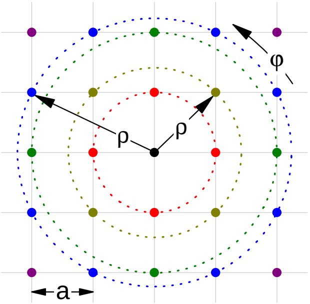
Ab initio nuclear physics on the lattice

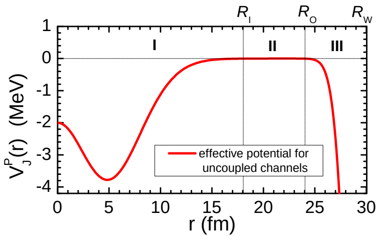


- In real world, rotational SO(3) symmetry is a strict symmetry.
- In a lattice world, due to **lattice artifacts**, some directions are **more preferred** than others.
- To solve this issue, we propose:
  - Improved kinetic energy
    B.L. et al., Phys. Rev. D 90, 034507 (2014)
  - Weighted average for energy
    B.L. et al., Phys. Rev. D 90, 034507 (2014)
  - W/ ave. for tensor operators
    B.L. et al., Phys. Rev. D 92, 014506 (2015)

Most lattice artifacts cancel out
when **averaging over lattice orientations**

Techniques for solving the lattice scattering problem





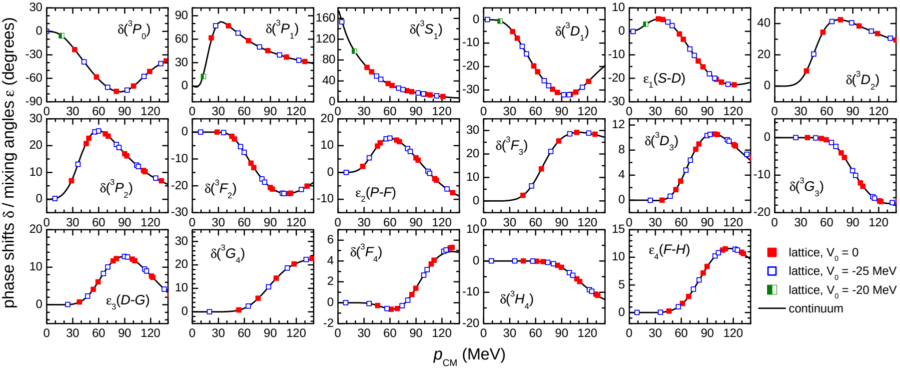
- Angular momentum projection: Expand wave functions on states with definite angular momentum,

$$|\rho\rangle_{L,L_z} = \sum_r Y_{L,L_z}(\hat{r})\delta_{\rho,|r|}|r\rangle$$

- Complex auxiliary potential: Twist radial wave functions with a potential at very large R. In asymptotic region $(r \to \infty)$:

$$\psi_k \approx A h^{+}_{J,k} - B h^{-}_{J,k},$$

B.L. et al., Phys. Lett. B 760 (2016) 309



- Phase shifts and mixing angles for a tensor pontential (toy model).
- Continuum results by solving the Lippmann-Schwinger equation.

B.L. et al., Phys. Lett. B 760 (2016) 309

Precision comparable with exact solutions

Chiral nuclear force up to N^{3}LO: lattice interactions

- We use a seperable form $V \cong O^\dagger O$ for short-range interactions:

$$O^{2M,s_{NL}}_{S,L,J,J_z,I,I_z}(n) = \sum_{S_z,L_z} \langle SS_z, LL_z|JJ_z\rangle \left[\psi(n)\nabla^{2M}_{1/2} R^*_{L,L_z}(\nabla)\psi(n)\right]^{s_{NL}}_{S,S_z,I,I_z}$$

$$R_{L,L_z}(r) = \sqrt{\frac{4\pi}{2L+1}}\, r^L Y_{L,L_z}(\theta,\phi)$$

The indices in O and $O^\dagger$ are all contracted to form scalars.

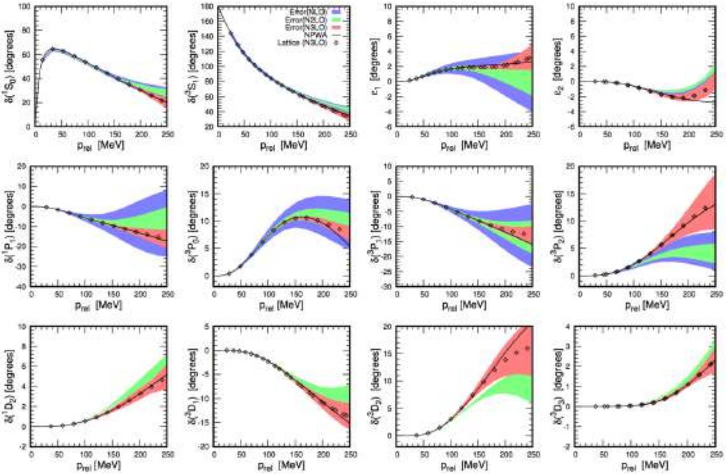
- Long-range interactions (1-pion, 2-pion) implemented using FFT:

$$V_{\rm OPE} = -\frac{g_A^2}{8F_\pi^2} \sum_{n',n,S',S,I} :\rho_{S',I}(n') f_{S'S}(n'-n)\rho_{S,I}(n):$$

$$f_{S'S}(n'-n) = \frac{1}{L^3}\sum_q \frac{q_{S'}q_S \exp\left[-iq\cdot(n'-n) - b_\pi(q^2+M_\pi^2)\right]}{q^2+M_\pi^2}$$

Ning Li, Elhatisari, Epelbaum, Lee, B.L., Meissner, PRC 98, 044002 (2018)

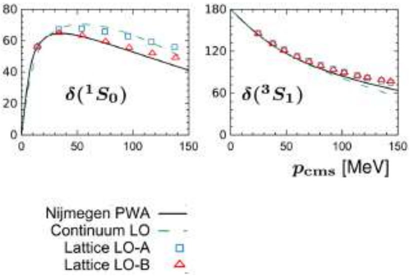
Chiral nuclear force up to N^{3}LO: fit on the lattice

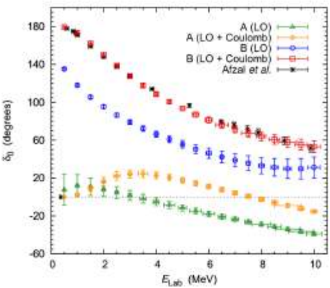


fit to N^{2}LO: Alarcon, Du, Klein, Lahde, Lee, Ning Li, B.L., Luu, Meissner, EPJA 53, 83 (2017)

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

- Both interaction A and B give the same N-N phase shift.
- A: **Non-local** B: **Local + non-local**





- Locality can only be probed by many-body calculations.
- What is the consequence for finite nuclei?

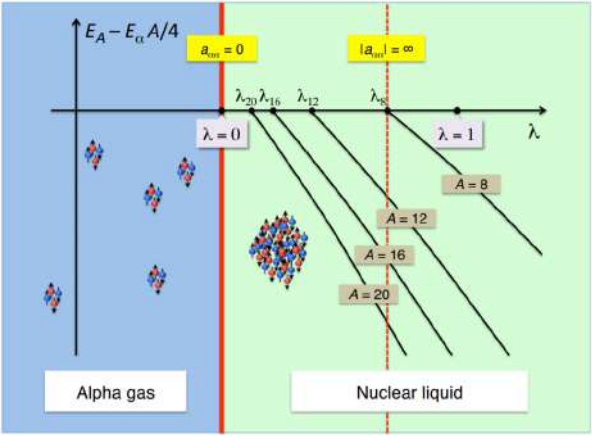
Elhatisari, Ning Li, Rokash, Alarcon, Du, Klein, B.L., Meißner, Epelbaum,

Krebs, Lähde, Lee, Rupak, PRL 117 (2016) 132501

Effects of locality: Zero-temperature phase diagram

$a_{\alpha\alpha}$: α-α scattering length. $E_A - E_\alpha A/4$: α-binding energy.

$\lambda = 0$: purely non-local $\lambda = 1$: reality



$\lambda_8 = 0.7(1)$

$\lambda_{12} = 0.3(1)$

$\lambda_{16} = 0.2(1)$

$\lambda_{20} = 0.2(1)$

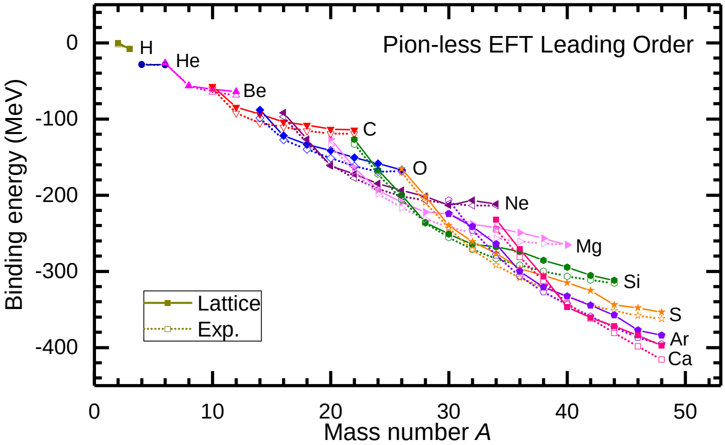
$\lambda_\infty = 0.0(1)$

Elhatisari, Ning Li, Rokash, Alarcon, Du, Klein, B.L., Meißner, Epelbaum,

Krebs, Lähde, Lee, Rupak, PRL 117 (2016) 132501

Essential elements for nuclear binding

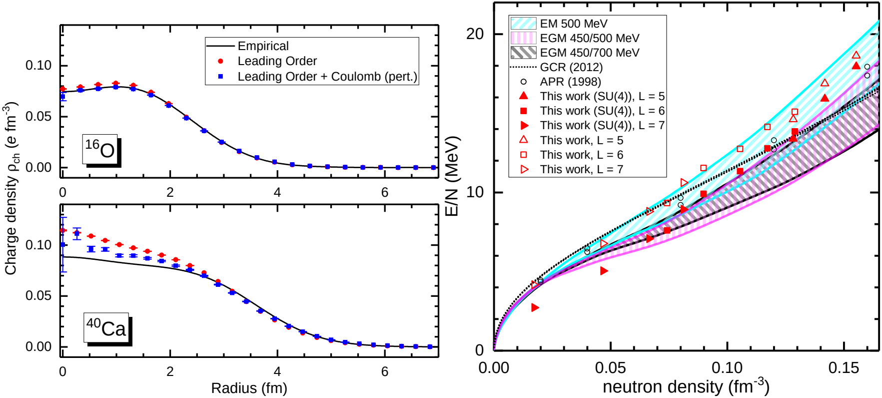
How many free parameters are essential for a proper nuclear force?
Answer: 4, Strength, Range, Three-body, Locality



B.L., Ning Li, Elhatisari, Lee, Epelbaum, Meißner, PLB 797, 134863 (2019)

Essential elements for nuclear binding

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



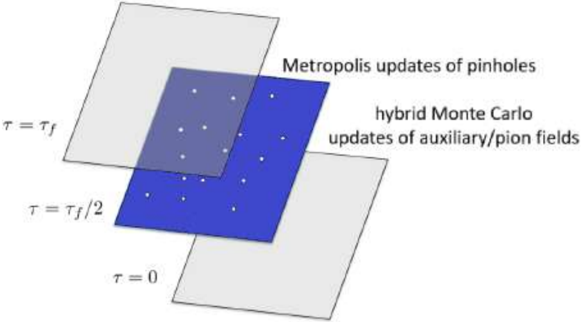
B.L., Ning Li, Elhatisari, Lee, Epelbaum, Meißner, PLB 797, 134863 (2019)

Pinhole algorithm: Sampling nucleon densities

The expectation of operator O can be expressed as a path integral:

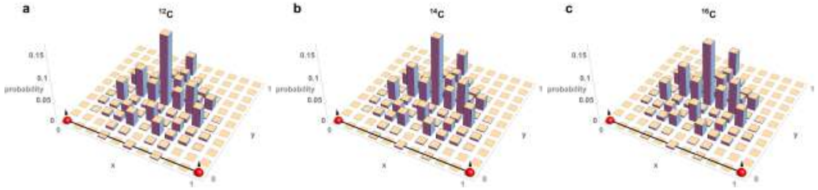
$$\langle O \rangle = \lim_{\tau\to\infty} \frac{\sum_{n_1,\cdots n_A} \int \mathscr{D}s\mathscr{D}\pi \langle \Psi_A | e^{-\frac{\tau}{2}H(s,\pi)} \rho_A(n_1,\cdots,n_A) e^{-\frac{\tau}{2}H(s,\pi)} | \Psi_A \rangle O(n_1,\cdots,n_A)}{\sum_{n_1,\cdots n_A} \int \mathscr{D}s\mathscr{D}\pi \langle \Psi_A | e^{-\frac{\tau}{2}H(s,\pi)} \rho_A(n_1,\cdots,n_A) e^{-\frac{\tau}{2}H(s,\pi)} | \Psi_A \rangle},$$

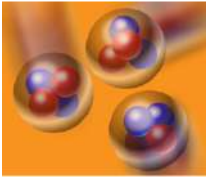
Density operator ρ_A can be sampled with **Metropolis algorithm**



Elhatisari, Epelbaum, Krebs, Lähde, Lee, Ning Li, B.L., Meißner, Rupak, PRL 119, 222505 (2017)

Positions of 3rd α-cluster relative to the other two in $^{12,14,16}C$

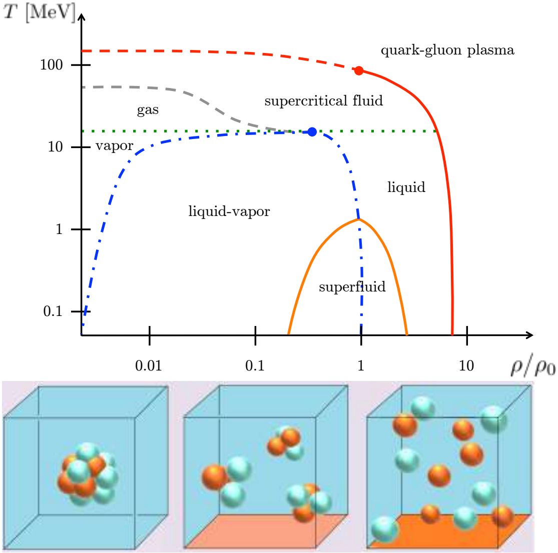




- **Hoyle state**: Triple-α resonance, essential for creating ^{12}C in stars (Hoyle, 1954). *Fine-tuning for life?* *Epelbaum et al., PRL 106, 192501 (2011)*
- *Question:* Are there **Hoyle-like states** in ^{14}C and ^{16}C? Consequence for element creation?

Visualize clustering in *ab inito* calculation

Elhatisari, Epelbaum, Krebs, Lähde, Lee, Ning Li, B.L., Meißner, Rupak, PRL 119, 222505 (2017)



A novel algorithm for simulating Finite-temperature nuclear matter from first principles

"*Ab initio*" means **phase transition** and **clustering** can emerge without model assumptions

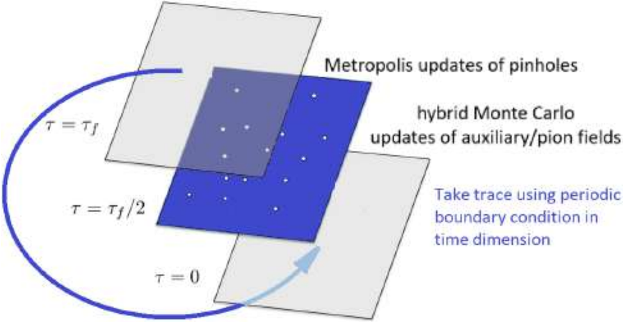
B.L., Ning Li, Elhatisari, Dean Lee, Drut, Lähde, Epelbaum, Meißner, PRL 125, 192502 (2020)

Pinhole trace algorithm

The pinhole states span the whole A-body Hilbert space.

Cannonical partition function can be expressed using pinholes:

$$Z_A = \mathrm{Tr}_A[\exp(-\beta H)] = \sum_{n_1,\cdots,n_A} \int \mathscr{D}s\mathscr{D}\pi \langle n_1,\cdots,n_A| \exp[-\beta H(s,\pi)] |n_1,\cdots,n_A\rangle$$

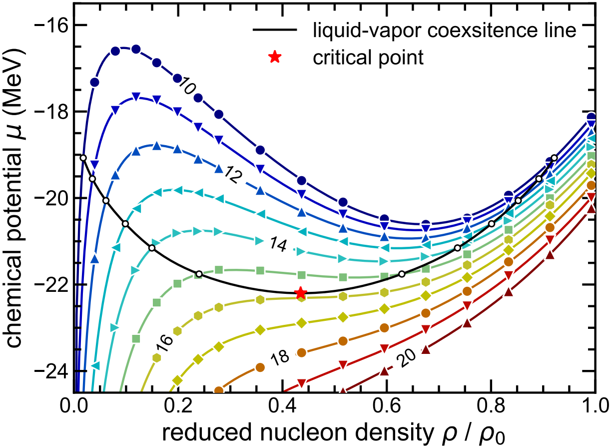


B.L., Ning Li, Elhatisari, Dean Lee, Drut, Lähde, Epelbaum, and Meißner, PRL 125, 192502 (2020)

Finite nuclear systems: Liquid-vapor coexistence line

Widom insertion method: Measure μ by inserting test particles

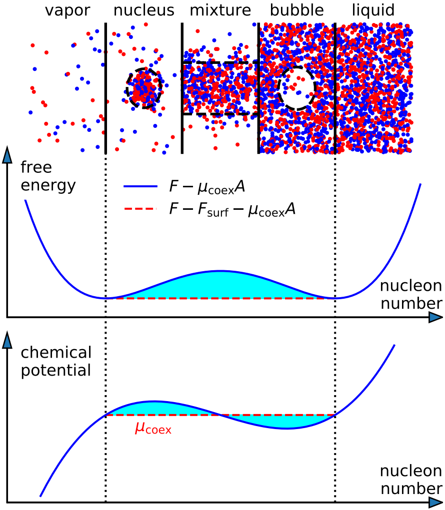
B. Widom, J. Chem. Phys. 39, 2808 (1963)



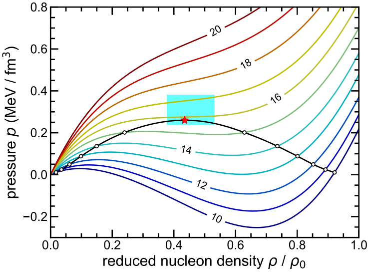
B.L., Ning Li, Elhatisari, Dean Lee, Drut, Lähde, , Epelbaum, and Meißner, PRL 125, 192502 (2020)

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



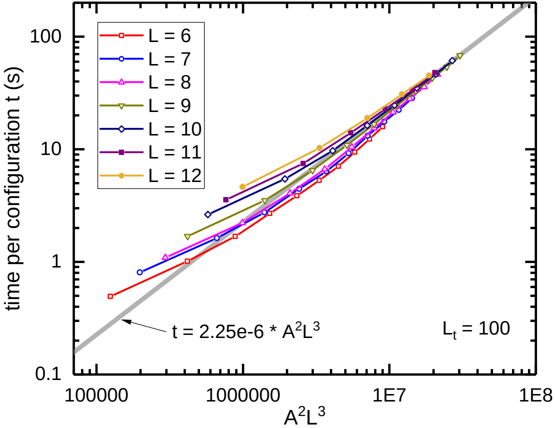
T_c, P_c and ρ_c of neutral symmetric nuclear matter

Experimental values and mean field results taken from [Elliott, Lake, Moretto, Phair, PRC 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		

Performance of PT algorithm: Time complexity

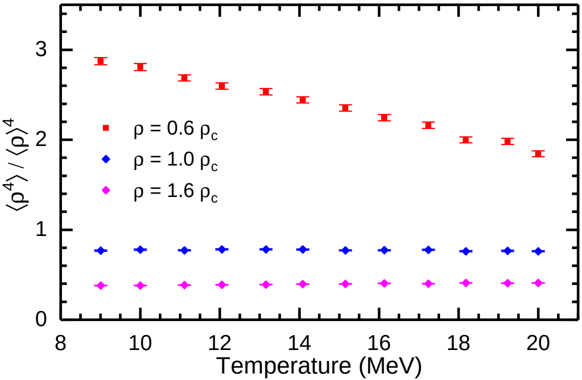
Time complexity $\sim \mathcal{O}(A^2 L^3)$, Grand canonical ensemble $\sim \mathcal{O}(L^6)$



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

B.L., Ning Li, Elhatisari, Dean Lee, Drut, Lähde, , Epelbaum, and Meißner, PRL 125, 192502 (2020)

Ratio $\langle \rho^4 \rangle / \langle \rho \rangle^4$ signifies the clustering correlation



B.L., Ning Li, Elhatisari, Dean Lee, Drut, Lähde, , Epelbaum, and Meißner, PRL 125, 192502 (2020)

Summary and Perspective

- Lattice Effective Field Theory is a unified framework for nuclear *ab initio* calculations.
- Based on Markov Chain Monte Carlo method.
  - Challenges: reduce statistical errors.
- Unlimited configuration space.
  - Able to describe phase transition, nuclear fragmentation, clustering,...
- TODO list: refined N^3LO chiral interaction, advanced lattice algorithms, numerical extrapolations, ...
- Future projects: $0\nu\beta\beta$ calculations, independent of other *ab initio* methods, reduce systematic errors. Possible connection with Lattice QCD.


谢谢各位老师!