Lattice simulations for nuclear structure and scattering

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Nuclear Lattice EFT Collaboration
HISKP, Universität Bonn

CRC110 Workshop on
Nuclear Dynamics and Threshold Phenomena
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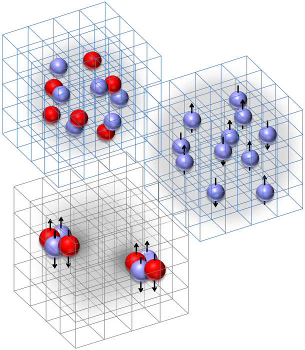

Nuclear Lattice Effective Field Theory collaboration

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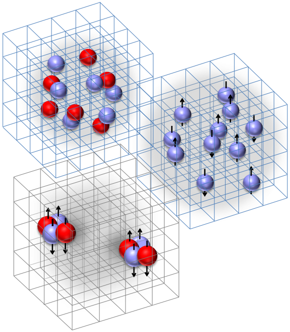
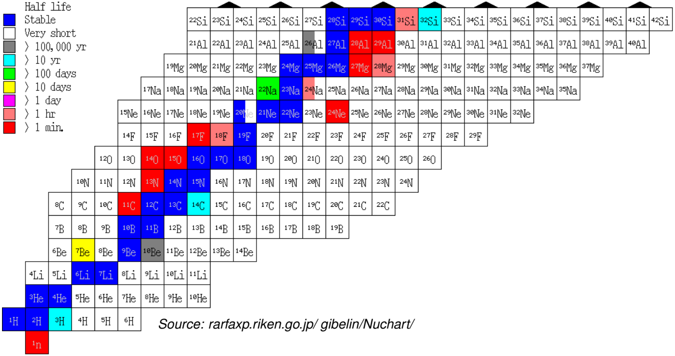
Outline

- Introduction
- Lattice effective field theory
- Adiabatic projection method
- Degree of locality of nuclear forces
- Pinhole Algorithm: density profiles for nuclei
- Summary



Ab initio nuclear structure and nuclear scattering

- *nuclear structure* :



Source: rarfaxp.riken.go.jp/ gibelin/Nuchart/

- *nuclear scattering* : ... processes relevant for stellar astrophysics
  - ▷ scattering of alpha particles : $^4\text{He}+^4\text{He}\rightarrow^4\text{He}+^4\text{He}$
  - ▷ triple-alpha reaction : $^4\text{He} + {}^4\text{He} + {}^4\text{He} \rightarrow {}^{12}\text{C} + \gamma$
  - ▷ alpha capture on carbon : $^4\text{He} + {}^{12}\text{C} \rightarrow {}^{16}\text{O} + \gamma$

⋮

Progress in *ab initio* nuclear structure and nuclear scattering

Unexpectedly large charge radii of neutron-rich calcium isotopes.
Garcia Ruiz *et al.*, Nature Phys. 12, 594 (2016).

Structure of ^{78}Ni from first principles computations.
Hagen, Jansen, & Papenbrock, PRL 117, 172501 (2016).

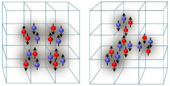
A nucleus-dependent valence-space approach to nuclear structure.
Stroberg *et al.*, PRL 118, 032502 (2017).

Ab initio many-body calculations of the ^{3}H(d, n)^{4}He and ^{3}He(d, p)^{4}He fusion.
Navratil & Quaglioni, PRL 108, 042503 (2012).

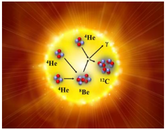
Elastic proton scattering of medium mass nuclei from coupled-cluster theory.
Hagen & Michel PRC 86, 021602 (2012).

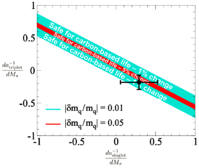
Coupling the Lorentz Integral Transform (LIT) and the Coupled Cluster (CC) Methods.
Orlandini, G. *et al.* , Few Body Syst. 55, 907-911 (2014).

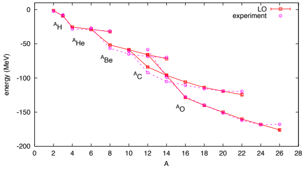
Nuclear LEFT: *ab initio* nuclear structure and scattering theory

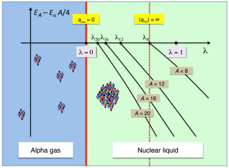


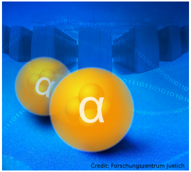
- Lattice EFT calculations for $A = 3, 4, 6, 12$ nuclei, PRL 104 (2010) 142501
- *Ab initio* calculation of the Hoyle state, PRL 106 (2011) 192501
- Structure and rotations of the Hoyle state, PRL 109 (2012) 252501
- Viability of Carbon-Based Life as a Function of the Light Quark Mass, PRL 110 (2013) 112502
- *Ab initio* calculation of the Spectrum and Structure of ^{16}O, PRL 112 (2014) 102501
- *Ab initio* alpha-alpha scattering, *Nature* 528, 111-114 (2015).
- Nuclear Binding Near a Quantum Phase Transition, PRL 117, 132501 (2016).
- *Ab initio* calculations of the isotopic dependence of nuclear clustering. arXiv:1702.05177.





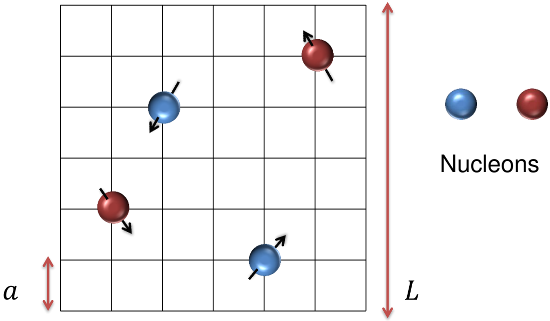






Lattice effective field theory

Lattice effective field theory is a powerful numerical method formulated in the framework of chiral effective field theory.



Chiral effective field theory for nucleons

Chiral effective field theory organizes the nuclear interactions as an expansion in powers of momenta and other low energy scales such as the pion mass (Q/Λ_χ) .

NN effective potential order by order...

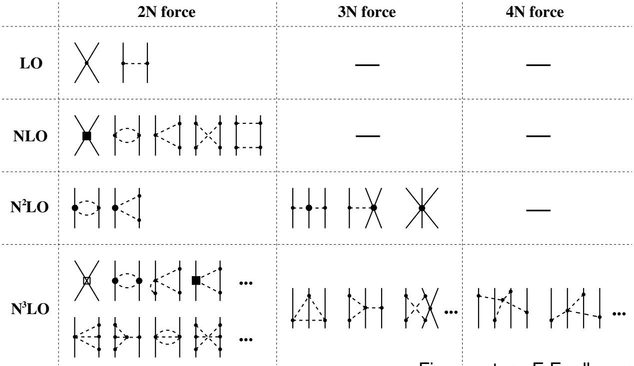


Fig. courtesy E.Epelbaum

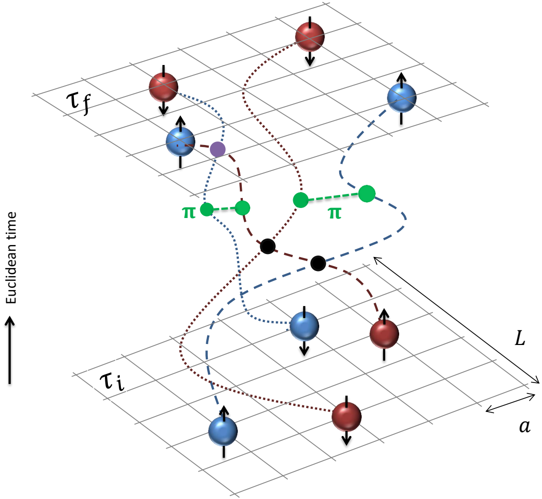
Ordonez et al. ’94; Friar & Coon ’94; Kaiser et al. ’97; Epelbaum et al. ’98,’03,’05,’15; Kaiser ’99-’01; Higa et al. ’03; ...

Lattice EFT: Euclidean time projection

$$e^{-H\tau}$$

$$\tau = L_t a_t$$

- evolve nucleons forward in Euclidean time
- allow them to interact



Lattice Monte Carlo calculations

Transfer matrix operator formalism $M =: \exp(-H\,a_t):$

Microscopic Hamiltonian $H = H_{\text{free}} + V$

$$Z^{(L_t)} = \text{Tr}(M^{L_t}) = \int Dc\,Dc^*\,\exp[-S(c,c^*)]$$

Creutz, Found. Phys. 30 (2000) 487.

The exact equivalence of several different lattice formulations.

Lee, PRC 78:024001, (2008); Prog.Part.Nucl.Phys., 63:117-154 (2009)

$$e^{-E_0\,a_t} = \lim_{L_t\to\infty} Z^{(L_t+1)}/Z^{(L_t)}$$

Lattice Monte Carlo calculations

Nuclear forces posses approximate SU(4) symmetry. $H_{\text{SU}(4)}$ acts as an approximate and inexpensive low energy filter at few first/last time steps. Significant suppression of sign oscillations. Chen, Lee, Schäfer, PRL 93 (2004) 242302

$$|\psi_I(\tau')\rangle = \exp\left[-H_{\text{SU}(4)}\,\tau'\right]|\psi_I\rangle \qquad \tau' = L_t'\,a_t$$

For time steps in midsection, the full H_{LO} Hamiltonian is used.

$$|\psi_I(\tau)\rangle = \exp\left[-H_{\text{LO}}\,\tau\right]|\psi_I(\tau')\rangle \qquad \tau = L_t\,a_t$$

$$Z_{\text{LO}}^{(L_t)} = \langle\psi_I(\tau/2)|\psi_I(\tau/2)\rangle \qquad Z_{\langle\mathcal{O}\rangle,\text{LO}}^{(L_t+1)} = \langle\psi_I(\tau/2)|\mathcal{O}|\psi_I(\tau/2)\rangle$$

These amplitudes are computed with the Hybrid Monte Carlo methods.

Phys. Lett. B195, 216-222 (1987), Phys. Rev. D35, 2531-2542 (1987).

Lattice Monte Carlo calculations

Higher order calculations (perturbative)

ho $=$ NLO, NNLO, $\cdots$

$$: \exp\left[-H_{\text{ho}}\, a_t\right] : \qquad\qquad : \exp\left[-H_{\text{ho}}\, a_t\right] :$$

$$\downarrow \qquad\qquad \downarrow$$

$$Z_{\text{ho}}^{(L_t)} = \langle \psi_I(\tau/2) | \psi_I(\tau/2) \rangle \qquad Z_{\langle \mathcal{O} \rangle,\text{ho}}^{(L_t+1)} = \langle \psi_I(\tau/2) | \mathcal{O} | \psi_I(\tau/2) \rangle$$

The observable $\mathcal{O}$ at (NLO, NNLO, $\cdots$)

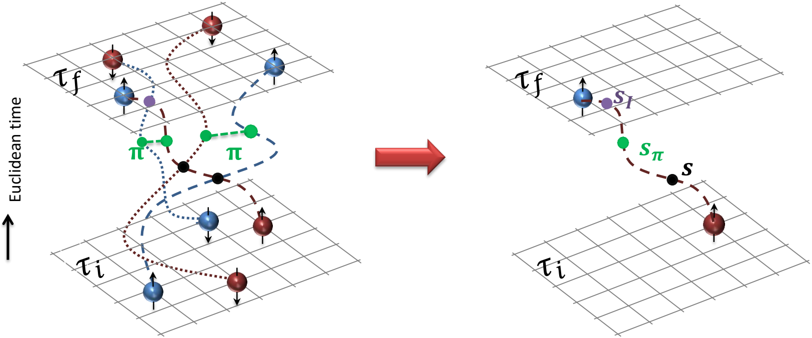
$$\langle \mathcal{O} \rangle_{0,\text{ho}} = \lim_{L_t \to \infty} \frac{Z_{\langle \mathcal{O} \rangle,\text{ho}}^{(L_t+1)}}{Z_{\text{ho}}^{(L_t)}}$$

Auxiliary field Monte Carlo

Use a Gaussian integral identity

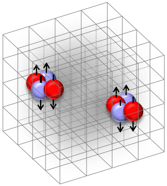
$$\exp\left[-\frac{C}{2}\left(N^{\dagger}N\right)^{2}\right] = \sqrt{\frac{1}{2\pi}}\int ds\, \exp\left[-\frac{s^{2}}{2} + \sqrt{C}\, s\left(N^{\dagger}N\right)\right]$$

s is an auxiliary field coupled to particle density. Each nucleon evolves as if a single particle in a fluctuating background of pion fields and auxiliary fields.

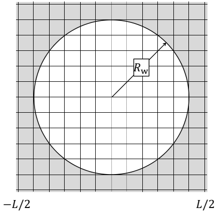


Two-cluster scattering: Adiabatic projection method

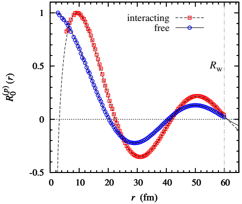
Split the problem into two parts



The first part
use Euclidean time projection to construct an *ab initio* low-energy cluster Hamiltonian, called the adiabatic Hamiltonian.



The second part
compute the two-cluster scattering phase shifts or reaction amplitudes using the adiabatic Hamiltonian.



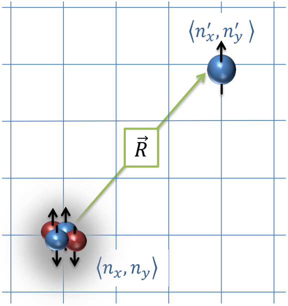
Rupak, Lee., PRL 111 (2013) 032502.
Pine, Lee, Rupak, EPJA 49 (2013) 151.
SE, Lee, PRC 90, 064001 (2014).
Rokash, Pine, SE, Lee, Epelbaum, Krebs, PRC 92,054612 (2015)
SE, Lee, Meißner, Rupak, EPJA 52: 174 (2016)

Two-cluster scattering: Adiabatic projection method

The method constructs a low energy effective theory for the clusters.

Use initial states parameterized by the relative spatial separation between clusters, and project them in Euclidean time.

$$|\vec{R}\rangle = \sum_{\vec{r}} |\vec{r} + \vec{R}\rangle_1 \otimes |\vec{r}\rangle_2$$



$$|\vec{R}\rangle_\tau = e^{-H\tau} |\vec{R}\rangle$$ dressed cluster state

The adiabatic projection in Euclidean time gives a systematically improvable description of the low-lying scattering cluster states.
In the limit of large Euclidean projection time the description becomes exact.

Two-cluster scattering: Adiabatic projection method

$$|\vec{R}\rangle_\tau = e^{-H\tau}\,|\vec{R}\rangle$$ dressed cluster state

Hamiltonian matrix

$$[H_\tau]_{\vec{R},\vec{R}'} = {}_\tau\langle\vec{R}|H|\vec{R}'\rangle_\tau$$

Norm matrix

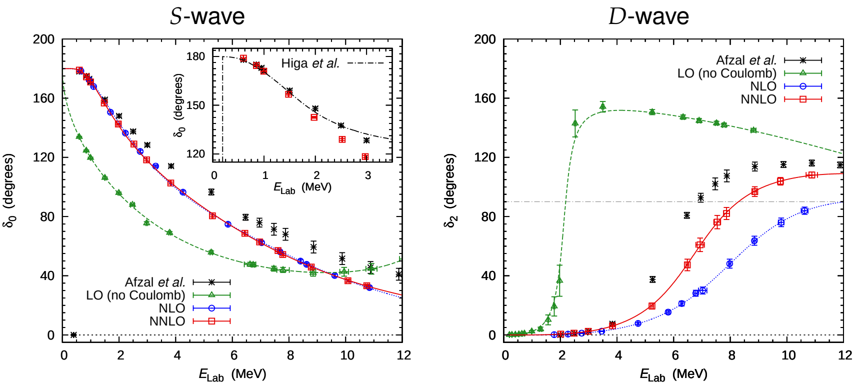
$$[N_\tau]_{\vec{R},\vec{R}'} = {}_\tau\langle\vec{R}|\vec{R}'\rangle_\tau$$

$$[H^a_\tau]_{\vec{R},\vec{R}'} = \sum_{\vec{R}'',\vec{R}'''}\left[N_\tau^{-1/2}\right]_{\vec{R}\vec{R}''}[H_\tau]_{\vec{R}''\vec{R}'''}\left[N_\tau^{-1/2}\right]_{\vec{R}'''\vec{R}'}$$

The structure of the adiabatic Hamiltonian, $[H^a_\tau]_{\vec{R},\vec{R}'}$, is similar to the Hamiltonian matrix used in recent calculations of ab initio NCSM/RGM for nuclear scattering and reactions.

Navratil, Quaglioni, PRC 83, 044609 (2011).
Navratil, Roth, Quaglioni, PLB 704, 379 (2011).
Navratil, Quaglioni, PRL 108, 042503 (2012).

Alpha-alpha scattering



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

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

SE, Lee, Rupak, Epelbaum, Krebs, Lähde, Luu, Meißner, *Nature* 528, 111-114 (2015)

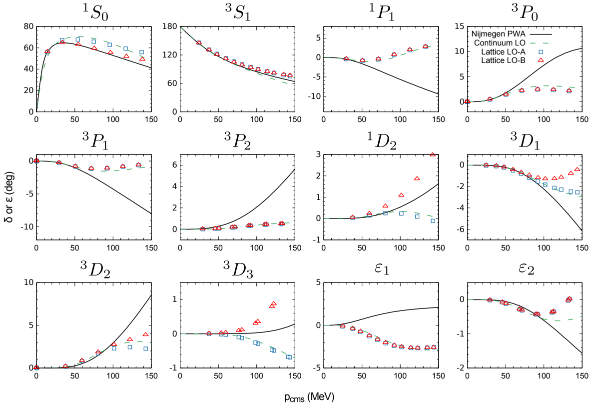
Degree of locality of nuclear forces

Interaction A

- Nonlocal short-range interactions $V(r,r')$
  - One-pion exchange interaction
    - (+ Coulomb interaction)

Interaction B

- Local short-range interactions $V(r,r') = U(r)\delta(r-r')$
  - Nonlocal short-range interactions $V(r,r')$
    - One-pion exchange interaction
      - (+ Coulomb interaction)



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Interaction B

- Local short-range interactions $V(r, r') = U(r)\delta(r - r')$
  - Nonlocal short-range interactions $V(r, r')$
    - One-pion exchange interaction
      - (+ Coulomb interaction)

Nucleus	A (LO)	B (LO)	A (LO + Coulomb)	B (LO + Coulomb)	Experiment
^{3}H	-7.82(5)	-7.78(12)	-7.82(5)	-7.78(12)	-8.482
^{3}He	-7.82(5)	-7.78(12)	-7.08(5)	-7.09(12)	-7.718
^{4}He	-29.36(4)	-29.19(6)	-28.62(4)	-28.45(6)	-28.296

SE, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, Lee, Rupak, PRL 117, 132501 (2016)

Introducing the nonlocal short-range interactions reduce the Monte Carlo sign oscillation significantly (the original motivation for studying the different interactions).

Degree of locality of nuclear forces

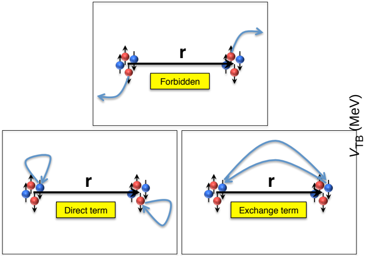
Interaction A

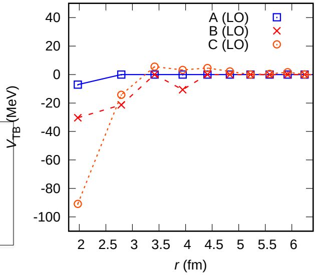
- Nonlocal short-range interactions $V(r, r')$
- One-pion exchange interaction
- (+ Coulomb interaction)

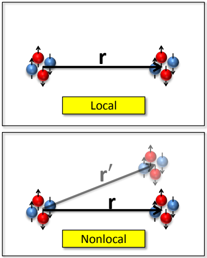
Interaction B

- Local short-range interactions $V(r, r') = U(r)\delta(r - r')$
- Nonlocal short-range interactions $V(r, r')$
- One-pion exchange interaction
- (+ Coulomb interaction)

Tight-binding approximation

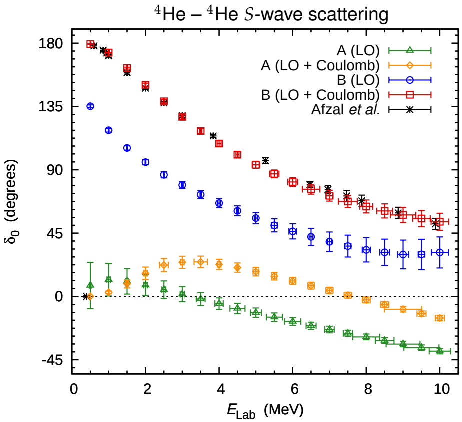






The alpha-alpha interaction is sensitive to the degree of locality of the interaction.

Degree of locality of nuclear forces



Nucleus	A (LO)	B (LO)	A (LO + Coulomb)	**B (LO + Coulomb)**	Experiment
^{8}Be	-58.61(14)	-59.73(6)	-56.51(14)	**-57.29(7)**	-56.591
^{12}C	-88.2(3)	-95.0(5)	-84.0(3)	**-89.9(5)**	-92.162
^{16}O	-117.5(6)	-135.4(7)	-110.5(6)	**-126.0(7)**	-127.619
^{20}Ne	-148(1)	-178(1)	-137(1)	**-164(1)**	-160.645

SE, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, Lee, Rupak, PRL 117, 132501 (2016)

Nuclear binding near a quantum phase transition

Nucleus	**A (LO)**	B (LO)	A (LO + Coulomb)	B (LO + Coulomb)	Experiment
^{4}He	**-29.36(4)**	-29.19(6)	-28.62(4)	-28.45(6)	-28.296
^{8}Be	**-58.61(14)**	-59.73(6)	-56.51(14)	-57.29(7)	-56.591
^{12}C	**-88.2(3)**	-95.0(5)	-84.0(3)	-89.9(5)	-92.162
^{16}O	**-117.5(6)**	-135.4(7)	-110.5(6)	-126.0(7)	-127.619
^{20}Ne	**-148(1)**	-178(1)	-137(1)	-164(1)	-160.645

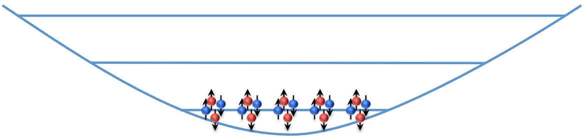
$$\frac{E_{^8\mathrm{Be}}}{E_{^4\mathrm{He}}} = 1.997(6)$$

$$\frac{E_{^{12}\mathrm{C}}}{E_{^4\mathrm{He}}} = 3.00(1)$$

$$\frac{E_{^{16}\mathrm{O}}}{E_{^4\mathrm{He}}} = 4.00(2)$$

$$\frac{E_{^{20}\mathrm{Ne}}}{E_{^4\mathrm{He}}} = 5.03(3)$$

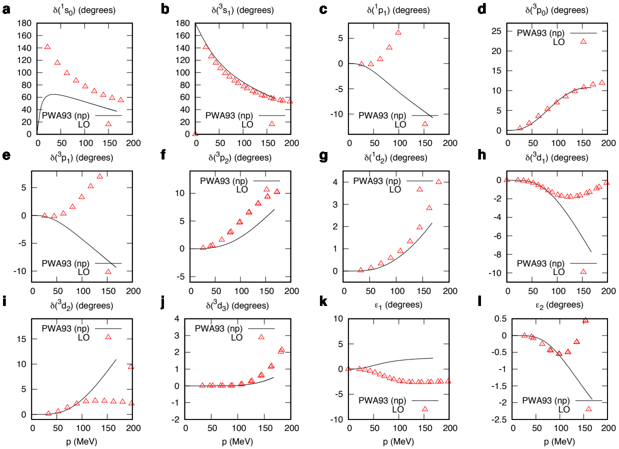
Bose condensate of alpha particles!



SE, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, Lee, Rupak, PRL 117, 132501 (2016)

New lattice action at LO

- Local interactions
- Nonlocal interactions
- OPE interaction
- (+ Coulomb interaction)



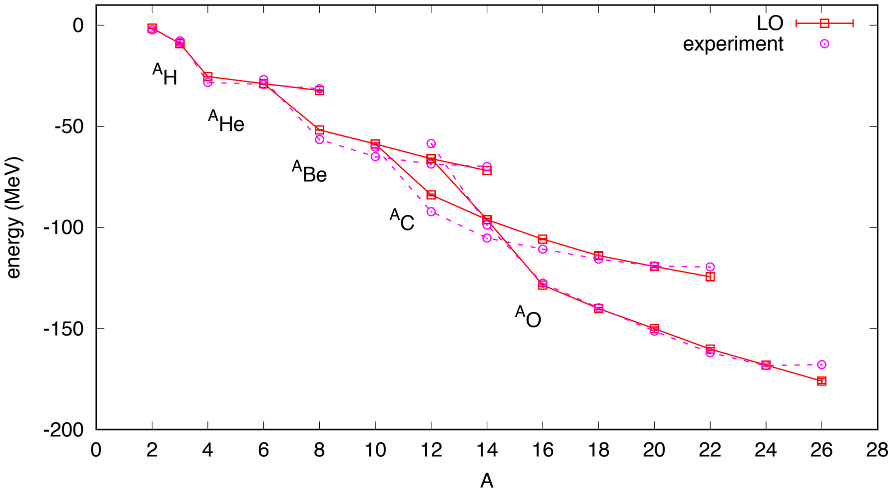
Average nucleon-nucleon S-wave scattering length

Average nucleon-nucleon S-wave effective range

Alpha-alpha S-wave scattering length

SE, Epelbaum, Krebs, Lähde, Lee, Li, Lu, Meißner, Rupak, arXiv:1702.05177

Ground state energies with the new lattice action at LO



SE, Epelbaum, Krebs, Lähde, Lee, Li, Lu, Meißner, Rupak, arXiv:1702.05177

Nuclear clusters: probing for alpha clusters

$\rho(\vec{n})$: the total nucleon density operator on the lattice site $\vec{n}$.

$\rho_4 = \sum_{\vec{n}} : \rho^4(\vec{n})/4! :$ is defined to construct a probe for alpha clusters.

Similarly ρ_3 is to construct a second probe for alpha clusters only in nuclei with even Z and even N where ^{3}H and ^{3}He clusters are not energetically favorable.

$$\rho_3 = \sum_{\vec{n}} : \rho^3(\vec{n})/3! :$$

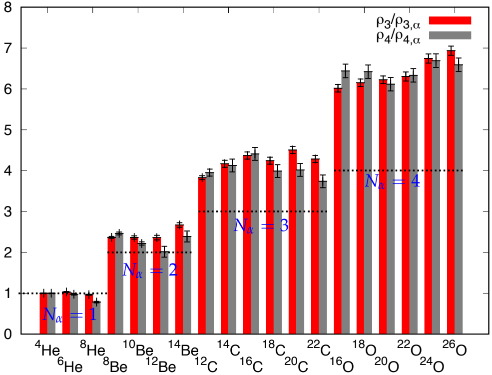
ρ_3 and ρ_4 depend on the short-distance regulator, the lattice spacing a. However the regularization-scale dependence of ρ_3 and ρ_4 does not depend on the nucleus being considered.

Therefore, by defining $\rho_{3,\alpha}$ and $\rho_{4,\alpha}$ as the corresponding values for the alpha particle, we consider the ratios $\rho_3/\rho_{3,\alpha}$ and $\rho_4/\rho_{4,\alpha}$ that are free from short-distance divergences and are model-independent quantities up to contributions from higher-dimensional operators in an operator product expansion.

Nuclear clusters: probing for alpha clusters

$\Delta_\alpha^{\rho_3}/N_\alpha$ the ρ_3-entanglement of the alpha clusters,

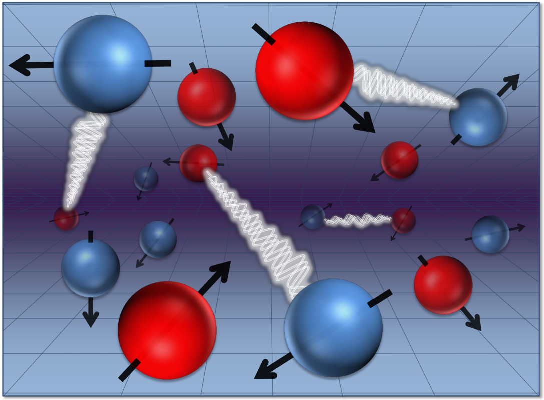
where $\Delta_\alpha^{\rho_3} = \rho_3/\rho_{3,\alpha} - N_\alpha$.



Nucleus	^{4,6,8}He	^{8,10,12,14}Be	^{12,14,16,18,20,22}C	^{16,18,20,22,24,26,28}O
$\Delta_\alpha^{\rho_3}/N_\alpha$	$0.0 - 0.03$	$0.20 - 0.35$	$0.25 - 0.50$	$0.50 - 0.75$

Nuclear clusters: probing for alpha clusters

Our results show that the transition from cluster-like states in light systems to nuclear liquid-like states in heavier systems should not be viewed as a simple suppression of multi-nucleon short-distance correlations, but rather an increasing entanglement of the nucleons involved in the multi-nucleon correlations.

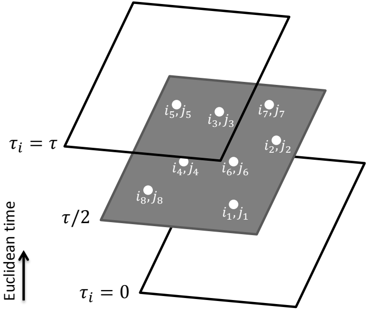


SE, Epelbaum, Krebs, Lähde, Lee, Li, Lu, Meißner, Rupak, arXiv:1702.05177

Density profiles for nuclei: pinhole algoritm

The simulations with auxiliary-field Monte Carlo methods involve quantum states that are superposition of many different center-of-mass positions. Therefore, the density distrubitions of the nucleons cannot be computed direclty.

Consider a screen placed at the middle time step having pinholes with spin and isospin labels that allow nucleons with the corresponding spin and isospin to pass.



Density profiles for nuclei: pinhole algoritm

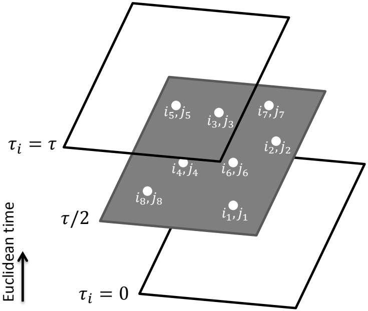
This opaque screen corresponds to the insertion of the normal-ordered A-body density operator,

$$\rho_{i_1,j_1,\ldots,i_A,j_A}(\vec{n}_1,\ldots,\vec{n}_A) =: \rho_{i_1,j_1}(\vec{n}_1)\ \ldots\ \rho_{i_A,j_A}(\vec{n}_A) :$$

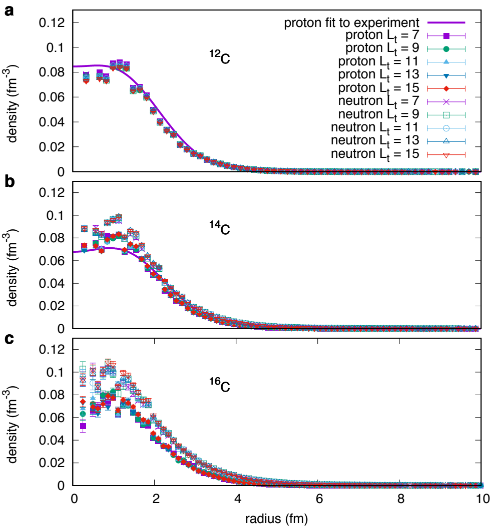
where $\rho_{i,j}(\vec{n}) = a^\dagger_{i,j}(\vec{n})a_{i,j}(\vec{n})$ is the density operator for nucleon with spin i and isospin j.

We performe Monte Carlo sampling of the amplitude,

$$A_{i_1,j_1,\ldots,i_A,j_A}(\vec{n}_1,\ldots,\vec{n}_A,L_t) = \langle\psi_I(\tau/2)|\rho_{i_1,j_1,\ldots,i_A,j_A}(\vec{n}_1,\ldots,\vec{n}_A)|\psi_I(\tau/2)\rangle$$



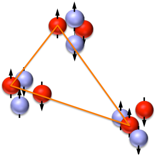
Pinhole algoritm: proton and neutron densities

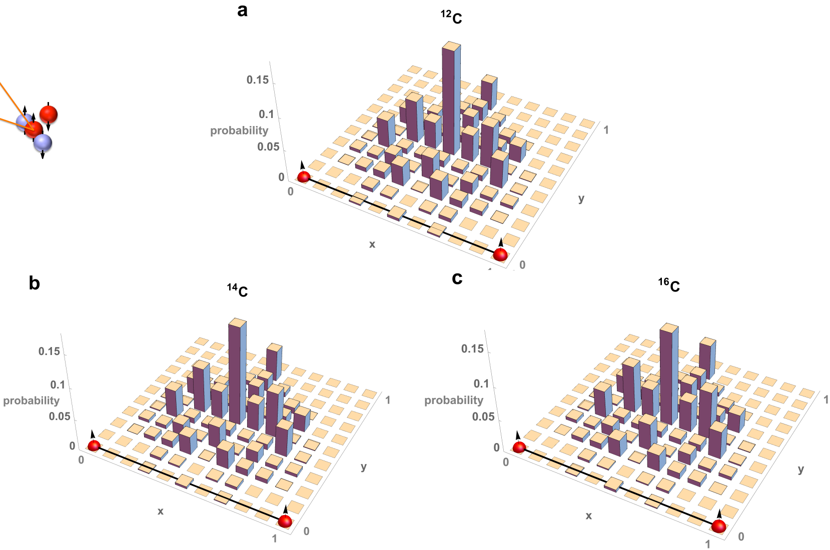


SE, Epelbaum, Krebs, Lähde, Lee, Li, Lu, Meißner, Rupak, arXiv:1702.05177

Pinhole algoritm: measure of alpha cluster geometry

Consider the triangular shape formed by the three spin-up protons.





SE, Epelbaum, Krebs, Lähde, Lee, Li, Lu, Meißner, Rupak, arXiv:1702.05177

Summary

- Scattering and reaction processes involving alpha particle are in reach of *ab initio* methods and this has opened the door towards using experimental data from collisions of heavier nuclei as input to improve *ab initio* nuclear structure theory.
- Understanding of the connection between the degree of locality of nuclear forces and nuclear structure has led to a more efficient set of lattice chiral EFT interactions (to be proven by the higher order corrections).
- The pinhole algorithm has been developed for the auxiliary-field Monte Carlo methods for the calculation of arbitrary density correlations with respect to the center of mass.

Thank you!

Extras