Lattice simulations for nuclear structure and reactions

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Nuclear Lattice EFT Collaboration

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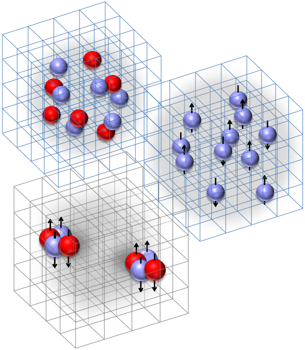

Nuclear Lattice Effective Field Theory collaboration

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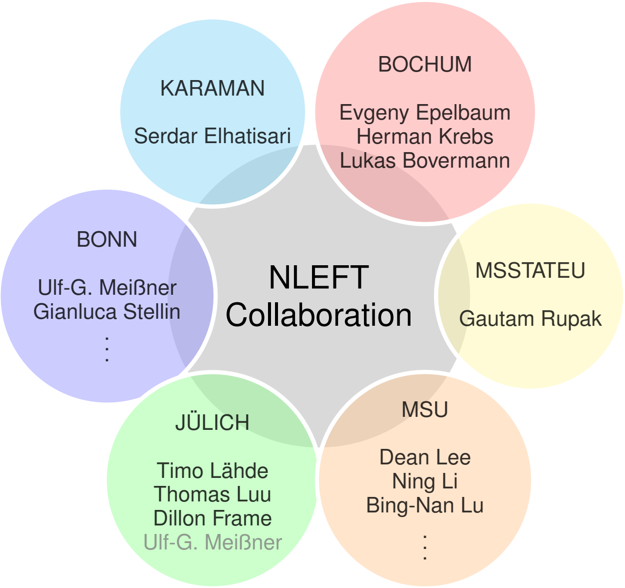
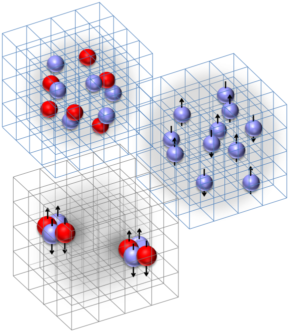


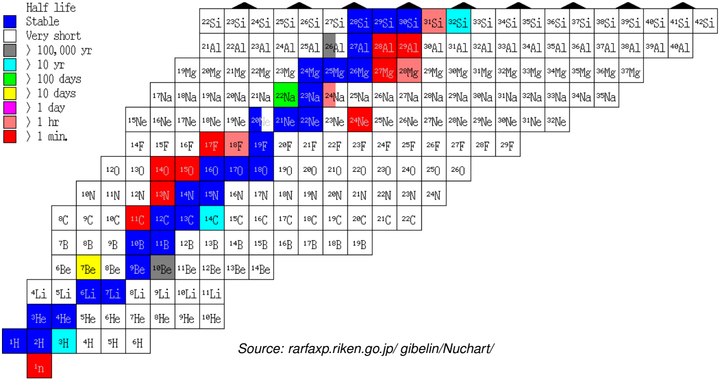
Outline

- Introduction
- Chiral effective field theory (χEFT)
- Lattice effective field theory
- Nuclear structure and reactions
- Degree of locality of nuclear forces
- Recent results
- Summary



Ab initio nuclear theory

The aim is to predict the properties of atomic nuclei from microscopic nuclear forces

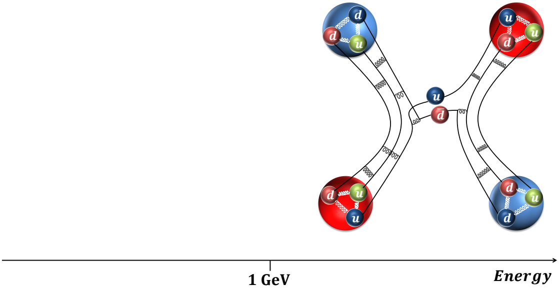


Source: rarfaxp.riken.go.jp/ gibelin/Nuchart/

- ☐ synthesis of the elements in the Universe (nucleosynthesis)
- ☐ mechanisms in stars and stellar explosions (nuclear processes)

Nuclear forces from QCD

Quantum chromodynamics (QCD) describes the strong forces by confining quarks (and gluons) into baryons and mesons.



$(\Lambda_\chi \sim$ chiral limit$)$
$m_u, m_d, m_s \to 0$

S. Weinberg, Phys. Lett. B 251 (1990) 288, Nucl. Phys. B363 (1991) 3, Phys. Lett. B 295 (1992) 114.

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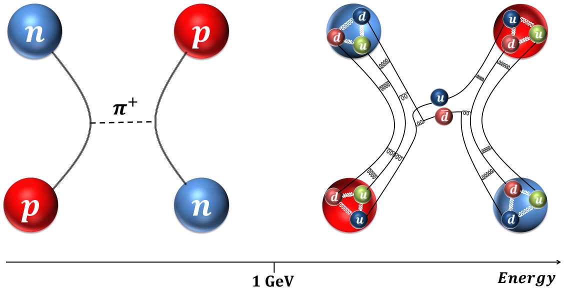


$$(\Lambda_\chi \sim \text{chiral limit})$$
$$m_u, m_d, m_s \to 0$$

"separation of scales"

S. Weinberg, Phys. Lett. B 251 (1990) 288, Nucl. Phys. B363 (1991) 3, Phys. Lett. B 295 (1992) 114.

Chiral EFT for nucleons: nuclear forces

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)

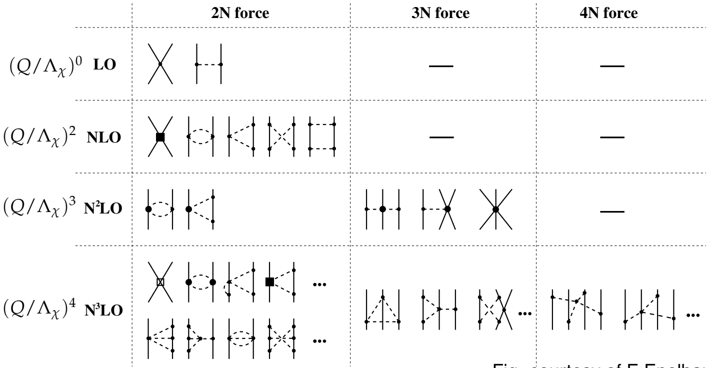
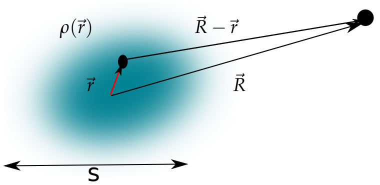


Fig. courtesy of E.Epelbaum

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; ...

A classical example: Multipole expansion

$$\Phi(r) = \frac{1}{4\pi\epsilon_0} \int_V \frac{\rho(\vec{r})dV}{|\vec{R}-\vec{r}|}$$



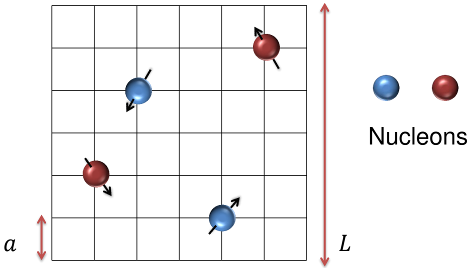
$$\frac{1}{|\vec{R}-\vec{r}|} = \frac{1}{\sqrt{R^2+r^2-2Rr\cos\theta}} = \frac{1}{R} + \frac{r}{R^2}\cos\theta + \frac{r^2}{R^3}\frac{3\cos^2\theta-1}{2} + \dots$$

$$\Phi(r) = \frac{1}{4\pi\epsilon_0}\left\{\frac{1}{R}\int_V \rho(\vec{r})dV + \frac{1}{R^2}\int_V \vec{r}\rho(\vec{r})dV + \frac{1}{R^3}\int_V (3r_ir_j - r^2\delta_{ij})\rho(\vec{r})dV\right\} + \mathcal{O}\left(\frac{1}{R^4}\right)$$

- ☐ We do not need to know the dynamics at the short distance to understand the dynamics at the long distance
- ☐ the sum converges for S $\ll R$
- ☐ long distances probes are determined by the bulk properties

Lattice effective field theory

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



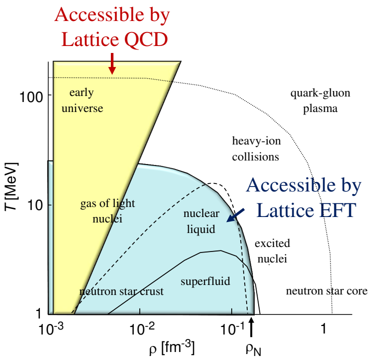


Fig. courtesy of D. Lee

Lattice formulation of χEFT

- a new lattice formulation of χEFT interactions:
  - a simpler decomposition into spin channels
  - the process of fitting to the empirical scattering phase shifts is simplified, and the resulting lattice phase shifts are more accurate.

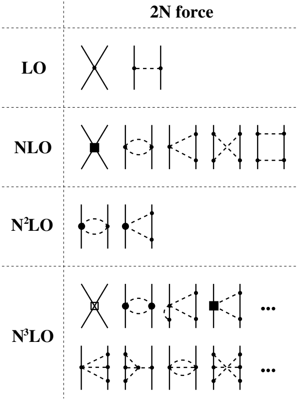
$$V^{S,I,J}_{L,L'}(\mathbf{n}) = \sum_{I_z,J_z}\sum_{S_z,L_z}\sum_{S'_z,L'_z}\left(\langle SS_z, LL_z|JJ_z\rangle \left[a(\mathbf{n})\ \nabla^{2M}\ R^*_{L,L_z}(\nabla)\ a(\mathbf{n})\right]^{s_{NL}}_{S,S_z,I,I_z}\right)^\dagger$$
$$\langle SS'_z, L'L'_z|JJ_z\rangle \left[a(\mathbf{n})\ \nabla^{2M}\ R^*_{L',L'_z}(\nabla)\ a(\mathbf{n})\right]^{s_{NL}}_{S,S'_z,I,I_z}$$

$$[a(\mathbf{n})\,a(\mathbf{n}')]^{s_{NL}}_{S,S_z,I,I_z} = \sum_{i,j,i',j'} a^{s_{NL}}_{i,j}(\mathbf{n})\, M_{ii'}(S,S_z)\, M_{jj'}(I,I_z)\, a^{s_{NL}}_{i,j}(\mathbf{n}')$$

Li, SE, Epelbaum, Lee, Lu, Meißner Phys. Rev. C 98, 044002 (2018)

χEFT for nucleons: *NN* scattering phase shifts

- formulate the lattice action in the framework of chiral effective field theory
- fit the unknown coefficients of the short-range lattice interactions to empirical phase shifts

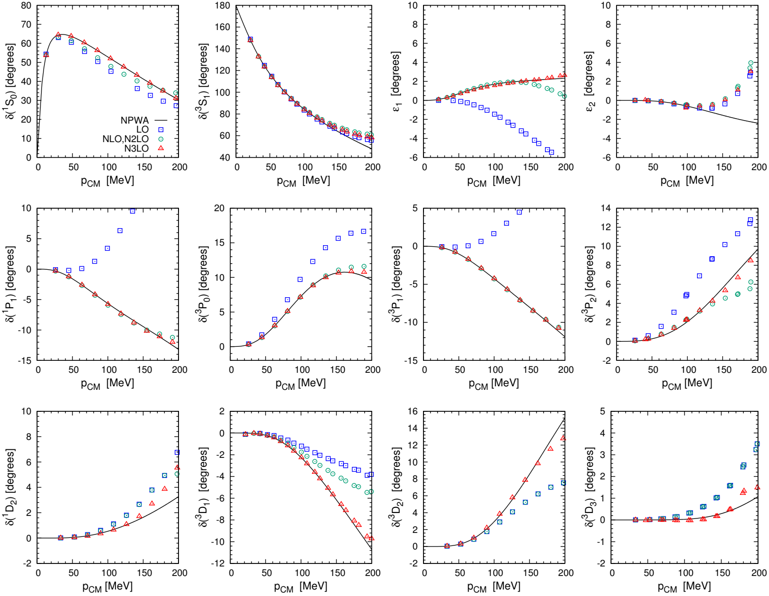


LO $\Longleftrightarrow$ $V_{0,{}^1S_0}$ $V_{0,{}^3S_1}$

NLO $\Longleftrightarrow$ $V_{2,{}^1S_0}$ $V_{2,{}^3S_1}$ $V_{2,{}^3SD}$ $V_{2,{}^1P_1}$ $V_{2,{}^3P_0}$ $V_{2,{}^3P_1}$ $V_{2,{}^3P_2}$

N³LO $\Longleftrightarrow$ $V^{(1)}_{4,{}^1S_0}$ $V^{(2)}_{4,{}^1S_0}$ $V^{(1)}_{4,{}^3S_1}$ $V^{(2)}_{4,{}^3S_1}$ $V^{(1)}_{4,{}^3SD}$ $V^{(2)}_{4,{}^3SD}$ $V_{4,{}^1P_1}$ $V_{4,{}^3P_0}$ $V_{4,{}^3P_1}$ $V_{4,{}^3P_2}$ $V_{4,{}^3PF}$ $V_{4,{}^1D_2}$ $V_{4,{}^3D_1}$ $V_{4,{}^3D_2}$ $V_{4,{}^3D_3}$

χEFT for nucleons: *NN* scattering phase shifts

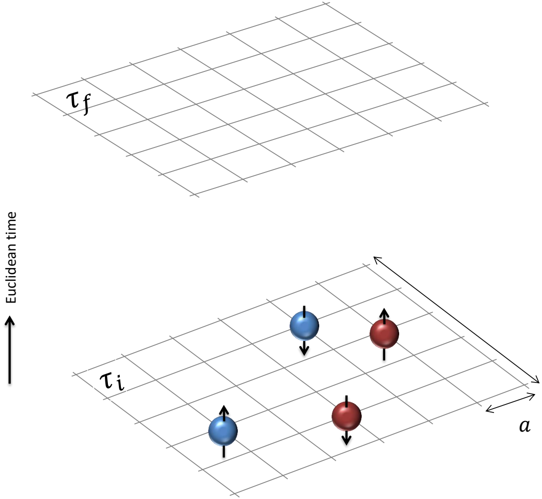


Li, SE, Epelbaum, Lee, Lu, Meißner Phys. Rev. C 98, 044002 (2018)

Many body quantum systems - *ab initio* nuclear theory

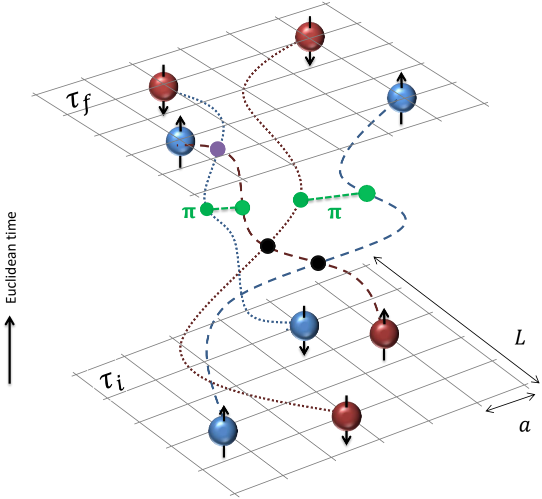
Lattice Monte Carlo calculations: Euclidean time projection

- ☐ construct a trial state of nucleons, $|\psi_I\rangle$, as a Slater determinant of free-particle standing waves on the lattice.



Lattice Monte Carlo calculations: Euclidean time projection

- ☐ construct a trial state of nucleons, $|\psi_I\rangle$, as a Slater determinant of free-particle standing waves on the lattice.
- ☐ evolve nucleons forward in Euclidean time, $e^{-H_{\rm LO}\,\tau}\,|\psi_I\rangle$, where $\tau = L_t a_t$.
- ☐ The evolution in Euclidean time automatically incorporates the induced deformation, polarization and clustering.



Lattice EFT: (Euclidean time) projection Monte Carlo

Transfer matrix operator formalism $\mathbf{M} =: \exp(-H_{\mathrm{LO}}\, a_t) :$

Microscopic Hamiltonian $H_{\mathrm{LO}} = H_{\mathrm{free}} + V_{\mathrm{LO}}$

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

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)

Lattice Monte Carlo calculations

Projection Monte Carlo uses a given initial state, $|\psi_I\rangle$, to evaluate a product of a string of transfer matrices $\mathbf{M}$.

$$Z(L_t) = \langle \psi_I \,|\mathbf{M}(L_t-1)\,\mathbf{M}(L_t-2)\,\ldots\mathbf{M}(1)\,\mathbf{M}(0)\,|\,\psi_I\rangle$$

In the limit of large Euclidean time the evolution operator $e^{-H_{\rm LO}\,\tau}$ suppress the signal beyond the low-lying states, and the ground state energy of our quantum system can be extracted by

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

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

perturbative higher order calculations

ho = NLO, NNLO, $\cdots$

$$\mathbf{M}_{\text{ho}} = : e^{-a_t(H_{\text{LO}}+V_{\text{ho}})} :$$

where the potential V_{ho} is treated perturbatively. Therefore, the higher order corrections to the ground state energy can be computed as,

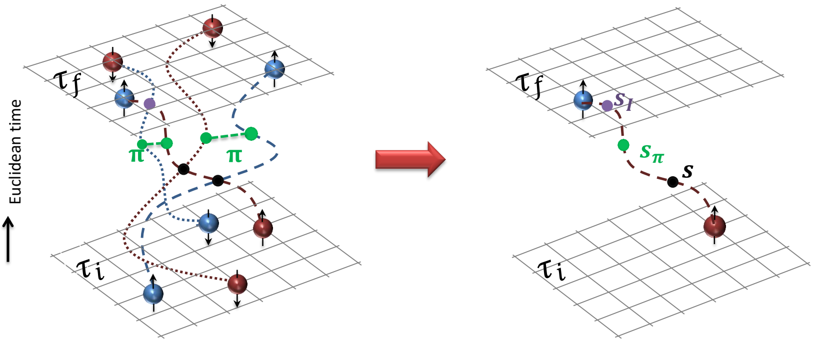
$$e^{-\Delta E_{\text{ho}}\, a_t} = \lim_{L_t\to\infty} \frac{\langle\psi_I|\, \mathbf{M}^{L_t/2}\, \mathbf{M}_{\text{ho}}\, \mathbf{M}^{L_t/2}\, |\psi_I\rangle}{\langle\psi_I|\, \mathbf{M}^{L_t}\, |\psi_I\rangle}$$

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.

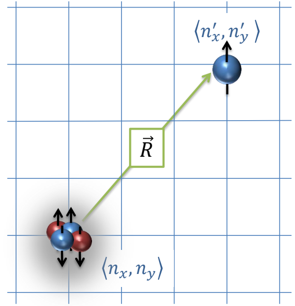


Scattering and reactions: Adiabatic projection method

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.

PRL 111 (2013) 032502; EPJA 49 (2013) 151; PRC 90, 064001 (2014); PRC 92,054612 (2015); EPJA 52: 174 (2016)

Scattering and reactions: Adiabatic projection method

$$|\vec{R}\rangle_\tau = e^{-H\tau}\,|\vec{R}\rangle$$ dressed cluster state (not orthogonal)

Hamiltonian matrix

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

Norm matrix

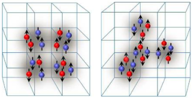
$$[N_\tau]_{\vec{R},\vec{R}'} = {}_\tau\langle\vec{R}|\vec{R}'\rangle_\tau$$

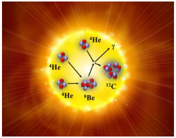
$$[H^a_\tau]_{\vec{R},\vec{R}'} = \sum_{\vec{R}'',\vec{R}'''}\left[N_\tau^{-1/2}\right]_{\vec{R}\vec{R}''}[H_\tau]_{\vec{R}''\vec{R}'''}\left[N_\tau^{-1/2}\right]_{\vec{R}'''\vec{R}'}$$

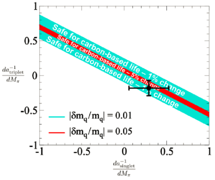
The structure of the adiabatic Hamiltonian, $[H^a_\tau]_{\vec{R},\vec{R}'}$, is similar to the Hamiltonian matrix used in calculations of ab initio no-core shell model/resonating group method (NCSM/RGM) for nuclear scattering and reactions.

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

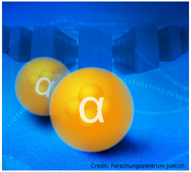
Nuclear LEFT: *ab initio* nuclear structure and scattering theory

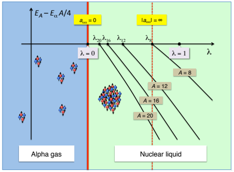


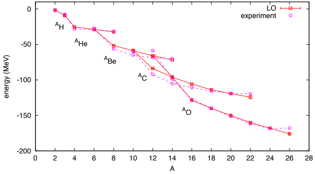




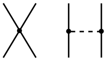
- Lattice EFT calculations for $A = 3, 4, 6, 12$ nuclei, PRL 104 (2010) 142501
- *Ab initio* calculation of the Hoyle state, PRL 106 (2011) 192501
- Structure and rotations of the Hoyle state, PRL 109 (2012) 252501
- Viability of Carbon-Based Life as a Function of the Light Quark Mass, PRL 110 (2013) 112502
- Radiative capture reactions in lattice effective field theory, PRL 111 (2013) 032502
- *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, PRL 119, 222505 (2017).
- Essential elements for nuclear binding, PLB 797 (2019) 134863.





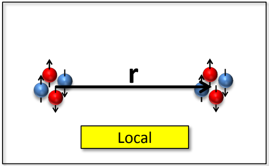


Degree of locality of nuclear forces

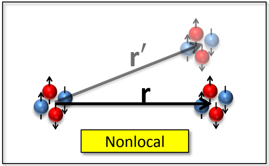
	2N force
LO	

$$V_{\rm LO} = V^{s_{NL},s_L}_{^1S_0,Q^0} + V^{s_{NL},s_L}_{^3S_1,Q^0} + V_{\rm OPE}$$

$$U(r) = V(r,r')\,\delta(r-r')$$



$$U(r,r') = V(r,r')$$

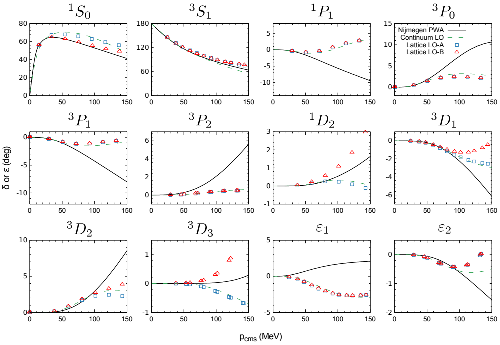


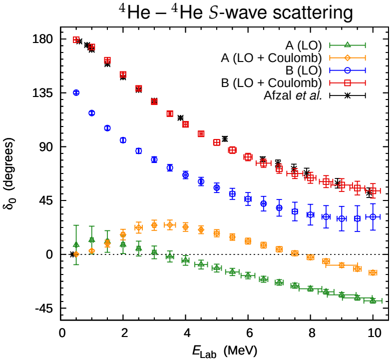
- ☐ Does every χEFT interaction give well controlled and reliable results for heavier systems?
- ☐ Is the convergence of higher-order terms under control?

Degree of locality of nuclear forces – I

$$V_{\rm LO}^{\rm A} = V^{s_{NL}}_{^1S_0,Q^0} + V^{s_{NL}}_{^3S_1,Q^0} + V_{\rm OPE}$$

$$V_{\rm LO}^{\rm B} = V^{s_{NL},s_L}_{^1S_0,Q^0} + V^{s_{NL},s_L}_{^3S_1,Q^0} + V_{\rm OPE}$$



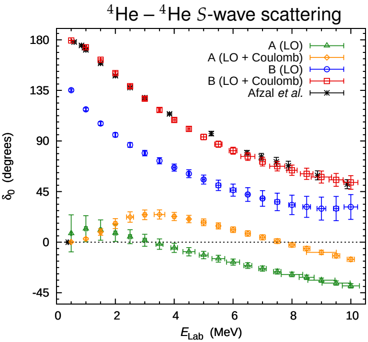


Nucleus	A (LO)	B (LO)	A (LO + Coulomb)	B (LO + Coulomb)	Experiment
^{3}H	-7.82(5)	-7.78(12)	-7.82(5)	-7.78(12)	-8.482
^{3}He	-7.82(5)	-7.78(12)	-7.08(5)	-7.09(12)	-7.718
^{4}He	-29.36(4)	-29.19(6)	-28.62(4)	-28.45(6)	-28.296

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

Degree of locality of nuclear forces – I

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



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

Degree of locality of nuclear forces – I

Nucleus	**A (LO)**	B (LO)	A (LO + Coulomb)	B (LO + Coulomb)	Experiment
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^{20}Ne	**-148(1)**	-178(1)	-137(1)	**-164(1)**	-160.645

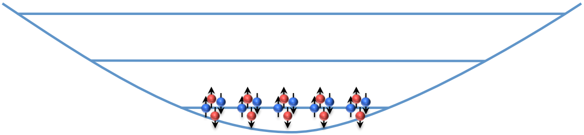
$$\frac{E_{^8\mathrm{Be}}}{E_{^4\mathrm{He}}} = 1.997(6)$$

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

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

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

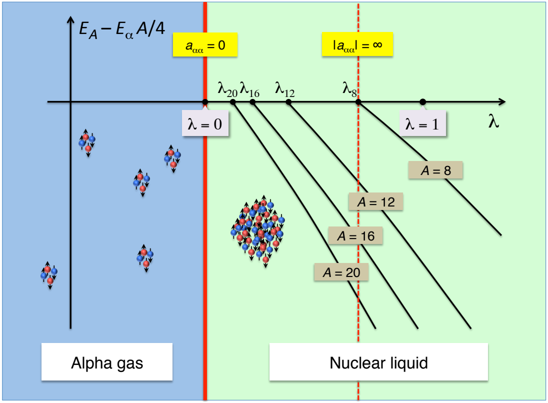
Bose condensate of alpha particles!



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

Nuclear binding near a quantum phase transition

Consider a one-parameter family of interactions: $V = (1-\lambda)\, V^A_{\text{LO}} + \lambda\, V^B_{\text{LO}}$



There is a quantum phase transition at the point where the α-α scattering length $a_{\alpha\alpha}$ vanishes, and it is a first-order transition from a Bose-condensed α-particle gas to a nuclear liquid.

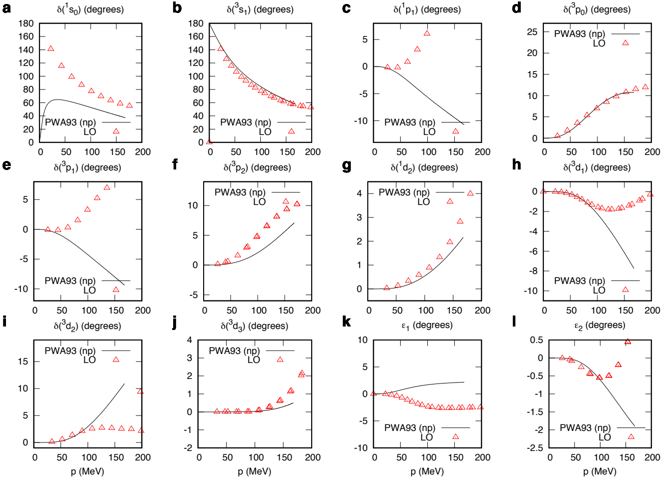
SE, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, Lee, Rupak, PRL 117, 132501 (2016)

Stoff, Phys. Rev. A 49 (1994) 3824

Degree of locality of nuclear forces – II

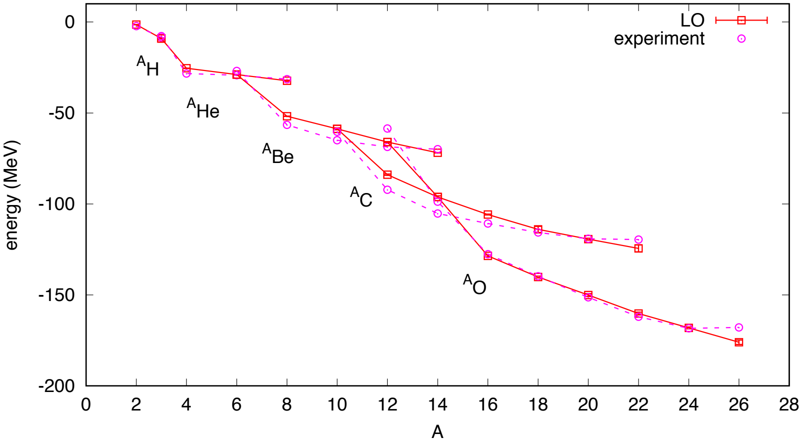
We can probe the degree of locality only by many-body calculations, and we consider an SU4-symmetric potential,

$$V_{\rm LO} = V_{\rm SU4}^{s_{NL}, s_L} + V_{\rm OPE}$$



Ground state energies at LO

$$V_{\mathrm{LO}} = V_{\mathrm{SU4}}^{s_{NL},s_L} + V_{\mathrm{OPE}} + V_{\mathrm{Coulomb}}$$



SE, Epelbaum, Krebs, Lähde, Lee, Li, Lu, Meißner, Rupak, PRL 119, 222505 (2017)

Degree of locality of nuclear forces – III

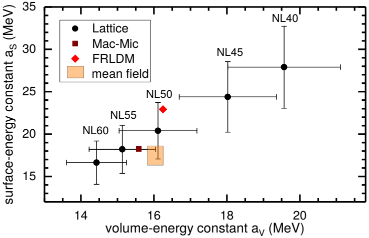
Consider the following potential in the framework of pionless effective field theory to probe the degree of locality from many-body calculations,

$$V_{\not\pi}^{\text{start}} = V_{\text{SU4}}^{C_2,s_{NL},s_L} + V_{\text{SU4}}^{C_3} + V_{\text{Coulomb}}$$

- ☐ C_2, s_L, and C_3 are tuned to get the few-body physics correct
- ☐ For $A \geq 16$, the binding energies are well-parameterized with the Bethe-Weizsäcker mass formula;

$$B(A) = a_V\, A - a_S\, A^{2/3} + E_{\text{Coulomb}} + (\text{symmetry} + \text{pairing} + \text{shellcorrection} + \ldots)$$

- ☐ Consider only $N = Z$ even-even nuclei, and obtain C_2, s_L, C_3 for various values of s_{NL}

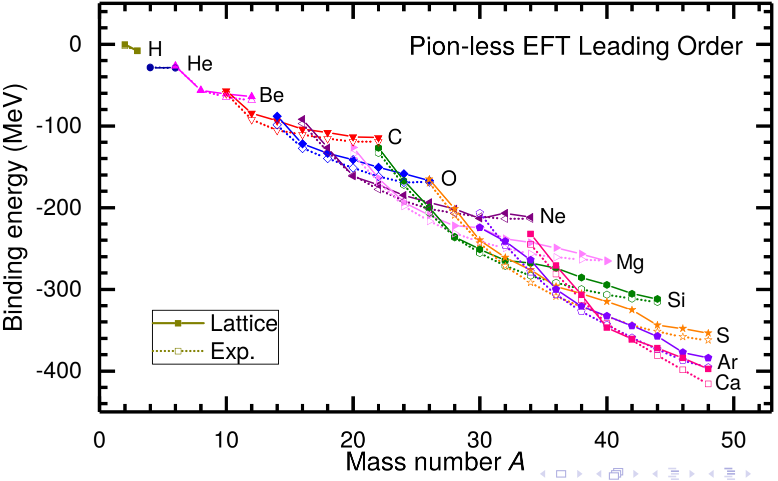


Lu, Li, SE, Lee, Epelbaum, Meißner, Phys. Lett. B, 797, 134863 (2019)

Essential elements for nuclear binding

- a lattice action with minimum number of parameters (four) which describes neutron matter up to saturation density and the ground state properties of nuclei up to calcium. $a = 1.32$ fm, $s_L = 0.0609$ (l.u.), and $s_{NL} = 0.5$ (l.u.)

Lu, Li, SE, Lee, Epelbaum, Meißner, Phys. Lett. B, 797, 134863 (2019)



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Lu, Li, SE, Lee, Epelbaum, Meißner, Phys. Lett. B, 797, 134863 (2019)

	B	Experiment	R_{ch}	Experiment
^{3}H	8.48(2)	8.48	1.90(1)	1.76
^{3}He	7.75(2)	7.72	1.99(1)	1.97
^{4}He	28.89(1)	28.3	1.72(1)	1.68
^{16}O	121.9(1)	127.6	2.74(1)	2.70
^{20}Ne	161.6(1)	160.6	2.95(1)	3.01
^{24}Mg	193.5(2)	198.3	3.13(1)	3.06
^{28}Si	235.8(4)	236.5	3.26(1)	3.12
^{40}Ca	346.8(6)	342.1	3.42(1)	3.48

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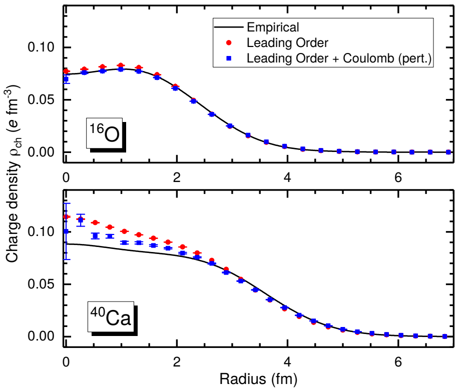
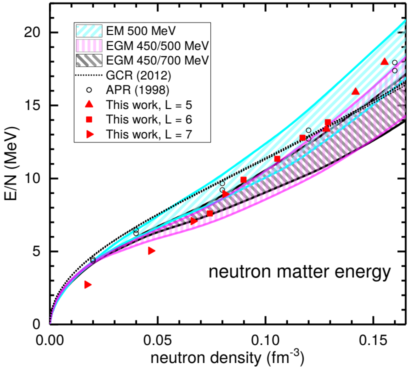
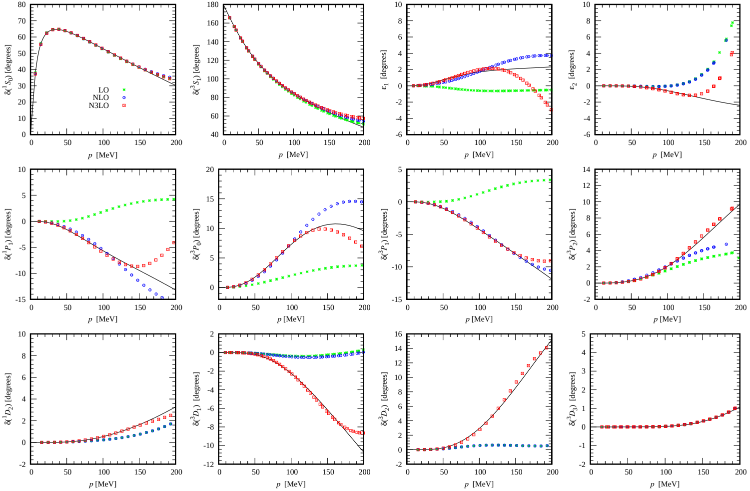




Ab initio nuclear structure: recent progress

We have constructed a new lattice formulation of chiral effective field theory interactions with a simpler decomposition into spin channels. Li, SE, Epelbaum, Lee, Lu, Meißner, Phys. Rev. C 98, 044002 (2018)

$a = 1.97$ fm, $s_L = 0.0336$ (l.u.), and $s_{NL} = 0.0839$ (l.u.) and $p_{\max} = \pi/a = 314$ MeV



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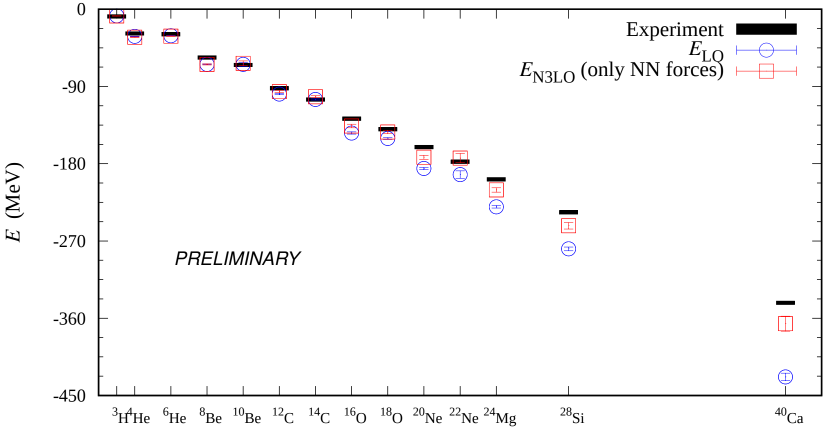
Preliminary results for the ground state energies of light and medium-mass nuclei:



- ☐ To determine the 3N forces, we consider several nuclear processes, such as triton beta-decay, neutron-alpha and alpha-alpha scattering, properties of ^{3}He and ^{4}He etc.

Triton beta-decay

$a = 1.97$ fm

Preliminary results for the 3-nucleon systems:

Bovermann, SE, Epelbaum, Krebs, Lee, Meißner [*work in progress*]

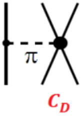
L (fm)	E_{LO} (MeV)	E_{NLO} (MeV)	E_{N3LO} (MeV)
11.84	-10.03	-9.07	-9.10
15.78	-9.55	-8.43	-8.47
19.73	-9.51	-8.36	-8.39

L (fm)	$\langle \mathbf{F} \rangle_{\mathrm{LO}}$	$\langle \mathbf{F} \rangle_{\mathrm{NLO}}$	$\langle \mathbf{F} \rangle_{\mathrm{N3LO}}$	$\langle \mathbf{GT} \rangle_{\mathrm{LO}}$	$\langle \mathbf{GT} \rangle_{\mathrm{NLO}}$	$\langle \mathbf{GT} \rangle_{\mathrm{N3LO}}$
11.84	1.0000	0.9995	0.9995	1.7045	1.6714	1.6725
15.78	1.0000	0.9996	0.9996	1.7111	1.6789	1.6796
19.73	1.0000	0.9997	0.9997	1.7134	1.6839	1.6845

$\langle \mathbf{F} \rangle_{\mathrm{emp}} = 0.9998$

$\langle \mathbf{GT} \rangle_{\mathrm{emp}} = 1.6474(23)$

Phys. Rev. C 95, no. 5, 059902 (2017)



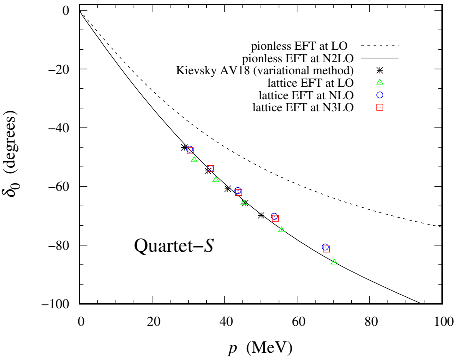
OPE

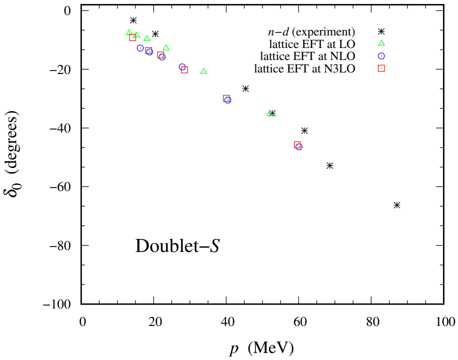
MEC

$n-d$ scattering

$a = 1.97$ fm

Preliminary results for the 3-nucleon systems:





Bovermann, SE, Epelbaum, Krebs, Lee, Meißner [*work in progress*]

variational method: Nucl. Phys. A 607, 402 (1996)

$n-d$ (experiment): Phys. Lett. 24B, 562 (1967)

pionless EFT: Nucl. Phys. A 675, 601 (2000)

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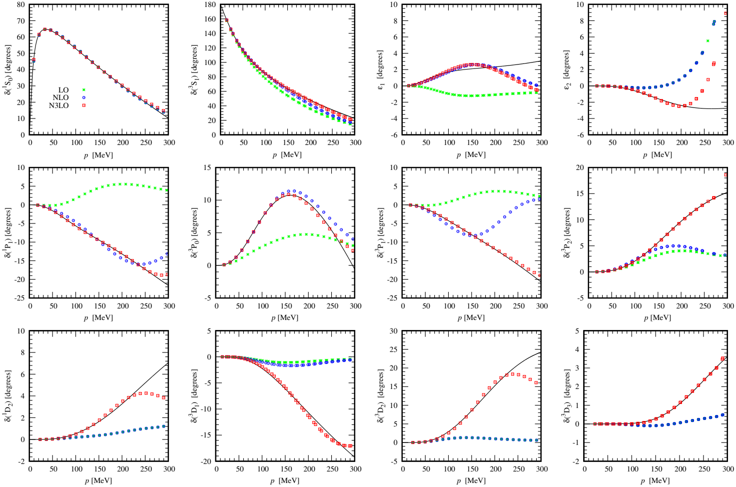

NLEFT collaboration [*work in progress*]

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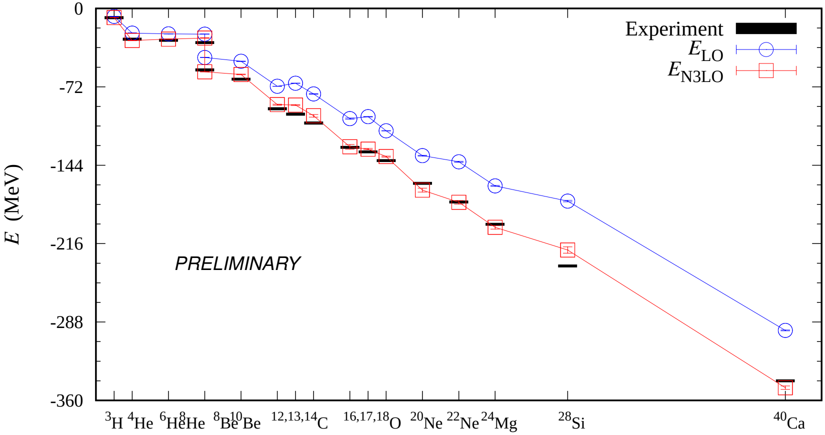

- To determine the 3N forces, we consider several nuclear processes, such as triton beta-decay, neutron-alpha and alpha-alpha scattering, properties of ^{3}He and ^{4}He etc.

Summary

- Nuclear forces in the framework of chiral effective field theory are well-established, and it is very important time for *ab initio* methods to make predictions in many-nucleon system using these forces.
- A new lattice formulation of chiral effective field theory interactions has improved our *ab initio* nuclear theory which describes the nuclear structure successfully as well as nuclear scattering and reaction processes.
- 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.
- 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.

Thanks!

Extras

Quantum Phase Transtition

In physics, a quantum phase transition (QPT) is a phase transition between different quantum phases (phases of matter at zero temperature). Contrary to classical phase transitions, quantum phase transitions can only be accessed by varying a physical parameter-such as magnetic field or pressure-at absolute zero temperature. The transition describes an abrupt change in the ground state of a many-body system due to its quantum fluctuations.