Nuclear lattice simulations with chiral effective field theory at N3LO

Serdar Elhatisari

Gaziantep S&T University
HISKP - Universität Bonn

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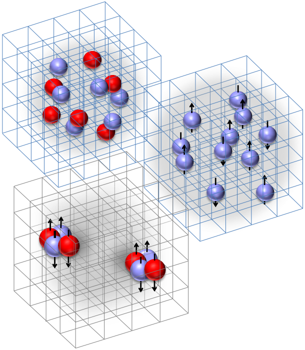
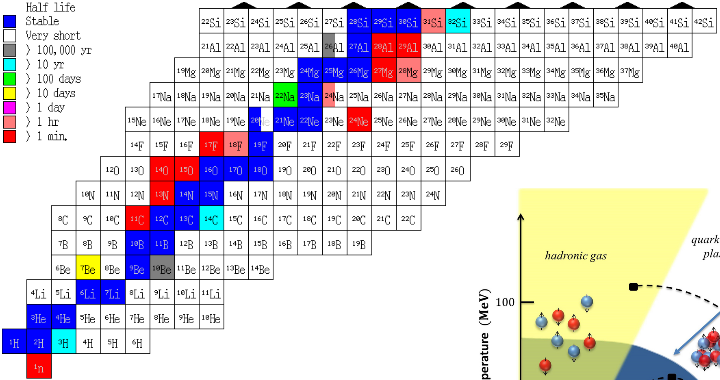
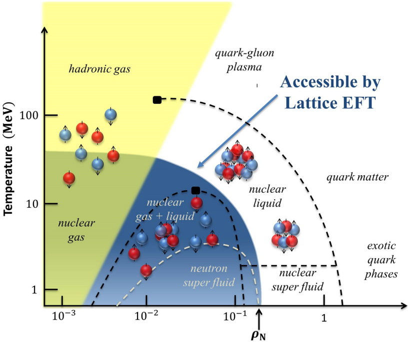


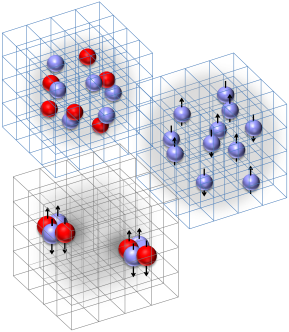
The aim is to predict the properties of nuclear systems from microscopic nuclear forces



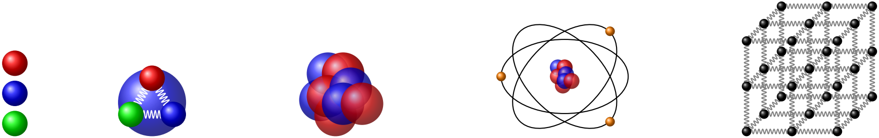


Outline

- Introduction
- Chiral effective field theory (chiral EFT)
- Lattice effective field theory
- A path to an ab-initio nuclear theory
- Wave function matching for quantum systems
- Recent progress in LEFT
- Summary



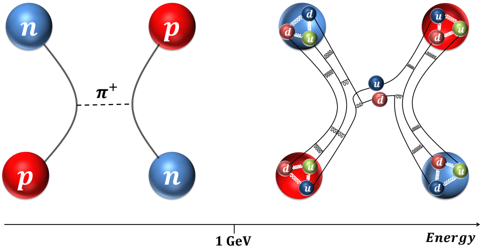
Nuclear forces from QCD



Quarks $< 10^{-16}$ | Nucleons $\sim 10^{-13}$ | Nucleus $\sim 10^{-12}$ | Atoms $\sim 10^{-8}$ cm | Matter

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

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



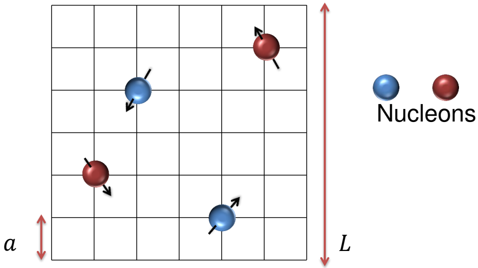
$(\Lambda_\chi \sim$ chiral limit$)$

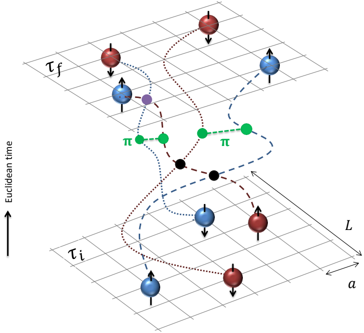
$m_u, m_d \to 0$

"separation of scales"

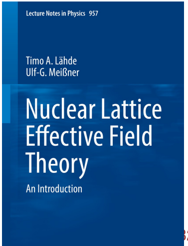
Lattice effective field theory

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





- 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.



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)

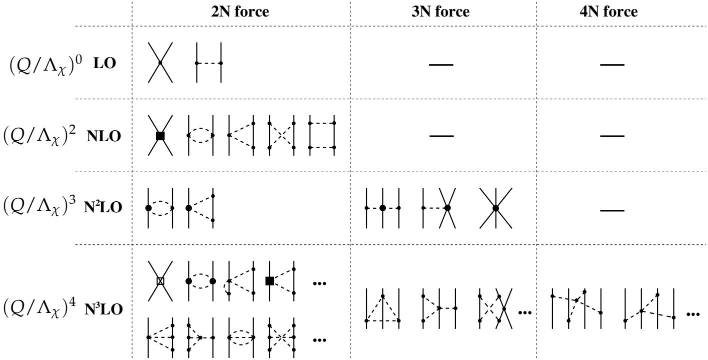
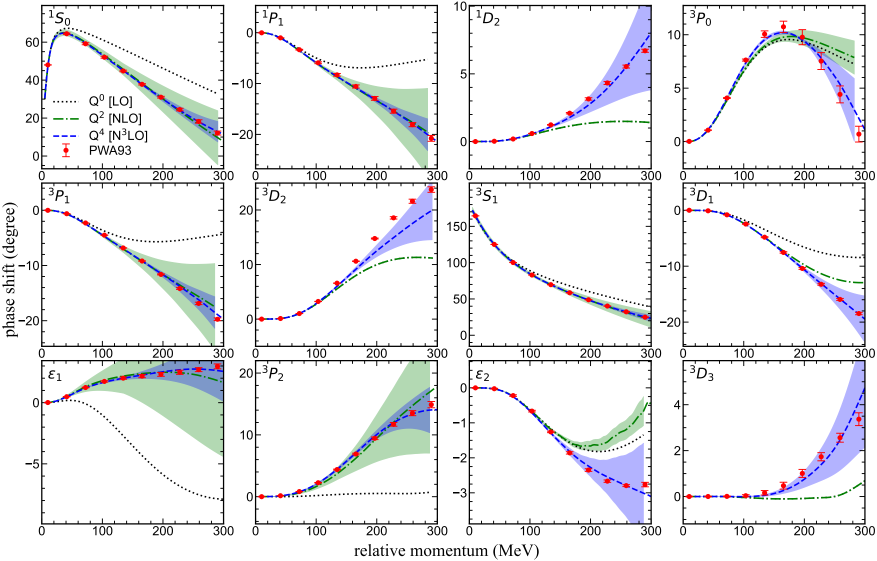


Fig. courtesy of E.Epelbaum

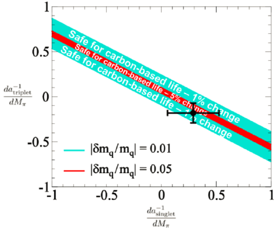
Ordonez et al. ’94; Friar & Coon ’94; Kaiser et al. ’97; Epelbaum et al. ’98,’03,’05,’15; Kaiser ’99-’01; Higa et al. ’03; ...

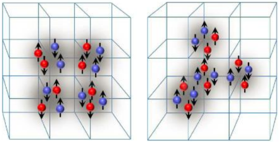
chiral EFT for nucleons: *NN* scattering phase shifts



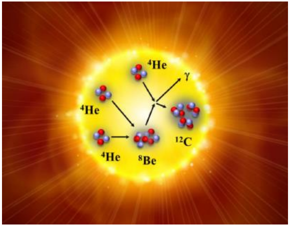
Li, SE, Epelbaum, Lee, Lu, Meißner *Phys. Rev. C* 98, 044002 (2018)

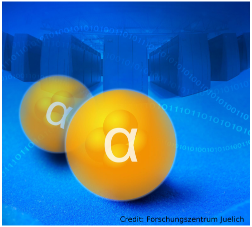
Nuclear LEFT: *ab initio* nuclear structure and scattering theory





- ☐ 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).





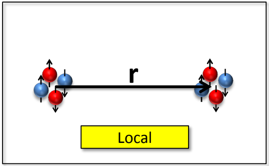
A path to an *ab-initio* nuclear theory:

degree of locality of nuclear forces

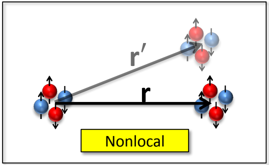
	2N force
LO	

$$V_{\mathrm{LO}} = V_{^1S_0}^{s_{\mathrm{NL}}, s_{\mathrm{L}}} + V_{^3S_1}^{s_{\mathrm{NL}}, s_{\mathrm{L}}} + V_{\mathrm{OPE}}$$

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



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



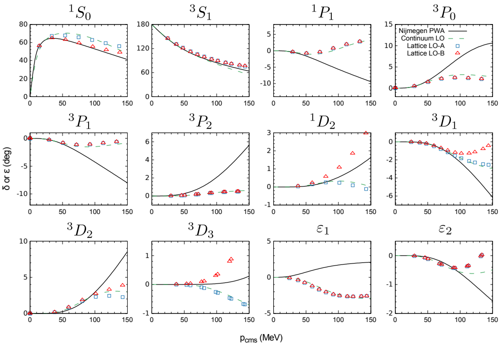
- ☐ Does every chiral EFT interaction give well controlled and reliable results for heavier systems?
- ☐ Is the convergence of higher-order terms under control?

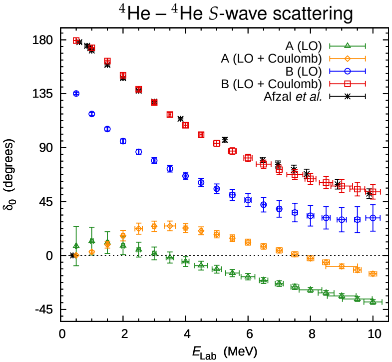
SE, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, Lee, Rupak, *PRL* 117, 132501 (2016)

Degree of locality of nuclear forces - I

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

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





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
^{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
^{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

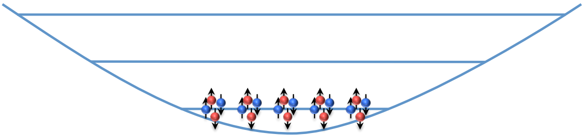
$$\frac{E_{^8\mathrm{Be}}}{E_{^4\mathrm{He}}} = 1.997(6)$$

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

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

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

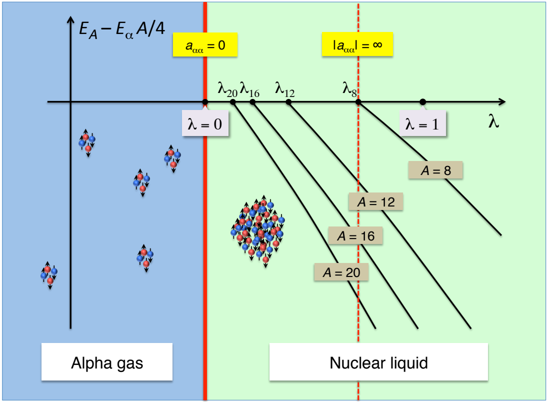
Bose condensate of alpha particles!



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

Nuclear binding near a quantum phase transition

Consider a one-parameter family of interactions: $V = (1-\lambda)\, V^{A}_{\rm LO} + \lambda\, V^{B}_{\rm LO}$



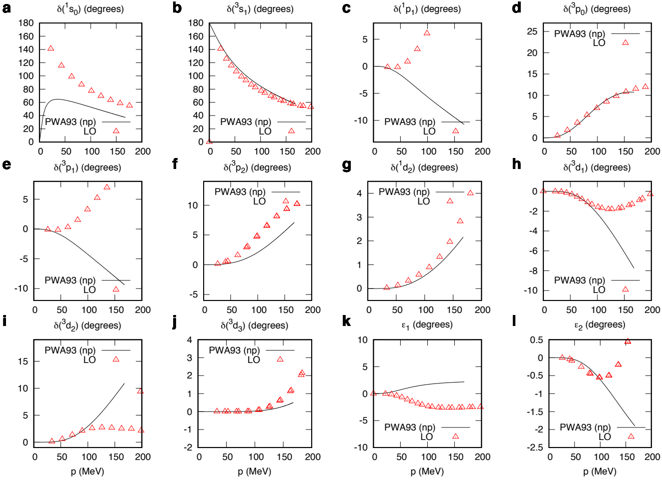
There is a quantum phase transition at the point where the α-α scattering length $a_{\alpha\alpha}$ vanishes, and it is a first-order transition from a Bose-condensed α-particle gas to a nuclear liquid.

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

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

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

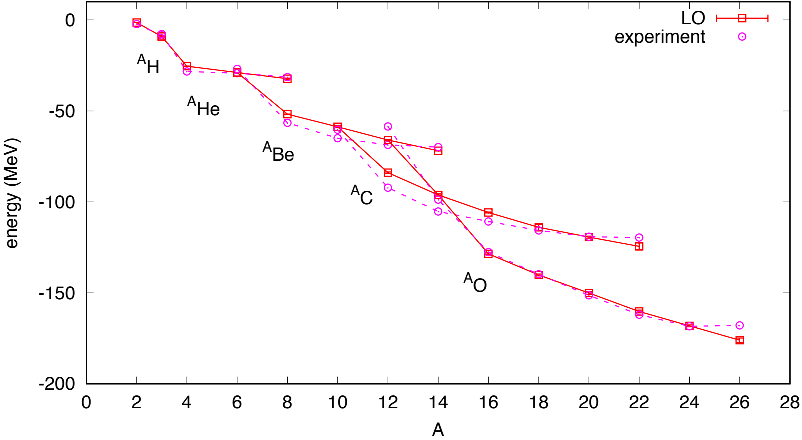
$$V_{\mathrm{LO}} = V_{\mathrm{SU4}}^{s_{NL}, s_L} + V_{\mathrm{OPE}}$$



Ground state energies at LO

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

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



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

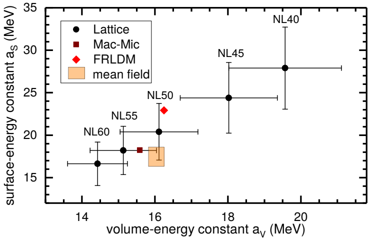
Degree of locality of nuclear forces – III

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 given s_{NL},
- ☐ This is repeated for s_{NL} = 0.1 - 0.6,
- ☐ For $A \geq 16$, the binding energies are well-parameterized with the Bethe-Weizsäcker mass formula;

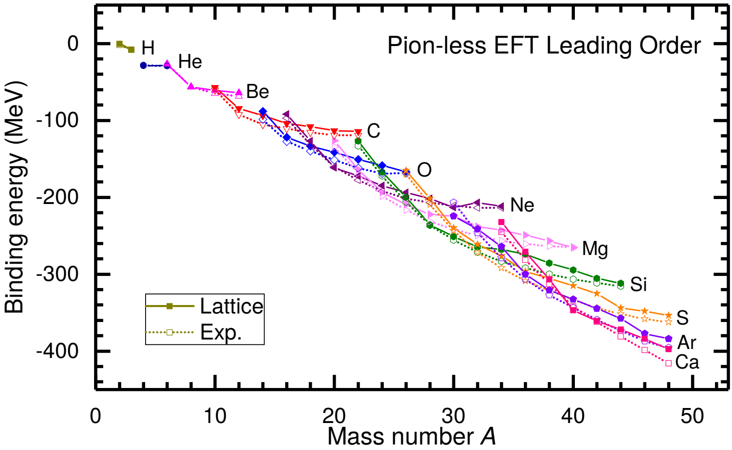
$$B(A) = a_V\, A - a_S\, A^{2/3} + E_{\text{Coulomb}} + (\text{symmetry} + \text{pairing} + \text{shellcorrection} + \ldots)$$



Essential elements for nuclear binding

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

$$V_{\not\pi}^{\mathrm{LO}} = V_{\mathrm{SU4}}^{C_2,s_{\mathrm{NL}},s_{\mathrm{L}}} + V_{\mathrm{SU4}}^{C_3} + V_{\mathrm{Coulomb}}$$

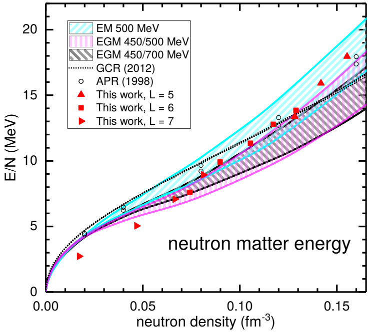


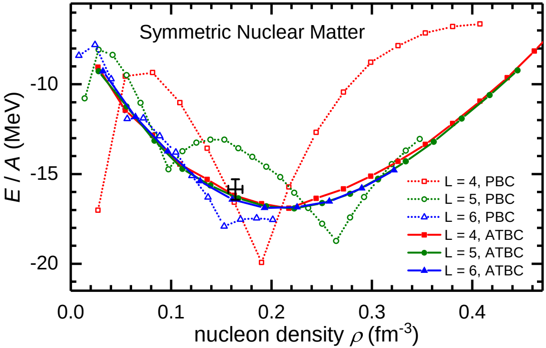
Lu, Li, SE, Lee, Epelbaum, Meißner, *Phys. Lett. B*, 797, 134863 (2019)

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, $s_{\mathrm{L}} = 0.061$ (l.u.), and $s_{\mathrm{NL}} = 0.5$ (l.u.)

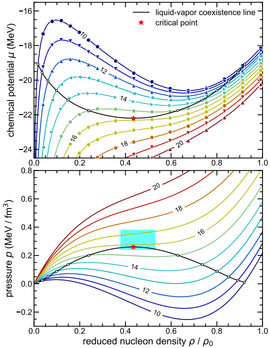
Lu, Li, SE, Lee, Epelbaum, Meißner, *Phys. Lett. B*, 797, 134863 (2019)

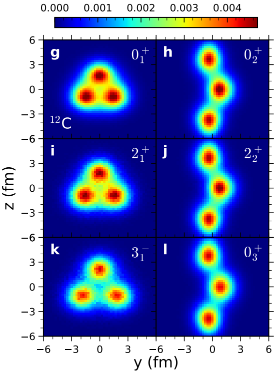


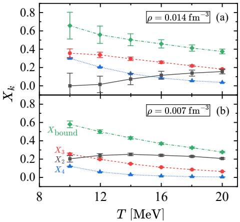


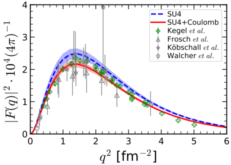
Lu, Li, SE, Lee, Drut, Lahde, Epelbaum, Meißner, *Phys. Rev. Lett.* 125, 192502 (2020)

Essential elements for nuclear binding





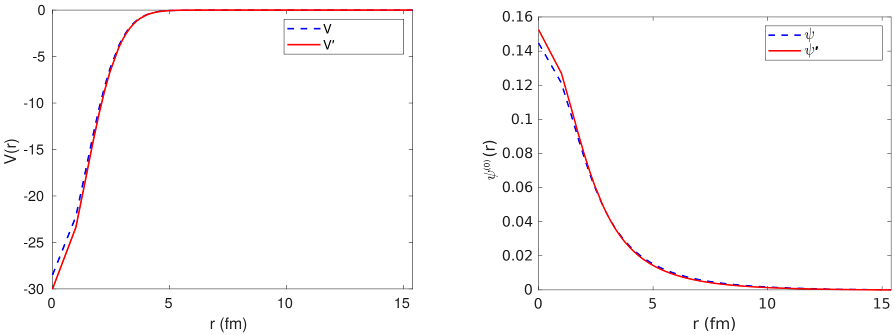




- ☐ *Ab-initio* nuclear thermodynamics,
  Phys. Rev. Lett. 125, 192502 (2020)
- ☐ Emergent geometry and duality in the carbon nucleus,
  Nature Commun. 14 (2023) 2777
- ☐ *Ab-initio* study of nuclear clustering in hot dilute nuclear matter,
  arXiv:2305.15037 [will be published in PLB]
- ☐ *Ab-initio* calculation of the alpha-particle monopole transition form factor, arXiv:2309.01558

Perturbative calculations

Toy model:

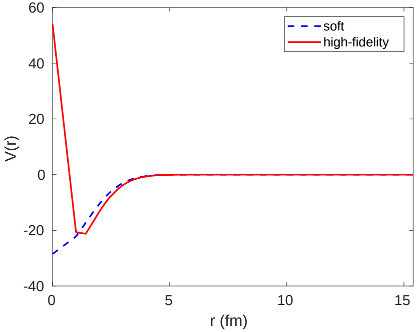


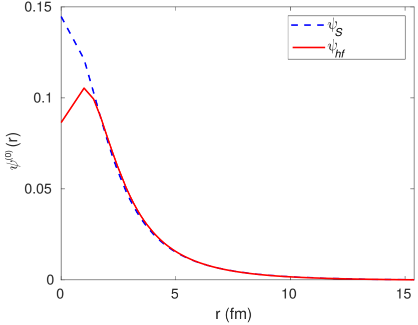
E	E'
-2.010472457971	-2.445743725635
1.775231321023	1.721517536958
6.206769197086	6.118307106128
12.776191791947	12.667625238436
21.337188185570	21.213065578266

Perturbative energies	
q	$\langle \psi^{(0)} \| H' \| \psi^{(q)} \rangle$
0	-2.43080610
1	-2.44610114
2	-2.44574140
3	-2.44575370

Perturbative calculations

Toy model:





E_{soft}	E_{hf}
-2.010472457971	-2.444693272597
1.775231321024	1.769682285996
6.206769197085	6.282284485051
12.776191791946	13.008087181009
21.337188185570	21.786534445492

Perturbative energies	
q	$\langle \psi_S^{(0)} \vert H \vert \psi_S^{(q)} \rangle$
0	-1.74722993
1	-2.89957307
2	-2.10036797
3	-2.26376481

Wavefunction Matching

- ☐ H_χ : –severe sign oscillation, –derived from the underlying theory.
- ☐ $H_{\rm soft}$: –tolerable sign oscillation, –many-body observables with a fair agreement.

Can unitary transformation create a new chiral Hamiltonian which is (first order) perturbation theory friendly?

$$H'_\chi = U^\dagger \, H_\chi \, U$$

- ☐ Let $|\psi_\chi^0\rangle$ be the normalized lowest eigenstate of H_χ.
- ☐ Let $|\psi_{\rm soft}^0\rangle$ be the normalized lowest eigenstate of $H_{\rm soft}$.

$$U_{R',R} = \theta(r-R)\,\delta_{R',R} + \theta(R'-r)\,\theta(R-r)\;|\psi_\chi^\perp\rangle\,\langle\psi_{\rm soft}^\perp|$$

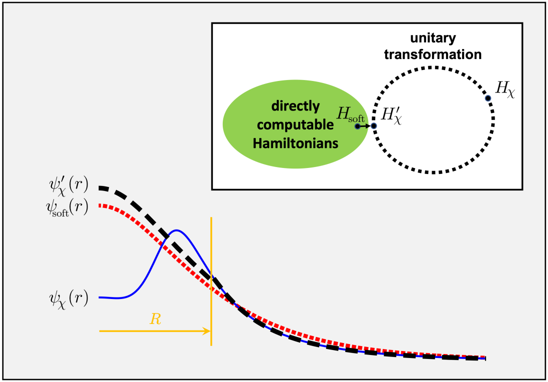
SE et al. [NLEFT collaboration] arXiv:2210.17488

Wavefunction Matching

- ☐ $H_{\rm soft}$: –tolerable sign oscillation, –many-body observables with a fair agreement.
- ☐ H_χ : –severe sign oscillation, –derived from the underlying theory.

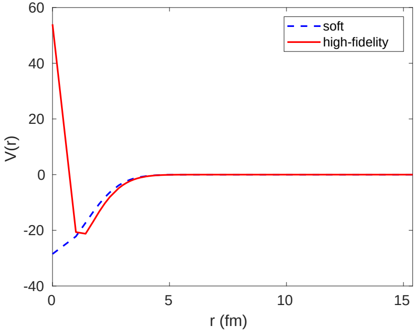
Unitary transformation can create a new chiral Hamiltonian which is (first order) perturbative friendly

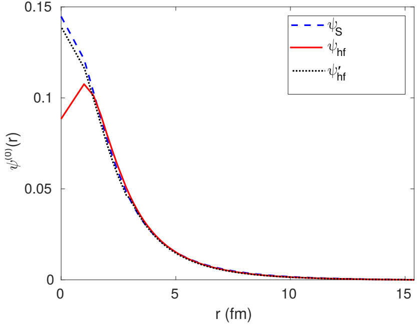
$$H'_\chi = U^\dagger \, H_\chi \, U$$



Wavefunction Matching: Perturbative calculations

Toy model:



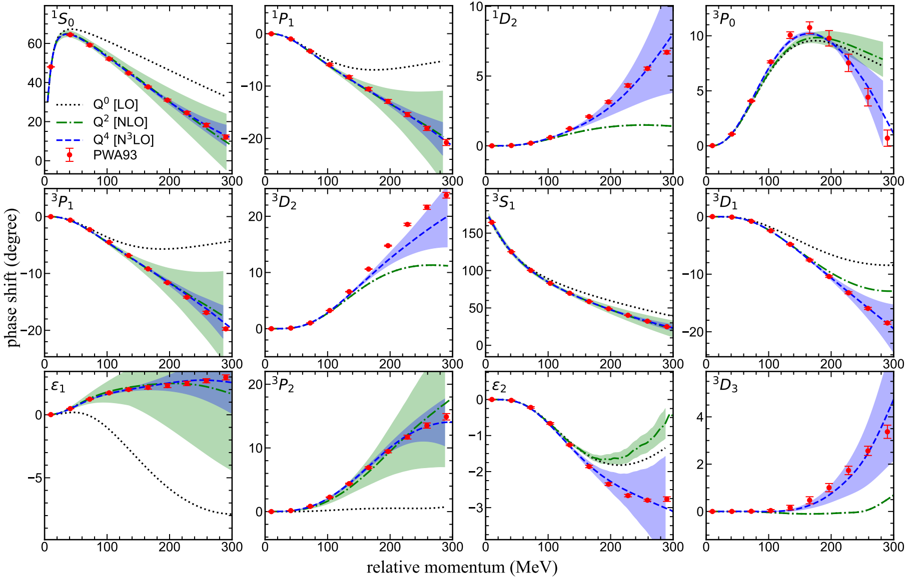


E_{hf}	E'_{hf}
−2.444693273	−2.444693273
1.769682286	1.769682286
6.282284485	6.282284485
13.008087181	13.008087181
21.786534446	21.786534446

q	$\langle\psi_S^{(0)}\|H'\|\psi_S^{(q)}\rangle$				
	$R = 0.00$	$R = 1.32$	$R = 1.86$	$R = 2.28$	$R = 3.22$ fm
0	−1.747230	−2.055674	−2.226685	−2.312220	−2.402507
1	−2.899573	−2.558509	−2.477194	−2.457550	−2.446214
2	−2.100368	−2.389579	−2.430212	−2.439585	−2.443339
3	−2.263765	−2.414809	−2.437676	−2.441072	−2.443233

Ab initio nuclear theory: recent progress in NLEFT

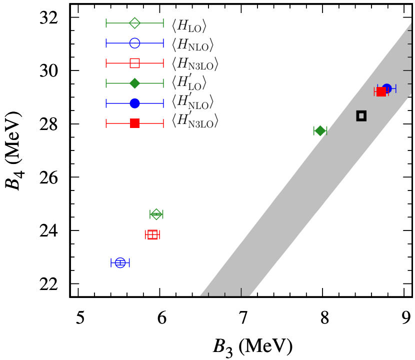
$a = 1.32$ fm and $p_{\max} = \pi/a = 471$ MeV



Ab initio nuclear theory: recent progress in NLEFT

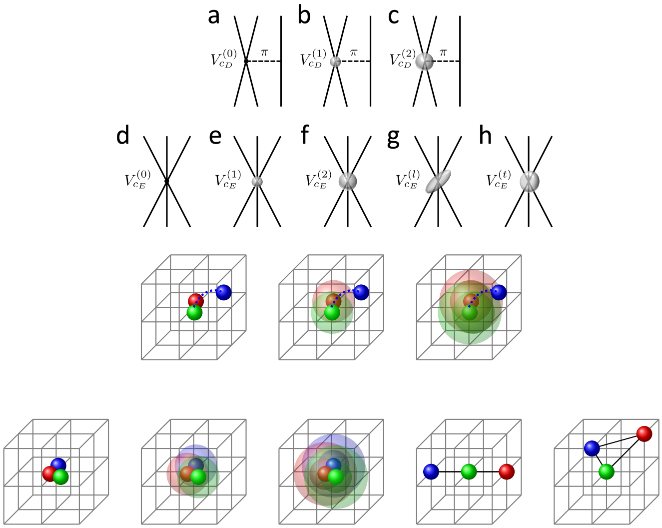
$a = 1.32$ fm and $p_{\max} = \pi/a = 471$ MeV

Nuclei	B_{Q0} MeV	B_{Q2} MeV	B_{Q4} MeV	Experiment
$E_{\chi,\mathrm{d}}$	1.7928	2.1969	2.2102	2.2246
$\langle\psi^0_{\mathrm{soft}}\| H_{\chi,\mathrm{d}} \|\psi^0_{\mathrm{soft}}\rangle$	0.4494	0.3445	0.6208	
$\langle\psi^0_{\mathrm{soft}}\| H'_{\chi,\mathrm{d}} \|\psi^0_{\mathrm{soft}}\rangle$	1.6496	1.9772	2.0075	



Ab initio nuclear theory: recent progress in NLEFT

$a = 1.32$ fm and $p_{\max} = \pi/a = 471$ MeV



SE et al. [NLEFT collaboration] arXiv:2210.17488

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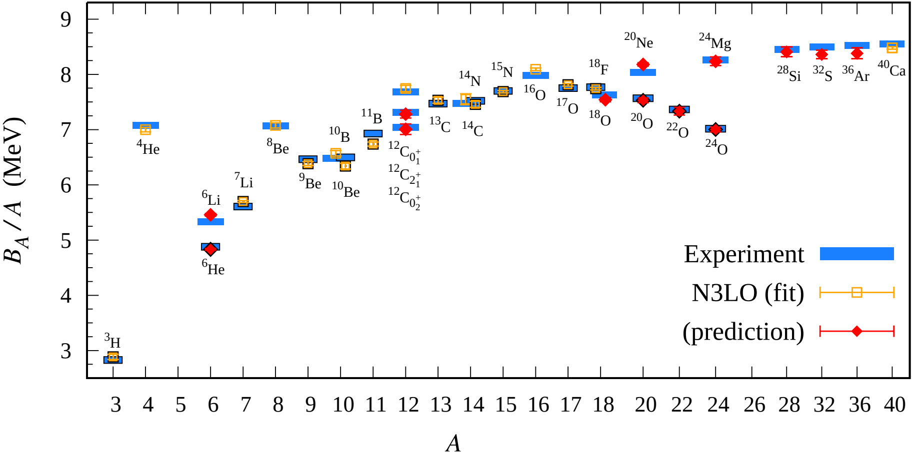

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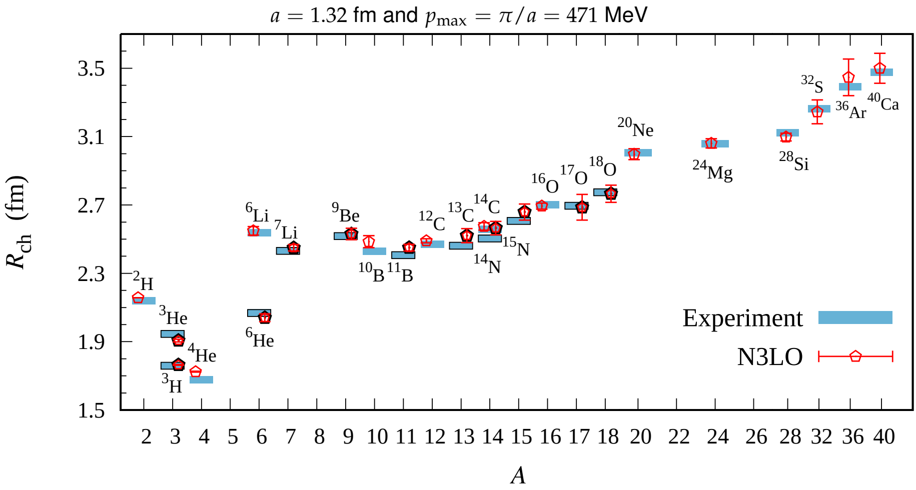

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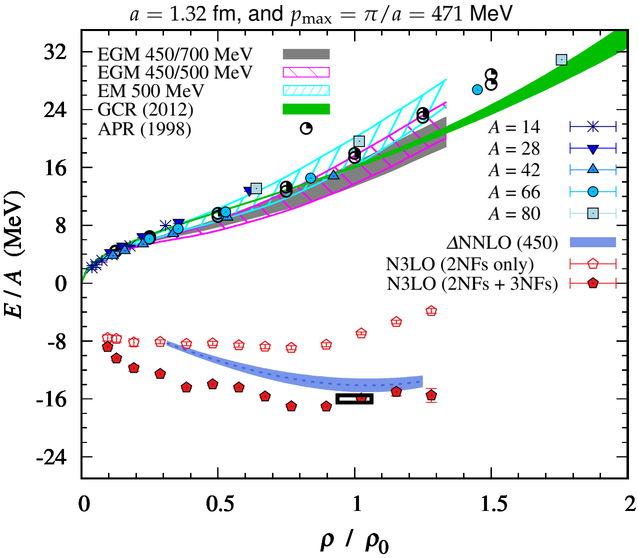

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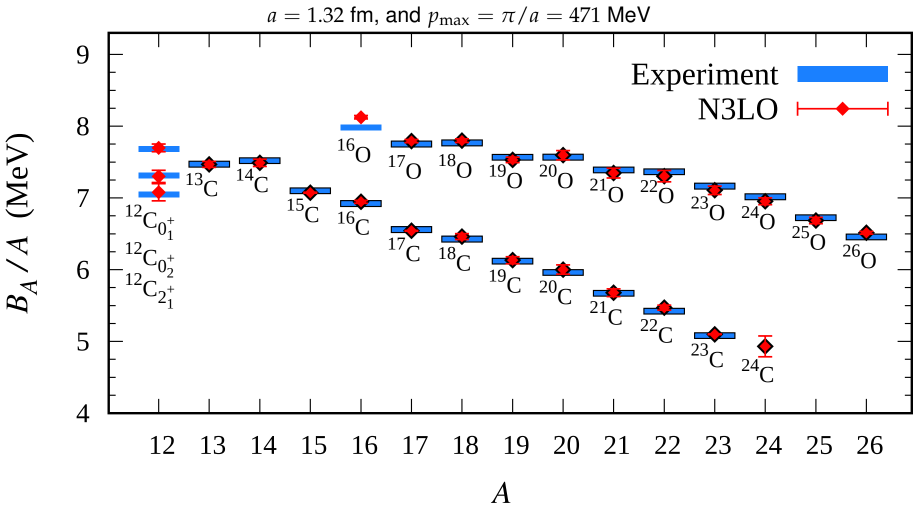

[NLEFT collaboration] in progress

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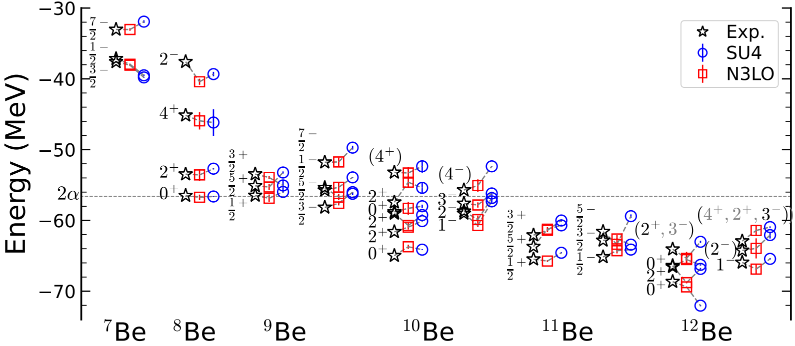

[NLEFT collaboration] in progress

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.
- 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.
- Improving QMC calculations with perturbation theory for many-body systems in nuclear physics is crucial to be able to use more realistic interactions in *ab initio* nuclear theory. Phys. Rev. Lett. 128, 242501 (2022)
- A recently developed method so called the wave function matching provides a rapid convergence in perturbation theory for many-body nuclear physics. Using this new method now we are able to calculate the nuclear binding energies, neutron matter, symmetric nuclear matter and charge radii of nuclei simultaneously in very good agreements with the experimental results.

Thanks!