Scattering processes in nuclear lattice simulations

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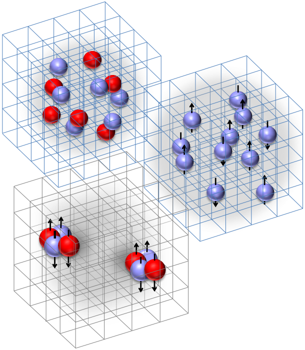
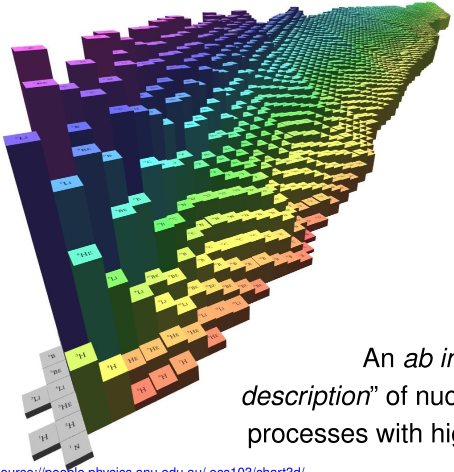
Bethe Forum
Frontiers in Nuclear Physics
Bonn, Germany
Nov 21-23, 2023

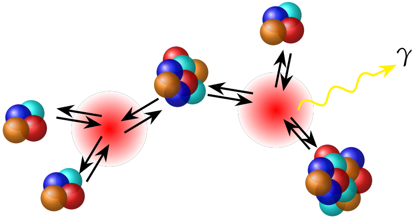


Ab initio nuclear theory

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



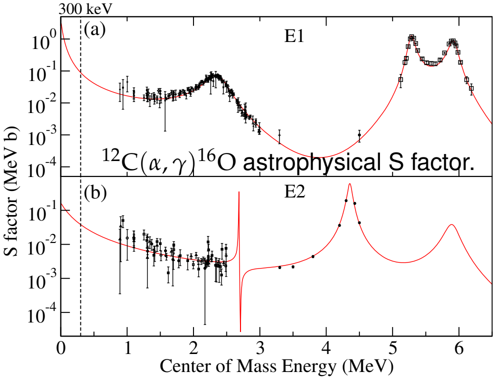
source://people.physics.anu.edu.au/ ecs103/chart3d/



An *ab initio* nuclear theory that has a “*unified description*” of nuclear structure and scattering/reaction processes with high predictive power.

Nuclear reactions

- ^{4}He: fuels the nucleosynthesis of the heavier elements. Direct measurements at the 300 keV, corresponding to helium-burning temperatures, are impossible due to the presence of the Coulomb barrier between nuclei.
- To accurately calculate the reaction rate for stellar burning simulations, the reaction cross section must be determined within the energy range of $0.15 - 3.4$ MeV.
- Therefore, the inaccessible reaction rate depends on extrapolating experimental data obtained at higher energies, leading to significant uncertainties in stellar evolution models.



$^{12}C(\alpha,\gamma)^{16}O$ astrophysical S factor.

deBoer *et al.*, *Rev. Mod. Phys.* 89, 035007

Progresses and challenges in *ab initio* scattering and reactions

- ☐ QMC calculations of n-^{4}He scattering.
  Nollett, Pieper, Wiringa, Carlson, & Hale, PRL 99, 022502 (2007).
- ☐ *Ab initio* many-body calculations of n-^{3}H, n-^{4}He, p-^{3,4}He,and n-^{10}Be scattering.
  Quaglioni & Navratil, PRL 101, 092501 (2008).
- ☐ Ab initio many-body calculations of the ^{3}H(d,n)^{4}He, ^{3}He(d,p)^{4}He fusion.
  Navratil & Quaglioni, PRL 108, 042503 (2012).
- ☐ Elastic proton scattering of medium mass nuclei from CC theory.
  Hagen & Michel PRC 86, 021602 (2012).
- ☐ Coupling the lorentz integral transform (LIT) and the CC Methods.
  Orlandini, G. et al. , Few Body Syst. 55, 907â911 (2014).
- ☐ *Ab initio* investigations of A=8 nuclei.
  Navratil, Kravvaris et al., J.Phys.Conf.Ser. 2586 (2023) 1, 012062
  Kravvaris and Volya, PRC 100, 034321 (2019)

Progresses and challenges in *ab initio* scattering and reactions

Ab initio calculations of scattering and reactions are limited by the computational scaling with the number of nucleons in target and projectile (clusters).

In general, for most of the many-body approaches it remains a challenge to address important processes relevant for stellar astrophysics.

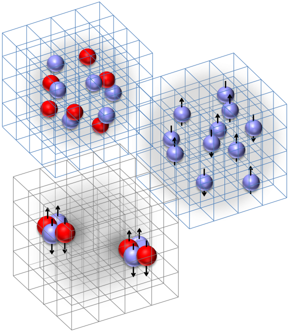
- ☐ Scattering of alpha particles: ${}^{4}\mathrm{He} + {}^{4}\mathrm{He} \to {}^{4}\mathrm{He} + {}^{4}\mathrm{He}$
- ☐ Triple- alpha reaction: ${}^{4}\mathrm{He} + {}^{4}\mathrm{He} + {}^{4}\mathrm{He} \to {}^{12}\mathrm{C} + \gamma$
- ☐ Alpha capture: ${}^{4}\mathrm{He} + {}^{12}\mathrm{C} \to {}^{16}\mathrm{O} + \gamma$

  ${}^{4}\mathrm{He} + {}^{16}\mathrm{O} \to {}^{20}\mathrm{Ne} + \gamma$

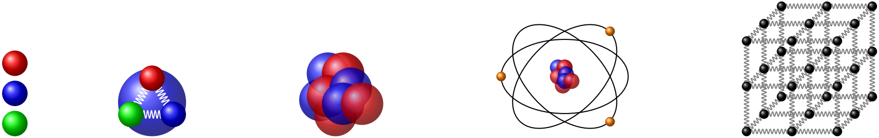
  $\vdots$

Outline

- Introduction
- Chiral effective field theory (chiral EFT)
- Lattice effective field theory
- Scattering on the lattice
- Adiabatic projection method
- Recent progress in LEFT
- Summary



Nuclear forces from QCD



Quarks $< 10^{-16}$

Nucleons $\sim 10^{-13}$

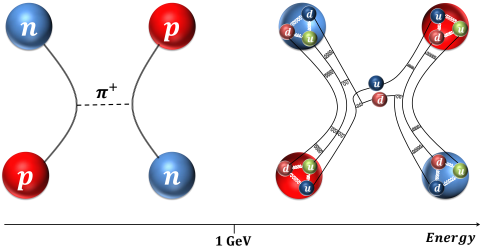
Nucleus $\sim 10^{-12}$

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.



chiral limit

$m_u, m_d \to 0$

"separation of scales"

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)

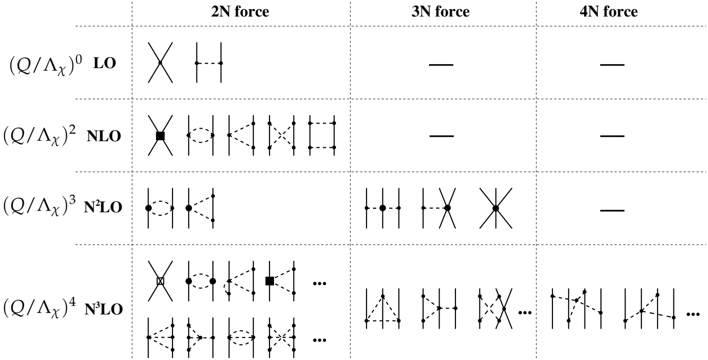
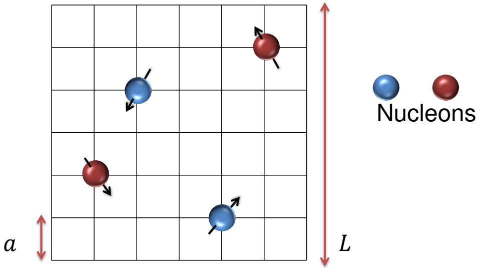


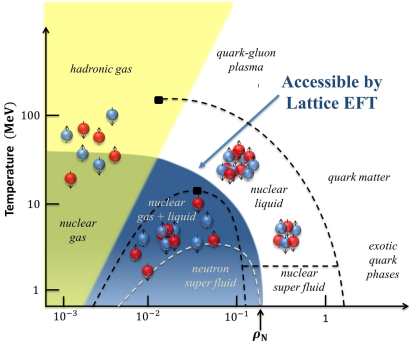
Fig. courtesy of E.Epelbaum

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; ...

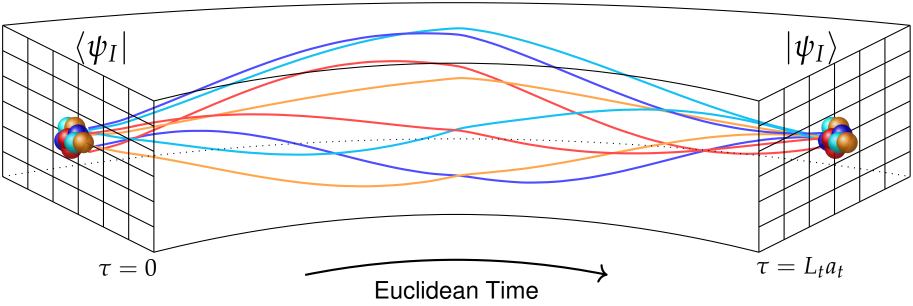
Lattice effective field theory

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





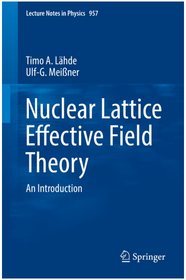
Lattice effective field theory



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

☐ evolve nucleons forward in Euclidean time, $e^{-H_{\mathrm{LO}}\,\tau}\,|\psi_I\rangle$, where $\tau = L_t a_t$.

☐ The evolution in Euclidean time automatically incorporates the induced deformation, polarization and clustering.


Lecture Notes in Physics 957

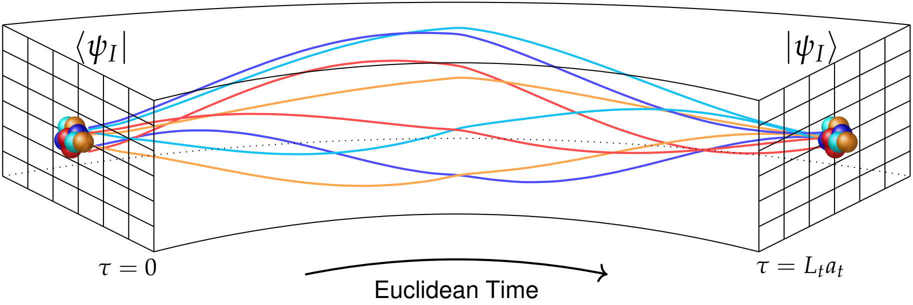
Timo A. Lähde
Ulf-G. Meißner

Nuclear Lattice Effective Field Theory

An Introduction

Springer

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 the particle density. Each nucleon evolves as if a single particle in a fluctuating background of pion fields and auxiliary fields.

Lattice EFT: (Euclidean time) projection Monte Carlo

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

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

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

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 $\hat{M}$.

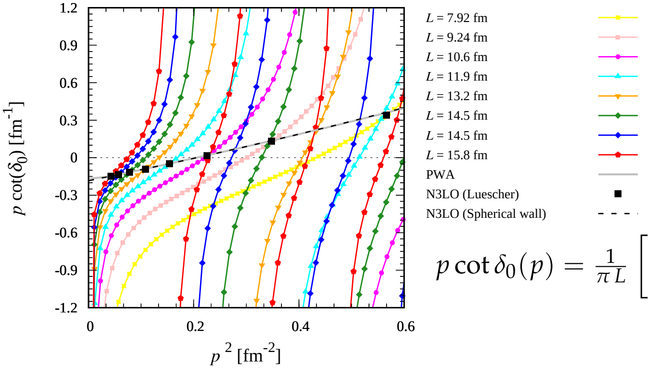
$$Z(L_t) = \langle \psi_I \,|\hat{M}(L_t - 1)\, \hat{M}(L_t - 2)\, \ldots \hat{M}(1)\, \hat{M}(0)\, |\, \psi_I \rangle$$

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 can be extracted by

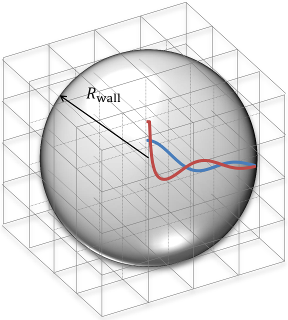
$$\lim_{L_t \to \infty} \frac{Z(L_t + 1)}{Z(L_t)} = e^{-E_0\, a_t}$$

$$\lim_{L_t \to \infty} \frac{\langle \psi_I |\, \hat{M}^{L_t/2}\, H_{\rm LO}\, \hat{M}^{L_t/2}\, |\psi_I \rangle}{\langle \psi_I |\, \hat{M}^{L_t}\, |\psi_I \rangle} = E_0$$

Scattering on the lattice



$$p\cot\delta_0(p) = \frac{1}{\pi L}\left[\sum_{\vec{n}}^{\Lambda}\frac{\theta\left(\Lambda^2-\vec{n}^2\right)}{\vec{n}^2-(Lp/2\pi)^2} - 4\pi\Lambda\right]$$



Lüscher’s finite volume method:

Lüscher, Comm. Math. Phys. 105 (1986) 153; NPB 354 (1991) 531

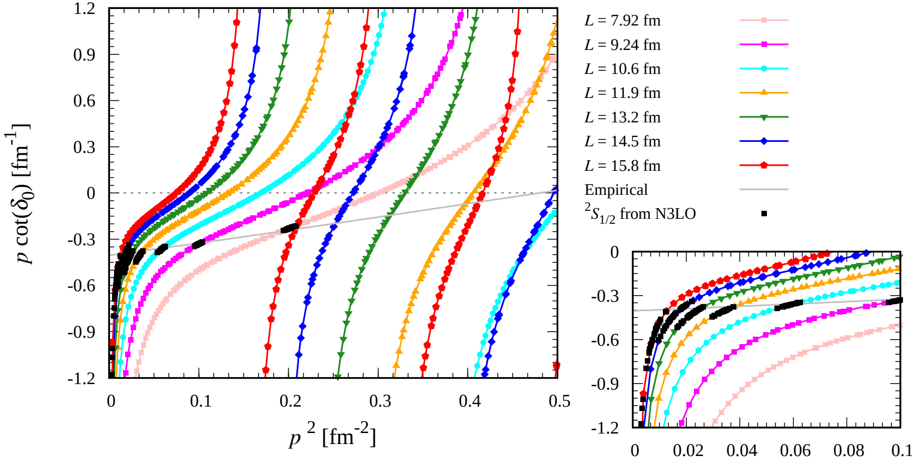
Spherical wall method:

$$R_\ell^{(p)}(r) = N_\ell(p)\times\begin{cases}\cot\delta_\ell(p)\,j_\ell(p\,r)-n_\ell(p\,r)\\ \cot\delta_\ell(p)\,F_\ell(p\,r)+G_\ell(p\,r)\end{cases}$$

Nucl. Phys. A 424, 47-59 (1984), Eur. Phys. J. A 34, 185-196 (2007).

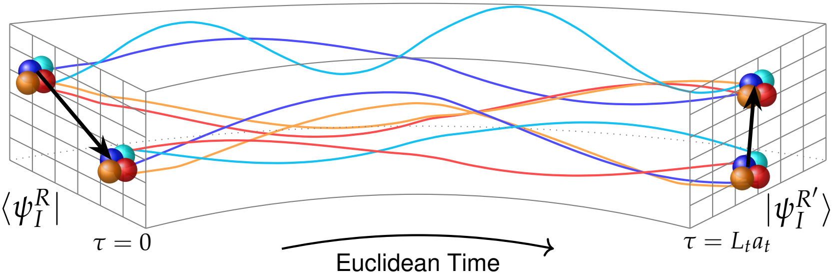
Scattering on the lattice

Neutron-alpha scattering at N3LO



S.E. and Meißner, [*in progress*].

Adiabatic projection method



The method constructs a low energy effective theory for the clusters by using initial states, $|\psi_I^R\rangle$ and $|\psi_I^{R'}\rangle$, parameterized by the relative spatial separation between clusters, and project them in Euclidean time to get dressed cluster states, $|\psi_I^R\rangle_\tau = e^{-H\tau}\ |\psi_I^R\rangle$.

Hamiltonian matrix

$$[H_\tau]_{R,R'}^{J,J_z} = {}_\tau^{J,J_z}\langle \psi_I^R | H | \psi_I^{R'}\rangle_\tau^{J,J_z}$$

Norm matrix

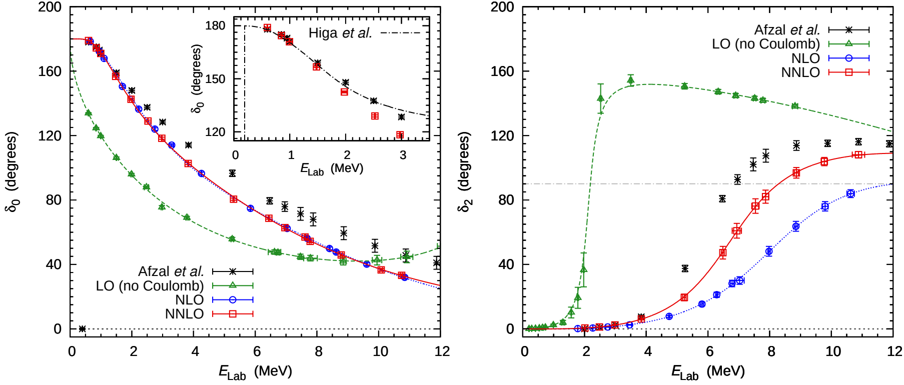
$$[N_\tau]_{R,R'}^{J,J_z} = {}_\tau^{J,J_z}\langle \psi_I^R | \psi_I^{R'}\rangle_\tau^{J,J_z}$$

$$[H_\tau^a]_{\vec{R},\vec{R}'}^{J,J_z} = \left[N_\tau^{-1/2}\ H_\tau\ N_\tau^{-1/2}\right]_{\vec{R}\,\vec{R}'}^{J,J_z}$$

Eur.Phys.J.A 52 (2016) 6, 174.

Eur.Phys.J.A 55 (2019) 8, 144.

Ab-initio alpha-alpha scattering N2LO



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

Higa, Hammer, van Kolck, *Nucl.Phys.* A809, 171 (2008), 0802.3426.

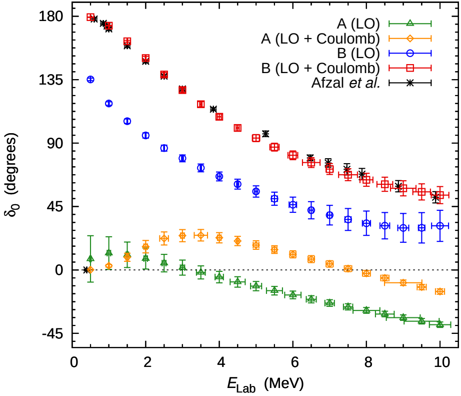
S.E., Lee, Rupak, Epelbaum, Krebs, Lähde, Luu, & Meißner. *Nature* 528, 111-114 (2015).

Ab-initio alpha-alpha scattering

Degree of locality of nuclear forces

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

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

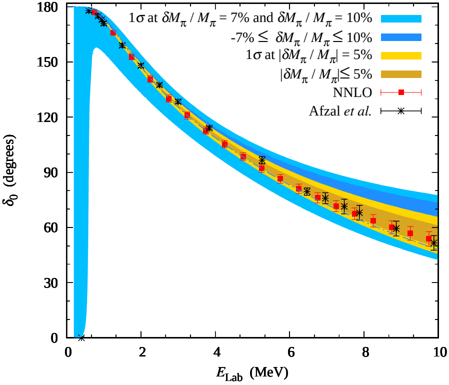


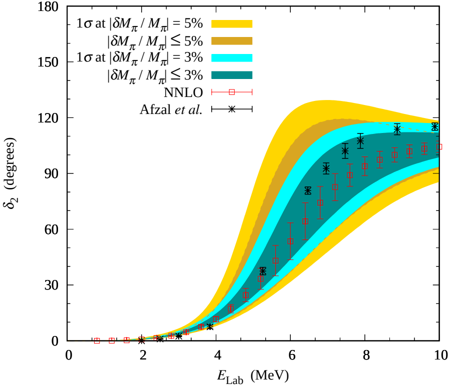
S.E., Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, Lee, Rupak, *PRL* 117, 132501 (2016)

Ab-initio alpha-alpha scattering in the Multiverse

Alpha-alpha scattering phase shifts under variations of the fundamental parameters of the Standard Model.

$$\left.\frac{\partial E_{\alpha\alpha}}{\partial M_\pi}\right|_{M_\pi^{\rm ph}} = \left.\frac{\partial E_{\alpha\alpha}(\tilde{M}_\pi, m_N(M_\pi), \tilde{g}_{\pi N}(M_\pi), C_0(M_\pi), C_I(M_\pi))}{\partial M_\pi}\right|_{M_\pi^{\rm ph}}$$





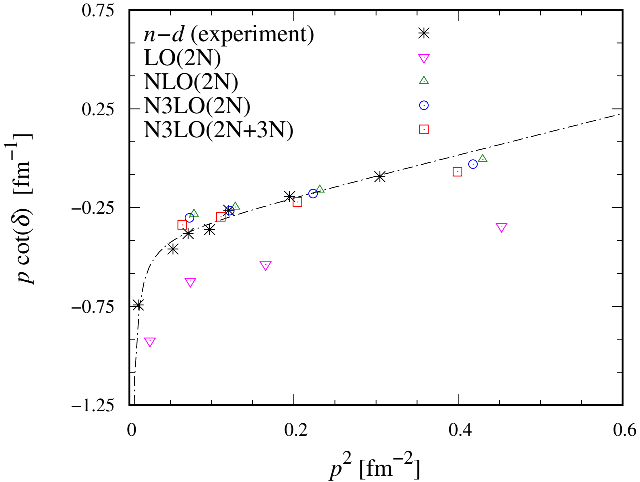
Afzal, Ahmad, Ali, *Rev. Mod. Phys.* 41, 247, (1969).

S.E., Lähde, Lee, Meißner, Vonk. *JHEP* 02 (2022) 001.

Chiral interactions at N3LO – 2NFs + 3NFs

Work	Constraints	Predictions
NCSM, Barrett *et al.*	BE of ^{3}H and ^{4}He	ES of ^{6}Li
NCSM, Nogga *et al.*	BE of ^{3}H and ^{4}He	Spectrum of ^{7}Li
NCSM, Navratil *et al.*	^{3}H, ^{6}Li, ^{10}B, ^{12}C	^{4}He, ^{6}Li, ^{10,11}B, ^{12,13}C
NCSM, Maris *et al.*	BE of ^{3}H and ^{3}H β decay	Structures of $A = 7, 8$
NCSM, Roth *et al.*	BE of ^{3}H and ^{3}H β decay	^{4}He, ^{6}Li, ^{12}C and ^{16}O
CC, Hagen *et al.*	BE of ^{3}H and ^{3}H β decay	EoS of nucleonic matter
BMBPT, Tichai *et al.*	BE of ^{3}H and ^{3}H β decay	BE of $^{16-26}$O, $^{36-60}$Ca and $^{50-78}$Ni
IT-NCSM, Roth *et al.*	BE of ^{3}H and ^{4}He, and ^{3}H β decay	BE of ^{4}He, ^{16}O, ^{40}Ca
CC, Roth *et al.*	BE of ^{3}H and ^{4}He, and ^{3}H β decay	BE of ^{16,24}O, ^{40,48}Ca
SCGF, Cipollone *et al.*	BE of ^{3}H and ^{4}He, and ^{3}H β decay	BE of ^{13,27}N, ^{14,28}O and ^{15,29}F
AFDMC, Lynn *et al.*	BE of ^{3}H and n-^{4}He P-wave phase shifts	EoS of nucleonic matter
CC, Carlsson *et al.*	BE of ^{3}H, ^{3,4}He, ^{14}Li and ^{16,22,24,25}O	R_c and BE of nuclei up to ^{40}Ca

Spin doublet S-wave neutron-deuteron scattering at N3LO



S.E., Hildenbrand and Meißner, [*in progress*].

Triton-β decay at N3LO

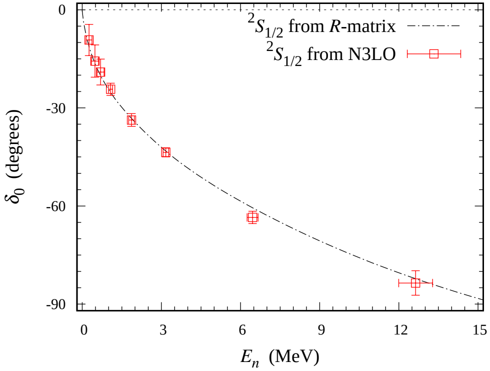
$$(1+\delta_R)\, t_{1/2}\, f_V = \frac{K/G_V^2}{\langle \mathbf{F} \rangle^2 + \frac{f_A}{f_V}\, g_A^2\, \langle \mathbf{GT} \rangle}$$

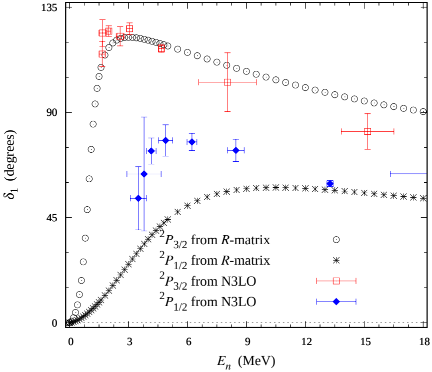
$$\langle \mathbf{F} \rangle = \sum_{n=1}^{3} \langle {}^3\mathrm{He} \| \tau_{n,+} \| {}^3\mathrm{H} \rangle = 0.9998 \qquad \langle \mathbf{GT} \rangle = \sum_{n=1}^{3} \langle {}^3\mathrm{He} \| \sigma_n \tau_{n,+} \| {}^3\mathrm{H} \rangle = 1.6474(23)\,.$$

L (fm)	$\langle \mathbf{F} \rangle$				$\langle \mathbf{GT} \rangle$			
	LO (2N)	NLO (2N)	N3LO (2N)	N3LO (2N+3N)	LO (2N)	NLO (2N)	N3LO (2N)	N3LO (2N+3N)
5.28	0.99996	0.99999	0.99999	0.99999	1.7167	1.6981	1.6976	1.7015
6.60	0.99984	0.99997	0.99997	0.99997	1.7115	1.6937	1.6919	1.6955
7.92	0.99969	0.99989	0.99990	0.99990	1.7099	1.6917	1.6886	1.6919
9.24	0.99967	0.99977	0.99977	0.99978	1.7107	1.6842	1.6801	1.6845
10.6	0.99973	0.99956	0.99958	0.99962	1.7125	1.6808	1.6763	1.6823
11.9	0.99980	0.99940	0.99958		1.7135	1.6764		

S.E., Hildenbrand and Meißner, [*in progress*].

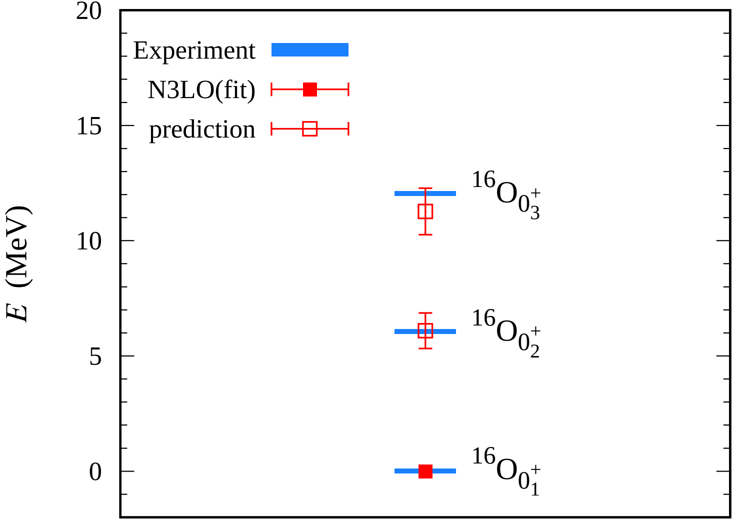
Neutron-alpha scattering at N3LO



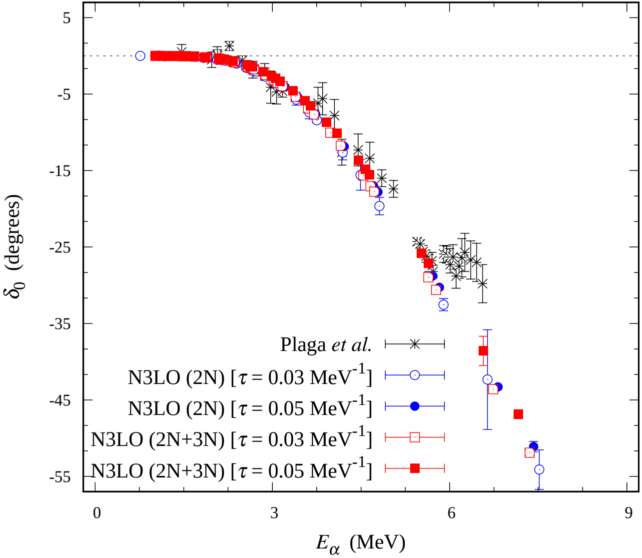


S.E. and Meißner, [*in progress*].

Alpha-carbon scattering at N3LO

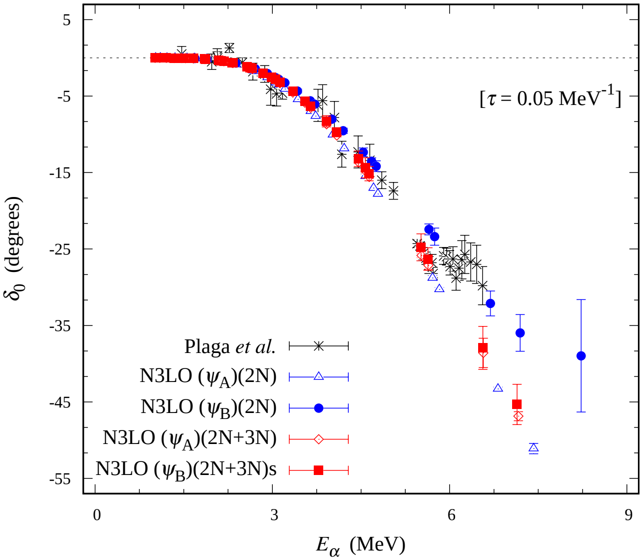


Ab initio alpha-carbon scattering at N3LO



S.E., Hildenbrand, Meißner, Lee, ... NLEFT [*in progress*].

Ab initio alpha-carbon scattering at N3LO



S.E., Hildenbrand, Meißner, Lee, ... NLEFT [*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.

☐ 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.

☐ With the recently developed N3LO lattice action and powerful numerical methods, we are ready to perform the first *ab initio* calculation of alpha-carbon scattering, “holy grail” of nuclear astrophysics.

Thanks!