Advancing nuclear structure and scattering calculations using NLEFT

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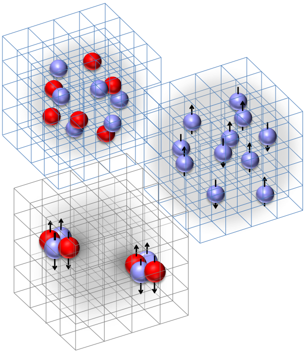
(GIBTU & KFUPM)

Frontiers in Nuclear Lattice EFT:
From Ab Initio Nuclear Structure to Reactions
Beihang University, Beijing
Mar 1-3, 2025

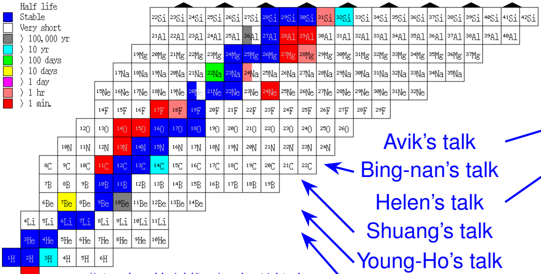


Ab initio nuclear theory

☐ Nuclear structure and nuclear reactions from the first principibles, without relying on any adjustable parameters.

Stellar nucleosynthesis

(Formation of heavier elements in stars)



source://atom.kaeri.kr/old/ton/nuchart1.html

Avik's talk

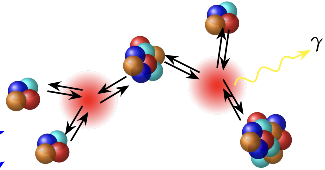
Bing-nan's talk

Helen's talk

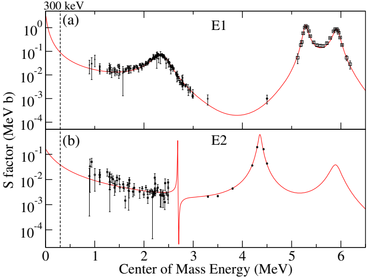
Shuang's talk

Young-Ho's talk

Zhengxue's talk



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



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

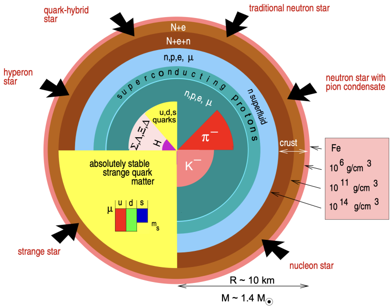
☐ Ab-initio theory: describing nuclear systems directly from fundamental interactions.

■ Challenges:

→ Complex nature of nuclear forces.

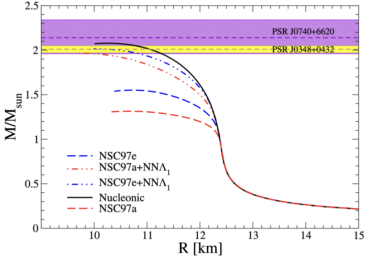
→ Scaling effectively to handle systems across the entire nuclear chart

Ab initio nuclear theory: Towards neutron stars and hypernuclei



J. Weber (arXiv:astro-ph/0008376)

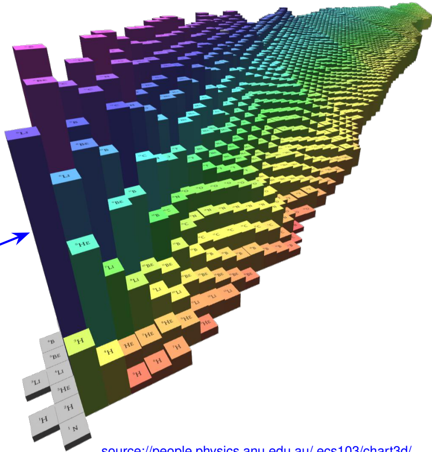
- ☐ Nuclear systems involving quarks beyond up and down quarks.
- ■ Challenges: "Hyperon puzzle".



Logoteta, Vidana, Bombaci (Eur. Phys. J. A (2019) 55: 207)

Fabian's talk

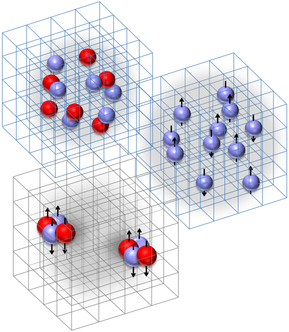
Hui's talk



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

Outline

- Introduction
- Nuclear forces from QCD
- Lattice effective field theory
- Wavefunction matching method
- Alpha-carbon scattering
- Neutron-alpha scattering
- Three-nucleon forces
- Nuclear thermodynamics
- Summary



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).

The nuclear interactions as a series of increasing complexity:

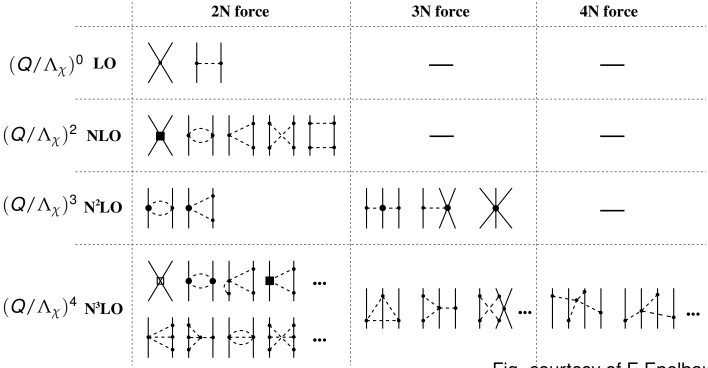


Fig. courtesy of E.Epelbaum

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 formulation of chiral EFT

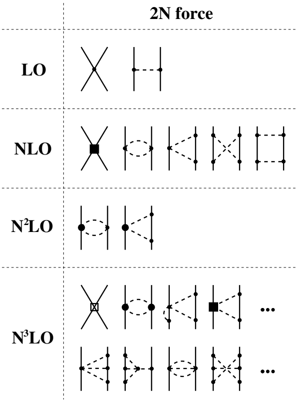
- Lattice formulation of nuclear forces in the framework of chiral EFT:
  - a simpler decomposition into spin channels
  - accurate phase shifts and binding energies.

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

$$\times \langle SS'_z, L'L'_z | JJ_z \rangle \left[a(\mathbf{n})\ \nabla^{2M}\ R^{*}_{L',L'_z}(\nabla)\ a(\mathbf{n}) \right]^{s_{NL}}_{S,S'_z,I,I_z}$$

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

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



LO ⟺ $V_{0,{}^1S_0}$ $V_{0,{}^3S_1}$

NLO ⟺ $V_{2,{}^1S_0}$ $V_{2,{}^3S_1}$ $V_{2,{}^3SD}$

$V_{2,{}^1P_1}$ $V_{2,{}^3P_0}$ $V_{2,{}^3P_1}$ $V_{2,{}^3P_2}$

N²LO, N³LO }

$V^{(1)}_{4,{}^1S_0}$ $V^{(2)}_{4,{}^1S_0}$ $V^{(1)}_{4,{}^3S_1}$ $V^{(2)}_{4,{}^3S_1}$

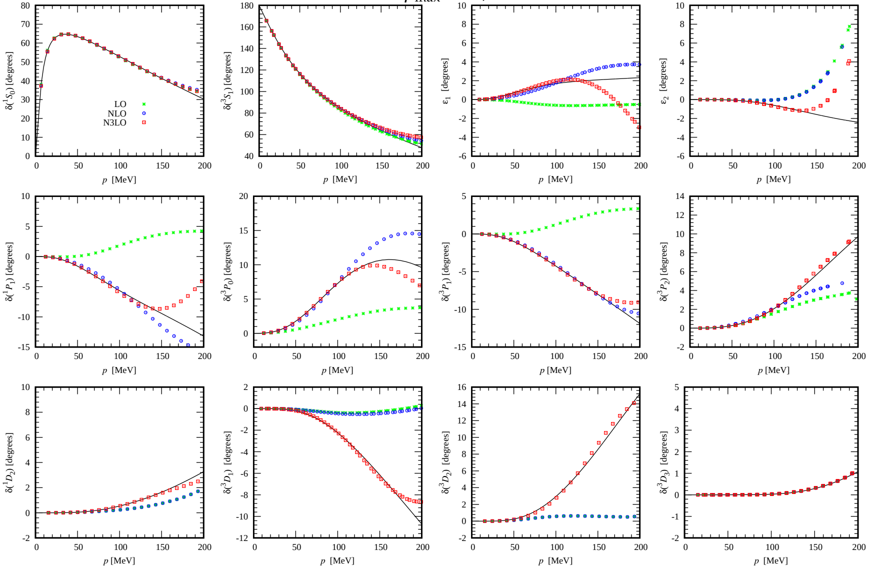
$V^{(1)}_{4,{}^3SD}$ $V^{(2)}_{4,{}^3SD}$

$V_{4,{}^1P_1}$ $V_{4,{}^3P_0}$ $V_{4,{}^3P_1}$ $V_{4,{}^3P_2}$ $V_{4,{}^3PF}$

$V_{4,{}^1D_2}$ $V_{4,{}^3D_1}$ $V_{4,{}^3D_2}$ $V_{4,{}^3D_3}$

Chiral EFT for nucleons: *NN* scattering phase shifts

$a = 1.97$ fm and $p_{\max} = \pi / a = 314$ MeV



SE FB22 2018. Springer Proceedings in Physics, (2020)

Lattice Monte Carlo calculations: Euclidean time projection

Non-perturbative leading order calculations

A given initial state, $|\psi_I\rangle$, as a Slater determinant of free-particle standing waves on the lattice, is projected to evaluate a product of a string of transfer matrices $\hat{M}$.

$$\lim_{L_t\to\infty} \frac{\langle\psi_I| \quad \hat{M} \quad \hat{M} \quad \ldots \quad H_{\rm LO} \quad \ldots \quad \hat{M} \quad \hat{M} \quad |\psi_I\rangle}{\langle\psi_I| \quad \hat{M} \quad \hat{M} \quad \ldots \quad \hat{M} \quad \hat{M} \quad |\psi_I\rangle} = E_{\rm LO}$$

In the limit of large Euclidean time the evolution operator the signal beyond the low-lying states is suppressed, and the ground state energy can be extracted.

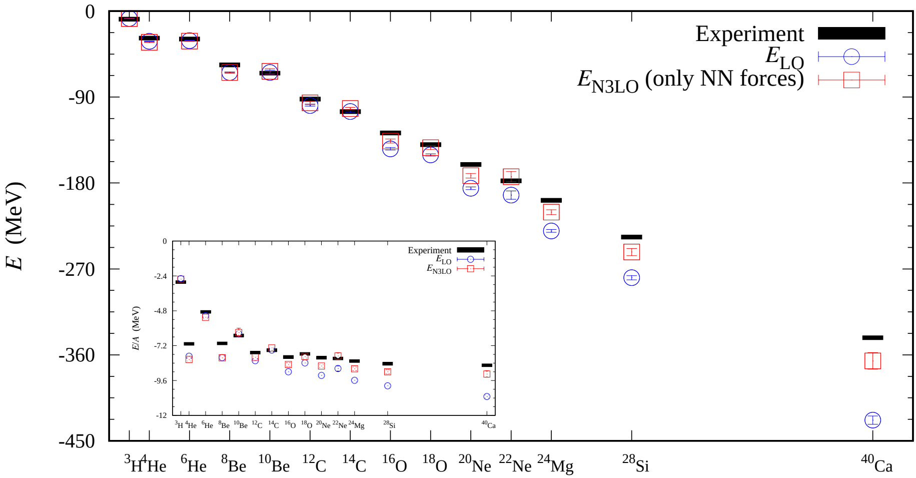
Perturbative higher order calculations

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

The higher order corrections to the ground state energy can be computed as,

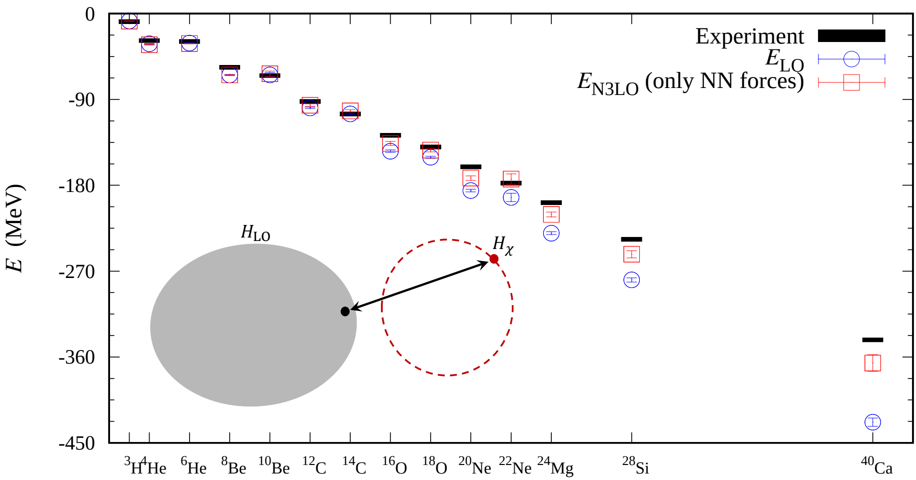
$$\lim_{L_t\to\infty} \frac{\langle\psi_I| \quad \hat{M} \quad \hat{M} \quad \ldots \quad H_{\rm ho} \quad \ldots \quad \hat{M} \quad \hat{M} \quad |\psi_I\rangle}{\langle\psi_I| \quad \hat{M} \quad \hat{M} \quad \ldots \quad \hat{M} \quad \hat{M} \quad |\psi_I\rangle} = \Delta E_{\rm ho}$$

$a = 1.97$ fm and $p_{\max} = \pi/a = 314$ MeV



SE FB22 2018. Springer Proceedings in Physics, (2020)

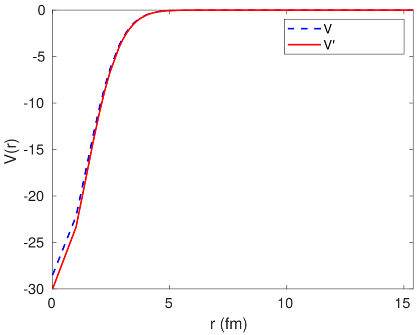
$a = 1.97$ fm and $p_{\max} = \pi / a = 314$ MeV

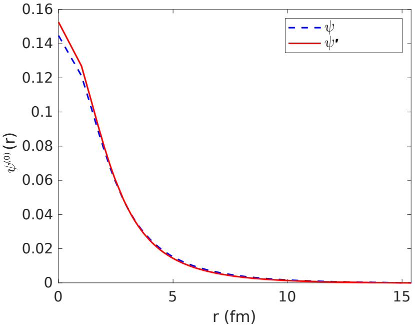


SE FB22 2018. Springer Proceedings in Physics, (2020)

Perturbative calculations

Toy model:



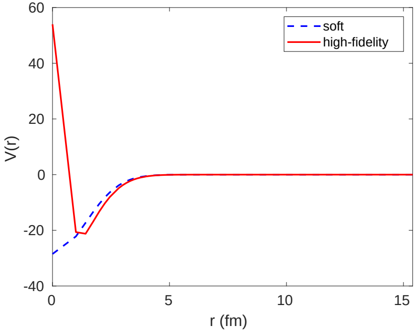


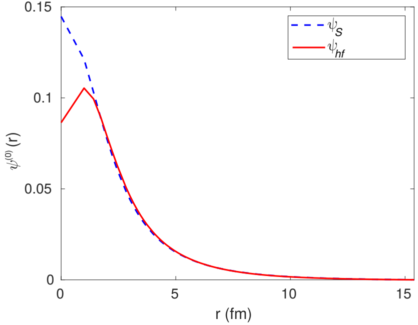
E	E'
−2.010472457971	−2.445743725635
1.775231321023	1.721517536958
6.206769197086	6.118307106128
12.776191791947	12.667625238436
21.337188185570	21.213065578266

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

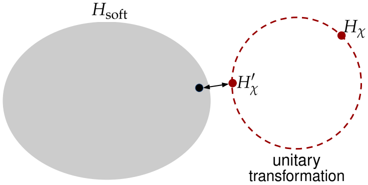
Perturbative energies	
q	$\langle \psi_S^{(0)} \| H \| \psi_S^{(q)} \rangle$
0	−1.74722993
1	−2.89957307
2	−2.10036797
3	−2.26376481

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

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

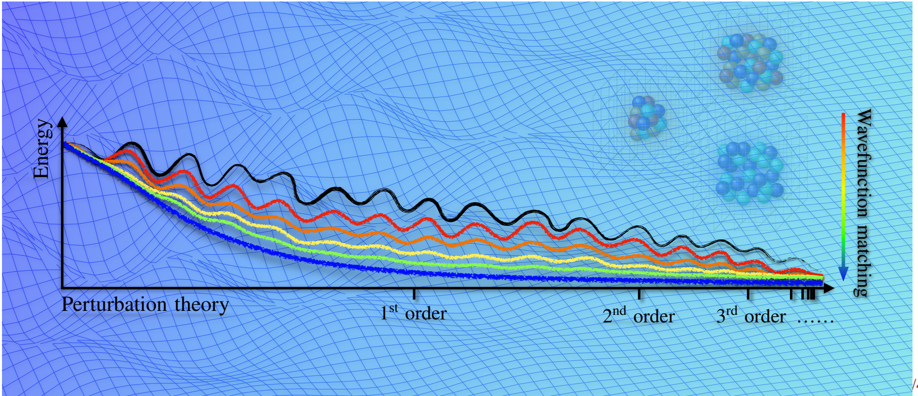
SE et al. *Nature* 630, 8015, 59-63 (2024)

- ☐ H_{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

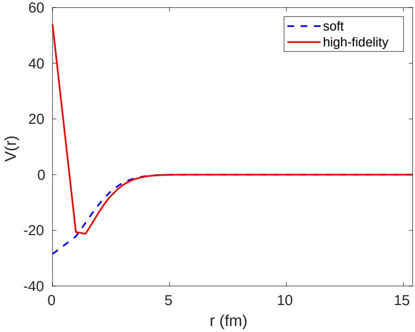
$$H'_{\chi} = U^{\dagger} H_{\chi} U \quad \rightarrow \quad H'_{\chi} = H_{\mathrm{soft}} + \boxed{(H'_{\chi} - H_{\mathrm{soft}})}$$

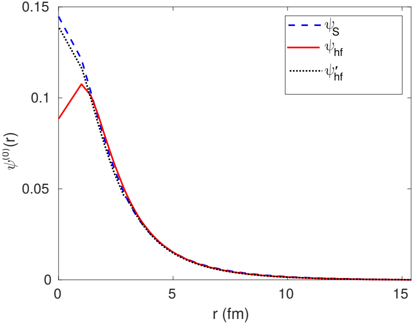
SE et al. *Nature* 630, 8015, 59-63 (2024)



Wavefunction Matching: Perturbative calculations

Toy model:

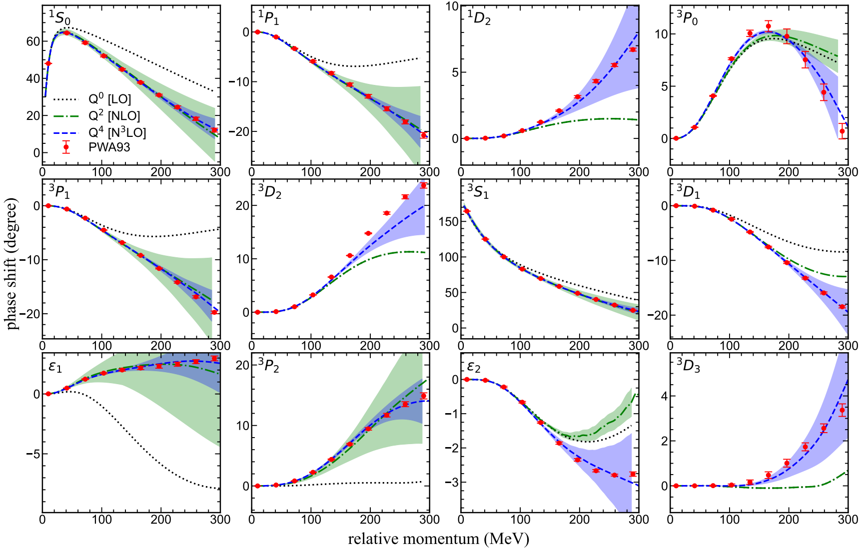




$E_{\rm hf}$	$E'_{\rm hf}$
−2.444693273	−2.444693273
1.769682286	1.769682286
6.282284485	6.282284485
13.008087181	13.008087181
21.786534446	21.786534446

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

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

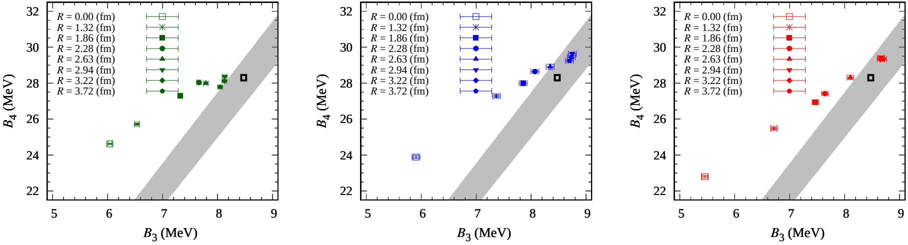


SE et al. *Nature* 630, 8015, 59-63 (2024)

Ab initio nuclear theory: recent progress in NLEFT

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

Nuclei	B_{Q^0} MeV	B_{Q^2} MeV	B_{Q^4} MeV	Experiment
$E_{\chi,\text{d}}$	1.7928	2.1969	2.2102	2.2246
$\langle\psi^0_{\text{soft}}\vert\, H_{\chi,\text{d}}\, \vert\psi^0_{\text{soft}}\rangle$	0.4494	0.3445	0.6208	
$\langle\psi^0_{\text{soft}}\vert\, H'_{\chi,\text{d}}\, \vert\psi^0_{\text{soft}}\rangle$	1.6496	1.9772	2.0075	



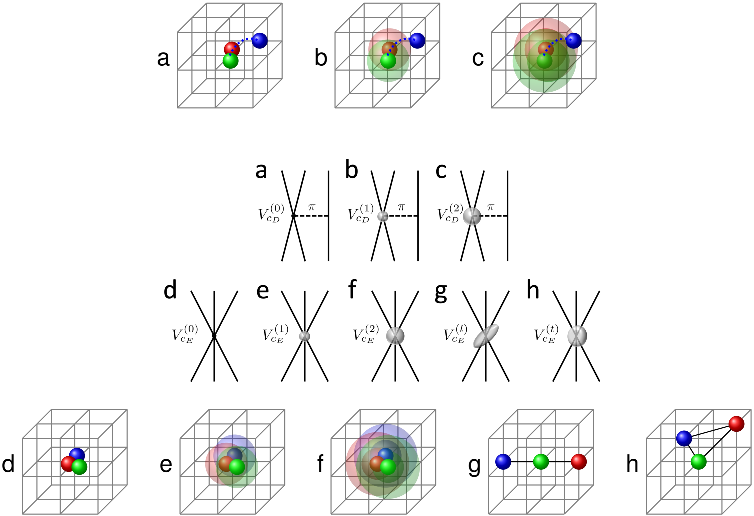
SE et al. *Nature* 630, 8015, 59-63 (2024)

Chiral interactions at N3LO – 2NFs + 3NFs

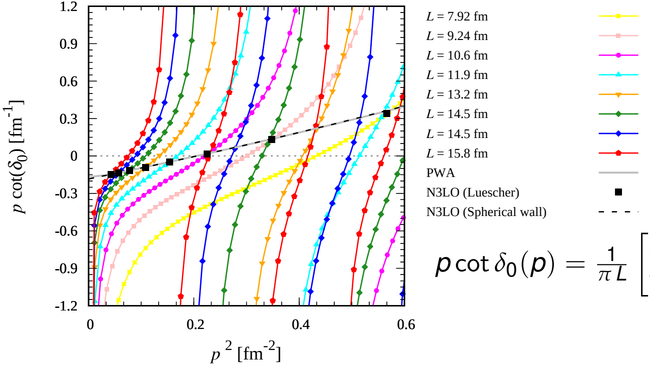
Work	Constraints	Predictions
NCSM, Barrett *et al.*, Nogga *et al.*	BE of ^{3}H and ^{4}He	Spectrum of ^{6}Li and ^{7}Li
NCSM, Navratil *et al.*	^{3}H, ^{6}Li, ^{10}B, ^{12}C	^{4}He, ^{6}Li, ^{10,11}B, ^{12,13}C
NCSM, Maris *et al.*, Roth *et al.*	BE of ^{3}H and ^{3}H β decay	Structures of $A = 7, 8$. ^{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
MBPT, Bogner *et al.*, Hebeler *et al.*, Drischler *et al.*, Wienholtz *et al.*, Simonis *et al.*	BE ^{3}H and R_c of ^{4}He	symmetric and asymmetric NM, BE of $^{48-58}$Ca, spectrum of *sd*-shell nuclei with $8 \leq Z, N \leq 20$, BE and R_c of open- and closed-shell nuclei up to $A = 78$
NCCI, Epelbaum *et al.*, Maris *et al.*	BE of ^3H, *nd* spin-doublet scattering length and the *pd* differential cross section	the spectrum of light nuclei with A = 3–16, elastic *nd* scattering and in the deuteron breakup reactions, properties of the $A = 3, 4$ nuclei, and for spectra of p-shell nuclei up to $A = 16$, BE and R_c of the oxygen and calcium isotope chains
CC, Carlsson *et al.*, Ekström *et al.*, Hagen *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, symmetric nuclear matter, neutron skin of ^{48}Ca, structure of ^{78}Ni
NCSM, IM-SRC, IM-NCSM, Hüther *et al.*	BE of ^{3}H and ^{16}O	R_c and BE of ^{4}He, $^{14-26}$O, $^{36-52}$Ca and $^{48-78}$Ni, the spectrum of ^{7}Li, ^{8}Be, ^{9}Be and ^{10}B
CC, Jiang *et al.*	properties of $A \leq 4$	properties of nuclei from $A = 16 - 132$

Ab initio nuclear theory: recent progress in NLEFT

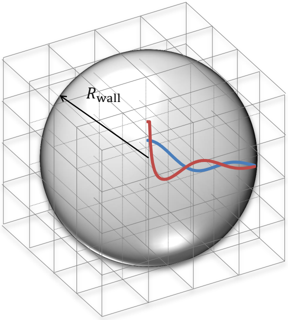
$a = 1.32$ fm and $p_{\max} = \pi / a = 471$ MeV



SE et al. *Nature* 630, 8015, 59-63 (2024)



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



Lüscher's finite volume method:

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

Spherical wall method:

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

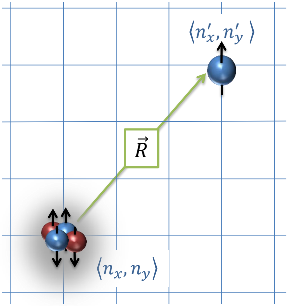
Nucl. Phys. A 424, 47-59 (1984), Eur. Phys. J. A 34, 185-196 (2007).

Scattering 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.

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



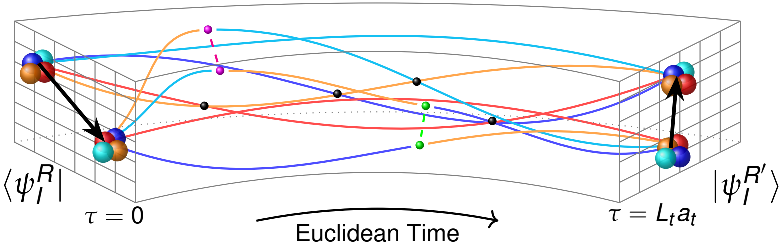
$$|\psi_I^R\rangle_\tau = e^{-H\tau}\,|\psi_I^R\rangle$$ dressed cluster state

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.

SE & Lee. *PRC* 90 064001 (2014).

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

SE, Lee, Meißner & Rupak *EPJA* 52, 6, 174 (2016).



Hamiltonian matrix

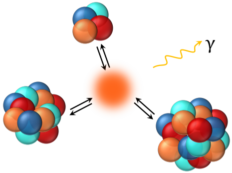
$$[H_\tau]^{J,J_z}_{R,R'} = {}^{J,J_z}_{\tau}\langle \psi_I^R | H | \psi_I^{R'} \rangle^{J,J_z}_{\tau}$$

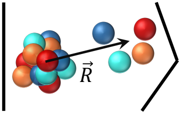
Norm matrix

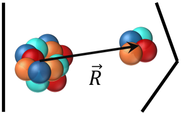
$$[N_\tau]^{J,J_z}_{R,R'} = {}^{J,J_z}_{\tau}\langle \psi_I^R | \psi_I^{R'} \rangle^{J,J_z}_{\tau}$$

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

Ab initio nuclear theory: alpha-Carbon scattering

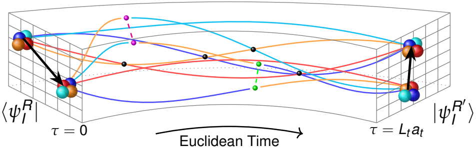


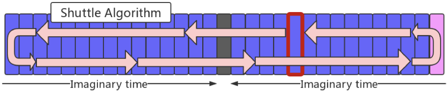
$$\left|\Psi_i^{^{16}\mathrm{O}}\right\rangle = \sum_{\vec{R}}$$ 

$$\left|\Psi_i^{^{16}\mathrm{A}}\right\rangle = \sum_{\vec{R}}$$ 

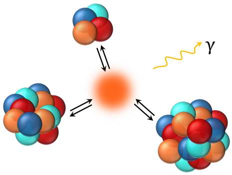
$$|\Psi_i\rangle \leftarrow |\Psi_i^{16\mathrm{O}}\rangle, \; |\Psi_i^{16A}\rangle$$

$$|\Psi_i\rangle = \theta(R-r)\,|\Psi_i^{16\mathrm{O}}\rangle + \theta(r-R)\,|\Psi_i^{16A}\rangle$$

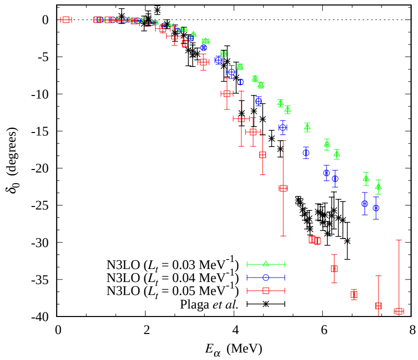


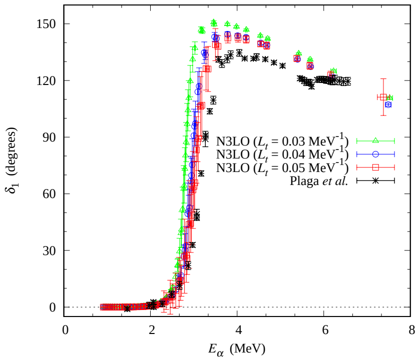


Ab initio nuclear theory: alpha-Carbon scattering



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

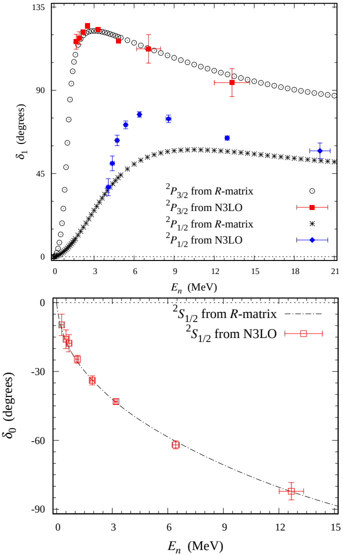


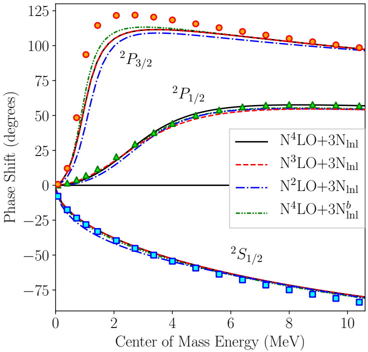


Work in progress.

Ab initio nuclear theory: neutron-alpha scattering

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

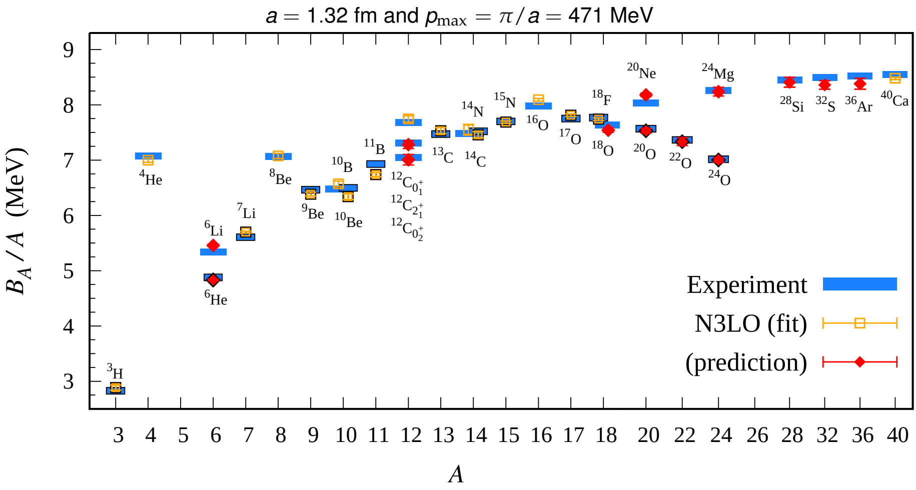




Kravvaris et al. PRC 102, 024616 (2020)

Work in progress.

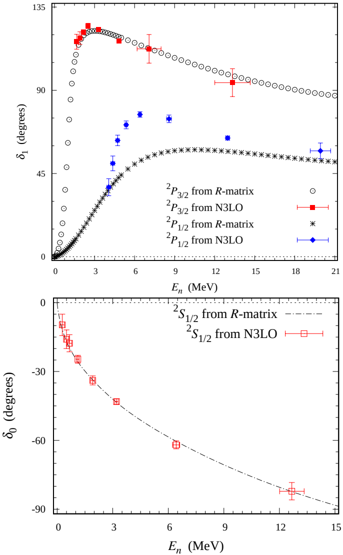
Ab initio nuclear theory: neutron-alpha scattering



SE et al. *Nature* 630, 8015, 59-63 (2024)

Ab initio nuclear theory: neutron-alpha scattering

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

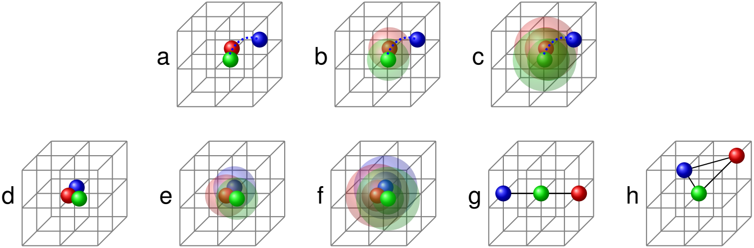


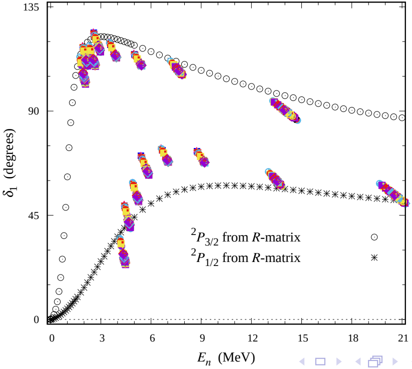
	N3LO	Experiment
^{9}Be, $\frac{3}{2}^-$	$-57.6(3)$	58.2
^{9}Be, $\frac{1}{2}^+$	$-58.2(1)$	56.5
^{9}Be, $\frac{1}{2}^-$	$-56.4(1)$	55.4

Shen et al. arXiv:2411.14935 (2024)

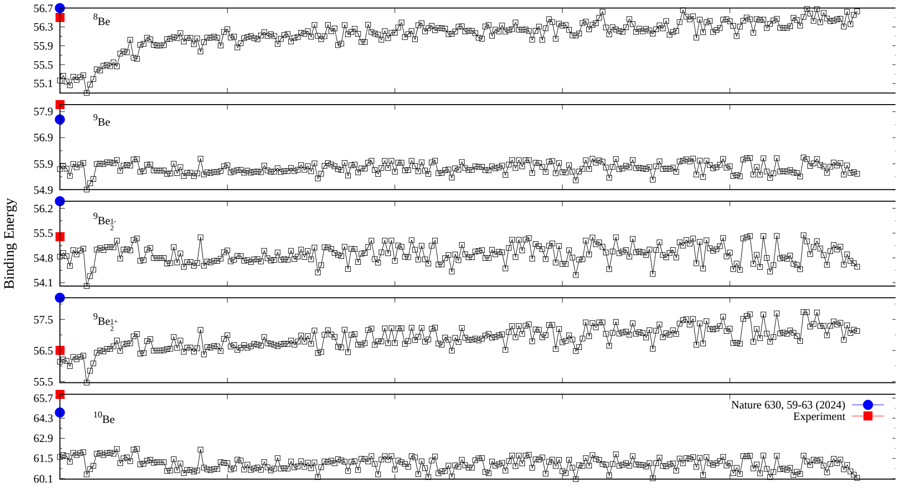
Work in progress.

Ab initio nuclear theory: neutron-alpha scattering



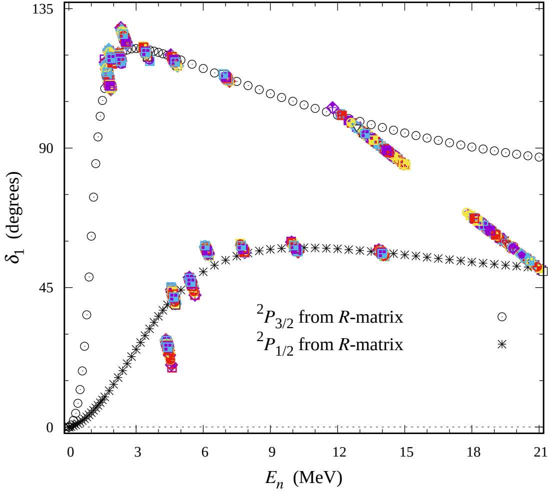


Ab initio nuclear theory: neutron-alpha scattering

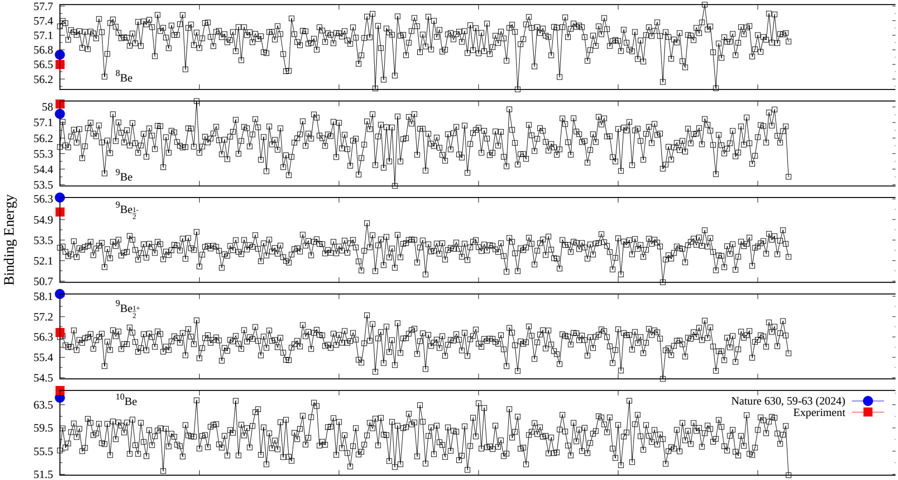


Ab initio nuclear theory: neutron-alpha scattering

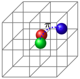
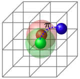
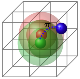
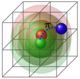
$V_{2,{}^1P_1}$, $V_{2,{}^3P_0}$, $V_{2,{}^3P_1}$, $V_{2,{}^3P_2}$, $V_{4,{}^1P_1}$, $V_{4,{}^3P_0}$, $V_{4,{}^3P_1}$, $V_{4,{}^3P_2}$, $V_{4,{}^3PF}$

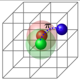
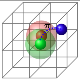
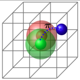


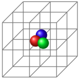
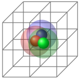
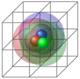
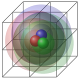
Ab initio nuclear theory: neutron-alpha scattering

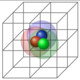
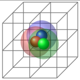
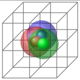


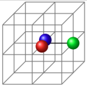
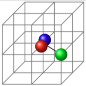
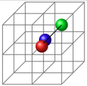
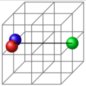
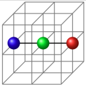
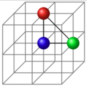
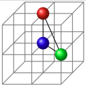
Ab initio nuclear theory: three-nucleon forces

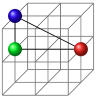
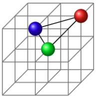
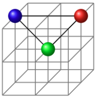
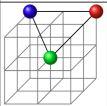
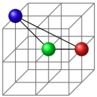
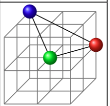
s_L / R_{s_L} (fm)	0.07 / 0.00	0.07 / 1.32	0.07 / 1.86	0.07 / 2.28
Shape				

s_{NL} / $R_{s_{NL}}$ (fm)	0.1 / 1.32	0.2 / 1.32	0.3 / 1.32
Shape			

s_L / R_{s_L} (fm)	0.07 / 0.00	0.07 / 1.32	0.07 / 1.86	0.07 / 2.28
Shape				

s_{NL} / $R_{s_{NL}}$ (fm)	0.1 / 1.32	0.2 / 1.32	0.3 / 1.32
Shape			

r_{RMS} (fm)	0.62	0.88	1.07	1.24	1.07	0.88	1.07
Shape							

r_{RMS} (fm)	1.39	1.07	1.24	1.39	1.24	1.39
Shape						

Ab initio nuclear theory: three-nucleon forces

The likelihood for the our model to be maximized is

$$\mathcal{L}(\vec{\beta}, \sigma^2) = \prod_{n \in \mathcal{S}_{\rm trn}} \frac{1}{(2\pi\sigma_n^2)^{1/2}} \exp\left\{ -\frac{1}{2\sigma_n^2} \left[z_n - z_{n,\rm NP}^{\rm theory} - \sum_{k \in \mathcal{F}_p} \beta_k \frac{\partial z_n^{\rm theory}}{\partial \beta_k} \right]^2 \right\},$$

Objective is to determine the optimal subsets $\mathcal{S}_{\rm trn}$ and $\mathcal{F}_p$, as well as regression coefficients $\vec{\beta}$.

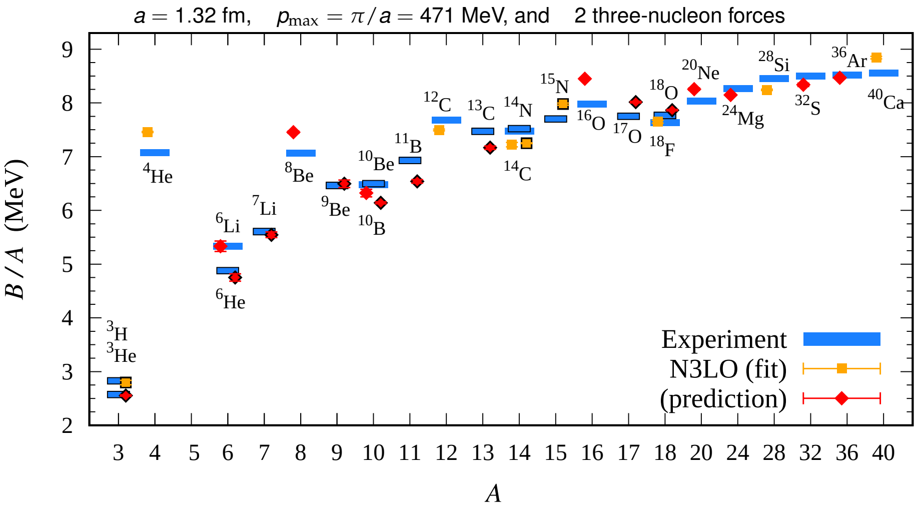
The acceptance probabilities for the new configurations $\mathcal{S}_{\rm trn}$ and $\mathcal{F}_p$,

$$\alpha_{\mathcal{S}} = \min\left(1, \frac{\mathcal{L}(\vec{\beta}', \sigma^2) q(\mathcal{S}'_{\rm trn}, \mathcal{F}_p | \mathcal{S}_{\rm trn}, \mathcal{F}_p)}{\mathcal{L}(\vec{\beta}, \sigma^2) q(\mathcal{S}_{\rm trn}, \mathcal{F}_p | \mathcal{S}'_{\rm trn}, \mathcal{F}_p)}\right), \quad \alpha_{\mathcal{F}_p} = \min\left(1, \frac{\mathcal{L}(\vec{\beta}', \sigma^2) q(\mathcal{S}_{\rm trn}, \mathcal{F}'_p | \mathcal{S}_{\rm trn}, \mathcal{F}_p)}{\mathcal{L}(\vec{\beta}, \sigma^2) q(\mathcal{S}_{\rm trn}, \mathcal{F}_p | \mathcal{S}_{\rm trn}, \mathcal{F}'_p)}\right).$$

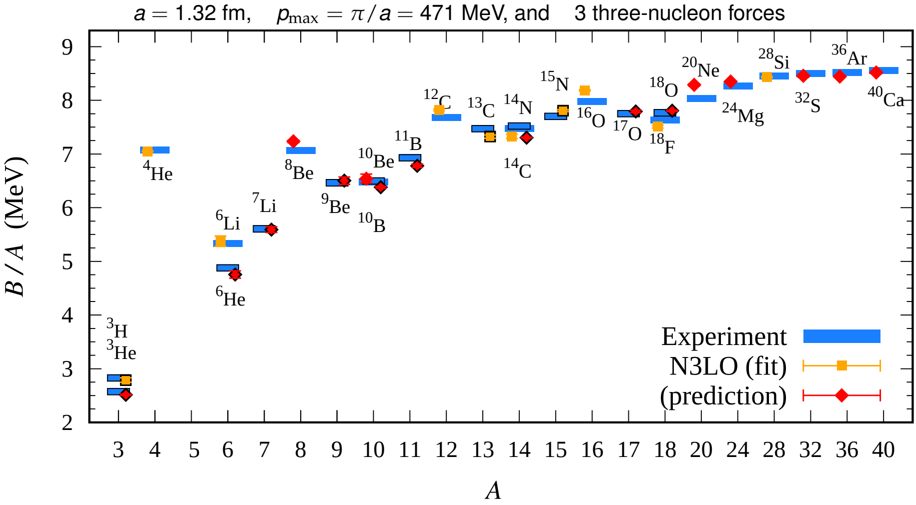
Then, evaluate the Root Mean Square Deviation (RMSD) as follows,

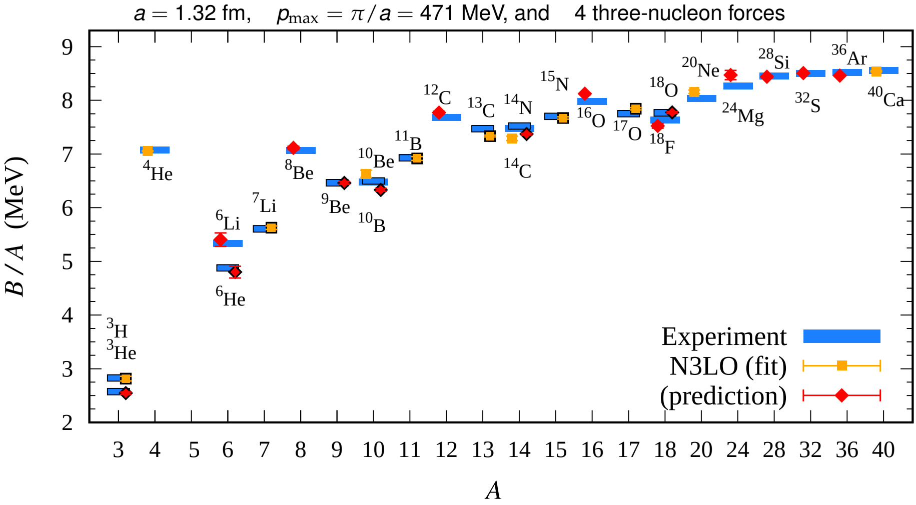
$$\mathrm{RMSD}(\mathcal{S}) = \sqrt{\frac{1}{M_{\mathcal{S}}} \sum_{i \in S} \left(\frac{z_i^{\rm theory} - z_i^{\rm exp}}{A_i} \right)^2}.$$

Ab initio nuclear theory: three-nucleon forces



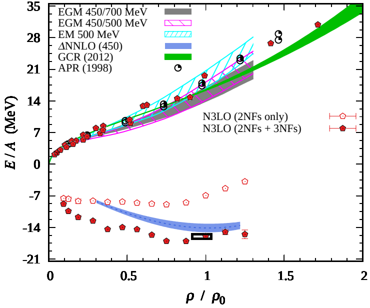
Ab initio nuclear theory: three-nucleon forces




a = 1.32 fm, p_max = π / a = 471 MeV, and 4 three-nucleon forces
B / A (MeV)
A
3H
3He
4He
6Li
6He
7Li
8Be
9Be
10Be
10B
11B
12C
13C
14N
14C
15N
16O
17O
18O
18F
20Ne
24Mg
28Si
32S
36Ar
40Ca
Experiment
N3LO (fit)
(prediction)

Ab initio nuclear theory: recent progress in NLEFT

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



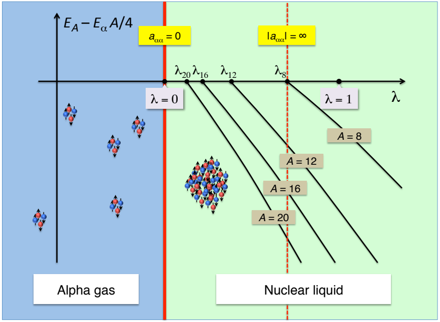
SE et al. *Nature* 630, 8015, 59-63 (2024)

The Equation of State (EoS) of nuclear matter:

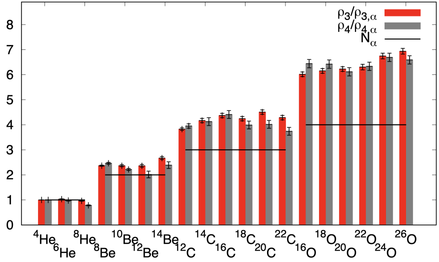
- Plays a fundamental role in understanding the structure and dynamics of neutron stars, the early universe, and heavy-ion collisions.
- Governs the behavior of nuclear matter under extreme conditions of density and temperature.

The challenge is to accurately capture **strong correlations** and **nuclear clustering** while overcoming sign problems and computational limitations, particularly at **finite temperature**.

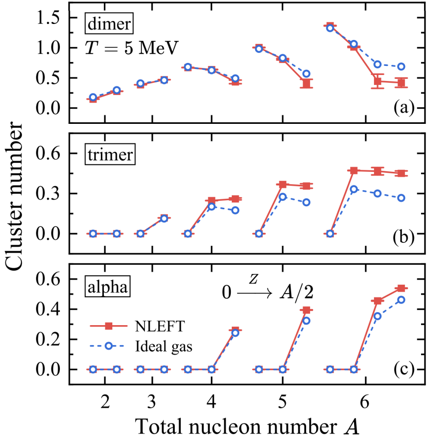
Ab initio nuclear theory: nuclear clustering



SE et al. *PRL* 117, 132501 (2016)



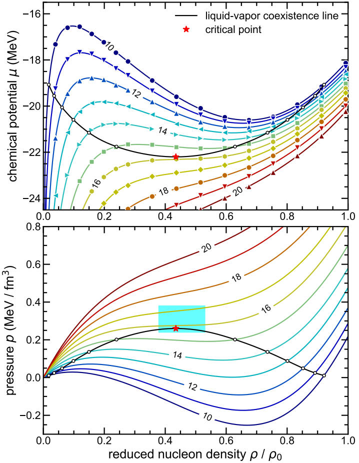
SE et al. *PRL* 119, 222505 (2017)



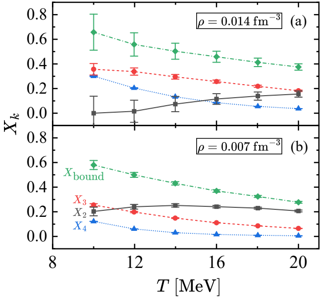
Ren et al. *PLB* 850 (2024) 138463

Ab-initio nuclear thermodynamics using NLEFT

- Pinhole Trace Algorithm (PTA): A novel approach enabling simulations of nuclear matter at nonzero temperature with a computational speed-up by orders of magnitude over grand canonical methods.



- First-principles calculations of nuclear thermodynamics using NLEFT.
- First-principles study of nuclear clustering in hot dilute nuclear matter.



Ren et al. PLB 850, 138463 (2024)

Lu et al. *Phys. Rev. Lett.* 125, 192502 (2020)

Ab initio nuclear theory: recent progress in NLEFT

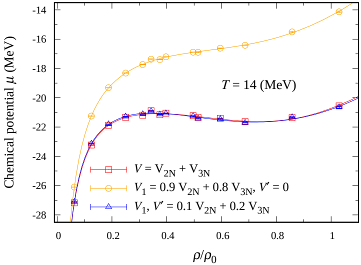
Work in progress.

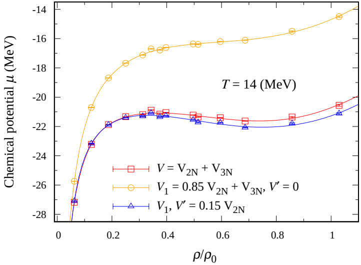
$$\mu = \frac{T}{2} \ln \left[A(A+1) \frac{\langle \mathcal{B}_{-1} \rangle_\Omega}{\langle \mathcal{B}_1 \rangle_\Omega} \right]$$

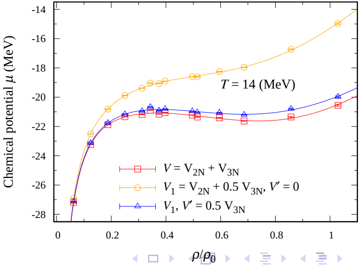
$$\mathcal{B}_1 = \sum_{c'} \langle \vec{c} \cup c' | M(s_{L_t}) \ldots M(s_1) | \vec{c} \cup c' \rangle \, / P(\vec{s}, \vec{c})$$

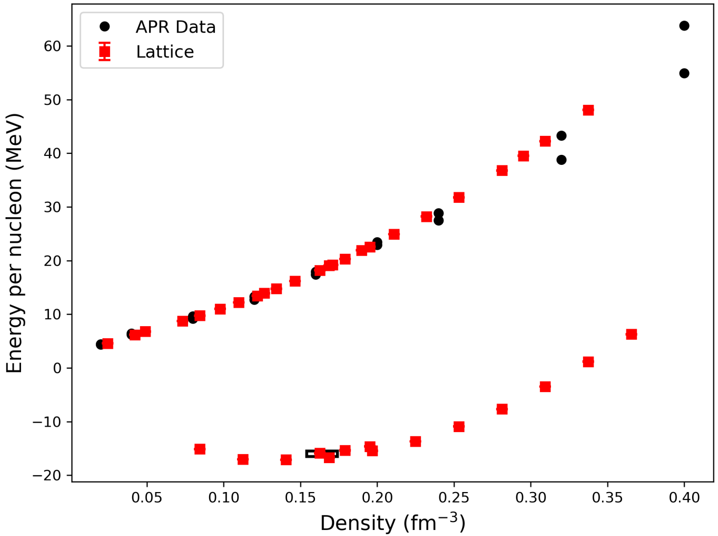
$$\mathcal{B}_{-1} = \sum_{c_i} \langle \vec{c} \setminus c_i | M(s_{L_t}) \ldots M(s_1) | \vec{c} \setminus c_i \rangle \, / P(\vec{s}, \vec{c})$$

$$\mathcal{B}_{\pm 1} = \frac{\mathcal{B}^{(0)}_{\pm 1}}{\mathcal{M}^{(0)}} + \frac{\mathcal{B}^{(1)}_{\pm 1}}{\mathcal{M}^{(0)}} - \frac{\mathcal{B}^{(0)}_{\pm 1} \mathcal{M}^{(1)}}{\mathcal{M}^{(0)} \mathcal{M}^{(0)}} + \mathcal{O}\left[(\mathcal{M}^{(1)})^2 \right]$$









Work 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.

- The wave function matching method offers rapid convergence in perturbation theory for many-body nuclear systems. It enables accurate calculations of nuclear binding energies, neutron matter, symmetric nuclear matter, and charge radii, all in excellent agreement with experimental data.

- The collaboration is advancing nuclear theory by performing calculations for nuclear structure, scattering and reactions.

- Our recent calculations will be complemented by improvements to nuclear forces on the lattice, such as including the explicit incorporation of the two-pion exchange potentials and more.

Thanks!