Nuclear Lattice EFT with Wave Function Matching for Light Nuclei

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— NLEFT collaboration —

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RUHR UNIVERSITÄT BOCHUM RUB

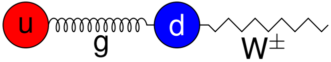
Workshop on Light Nuclei between
Single-Particle and Clustering Features

CEA-Saclay, Gif-sur-Yvette, France
3-6 December 2024

Light Nuclei Workshop CEA Paris-Saclay 2024

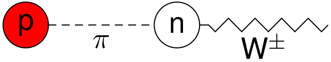
What is nuclear lattice effective field theory (EFT)?

QCD



non-perturbative for nuclei
⇒ take only symmetries

chiral EFT



continuum EFT: [E. Epelbaum et al. (2009)], [R. Machleidt, D. R. Entem (2011)]

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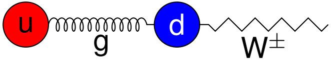

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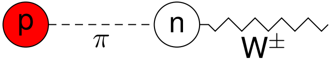
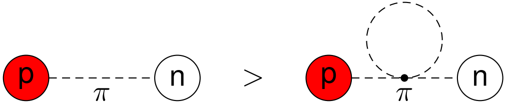


∞ many terms
$\Rightarrow$ power counting of
m_π, $\vec{p}_\pi$, m_{N}^{-1}, $\vec{p}_{\mathrm{N}}$, e,
$(m_{\mathrm{u}} - m_{\mathrm{d}})/(m_{\mathrm{u}} + m_{\mathrm{d}})$

expansion of nuclear Hamiltonian/current

no ∞ many terms at each order



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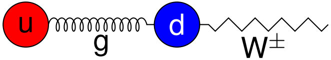

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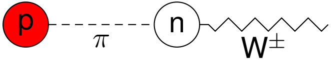

∞ many terms
⇒ power counting of
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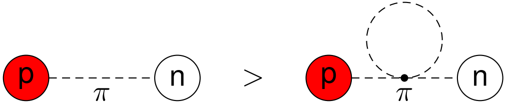
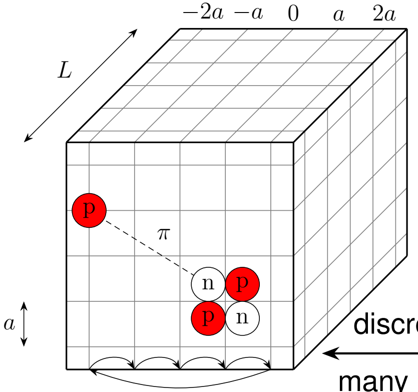


discretize for
many nucleons

nuclear lattice EFT (≠ lat. QCD)



continuum EFT: [E. Epelbaum et al. (2009)], [R. Machleidt, D. R. Entem (2011)]; lattice EFT: [D. Lee (2009)], [T. A. Lähde, Ulf-G. Meißner (2019)]

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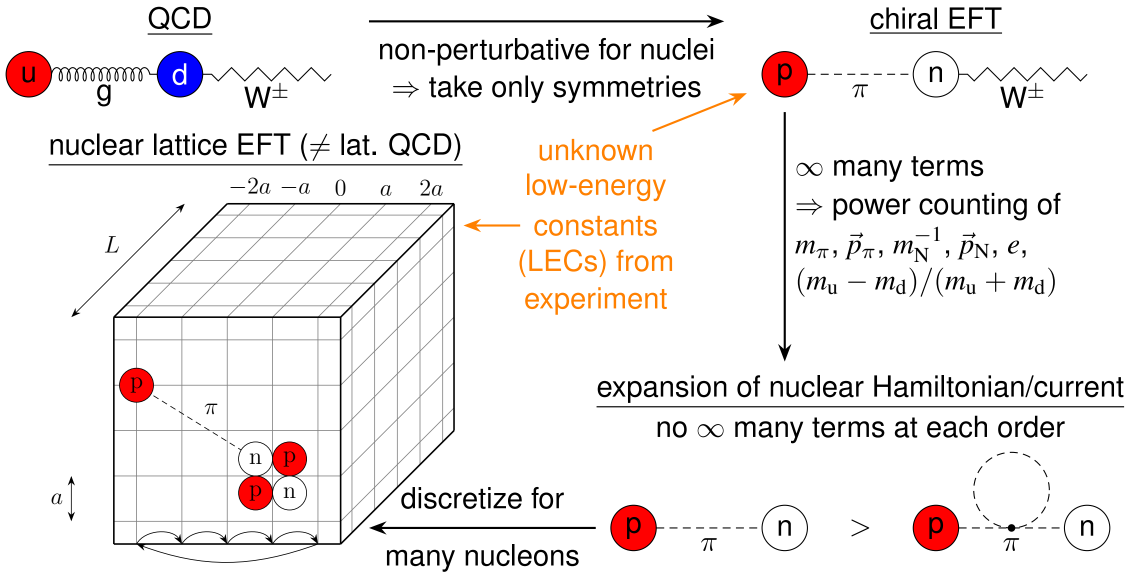

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Outline

PhD thesis

Non-perturbative three-nucleon simulation using chiral lattice EFT

Lukas Bovermann,[a,*] Evgeny Epelbaum,[a] Hermann Krebs[a] and Dean Lee[b]

[LB et al. (arXiv 2024)]

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Wave function matching for improvement of perturbation theory using unitary transformations

[LB (chapter of PhD thesis in progress)]

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from benchmark model to nuclei

papers based on WFM

Wavefunction matching for solving quantum many-body problems

https://doi.org/10.1038/s41586-024-07422-z

Received: 23 November 2022

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Serdar Elhatisari[1,2], Lukas Bovermann[3], Yuan-Zhuo Ma[4,5], Evgeny Epelbaum[3], Dillon Frame[6,7], Fabian Hildenbrand[6,7], Myungkuk Kim[8], Youngman Kim[8], Hermann Krebs[3], Timo A. Lähde[6,7], Dean Lee[4,✉], Ning Li[9], Bing-Nan Lu[10], Ulf-G. Meißner[2,6,7,11], Gautam Rupak[12], Shihang Shen[6,7], Young-Ho Song[13] & Gianluca Stellin[14]

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The triton lifetime from nuclear lattice effective field theory

Serdar Elhatisari [a,b,c], Fabian Hildenbrand [d,*], Ulf-G. Meißner [c,d,e]

[S. Elhatisari et al. (PLB 2024)]

use potential (fitted for $A \geq 3$) non-perturbatively for $A = 3$

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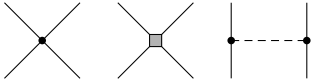
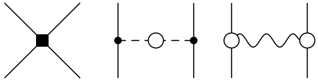
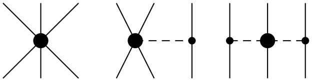
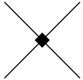
1. Non-perturbatively fitted potential for $A = 3$

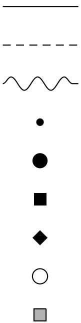
Non-perturbative three-nucleon simulation using chiral lattice EFT

Lukas Bovermann,[a,*] **Evgeny Epelbaum,**[a] **Hermann Krebs**[a] **and Dean Lee**[b]

[LB et al. (arXiv 2024)]

Few-nucleon Hamiltonian

	2NF (two-nucleon force)	3NF
leading order (LO)		
next-to-LO (NLO)		
N^2LO		
N^3LO		



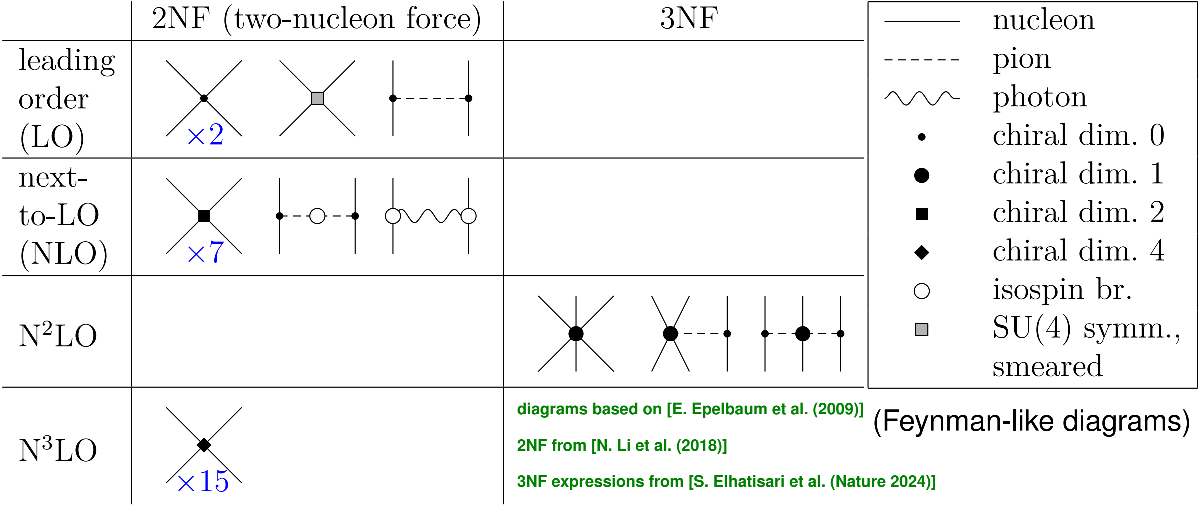
(Feynman-like diagrams)

diagrams based on [E. Epelbaum et al. (2009)]

2NF from [N. Li et al. (2018)]

3NF expressions from [S. Elhatisari et al. (Nature 2024)]

Few-nucleon Hamiltonian



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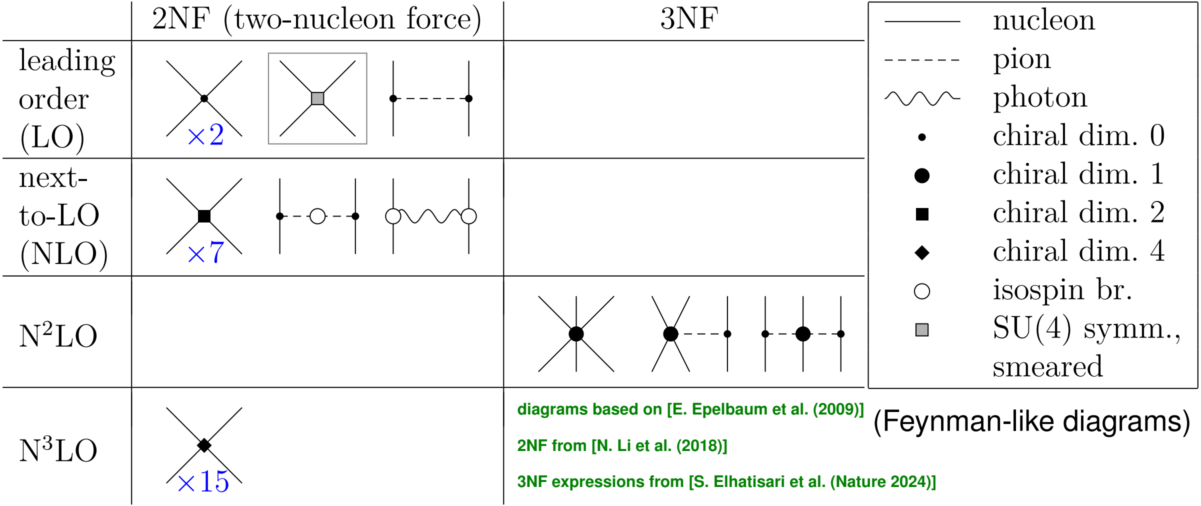
tuned to NN phase shifts, mixing angles & deuteron ground state (GS) energy;

Few-nucleon Hamiltonian



(Feynman-like diagrams)

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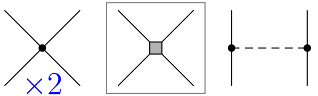
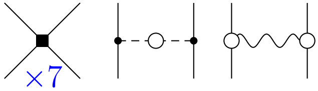
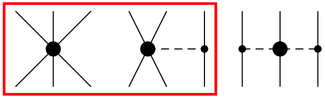
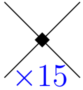
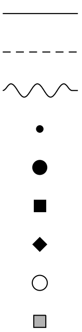
leading order (LO)		
next-to-LO (NLO)		LEC c_E LEC c_D
N^2LO		
N^3LO		diagrams based on [E. Epelbaum et al. (2009)] 2NF from [N. Li et al. (2018)] 3NF expressions from [S. Elhatisari et al. (Nature 2024)]



- nucleon
- pion
- photon
- chiral dim. 0
- chiral dim. 1
- chiral dim. 2
- chiral dim. 4
- isospin br.
- SU(4) symm., smeared

(Feynman-like diagrams)

tuned to NN phase shifts, mixing angles & deuteron ground state (GS) energy; redundant for 3N; tuned to triton GS energy & half-life;

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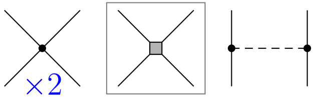
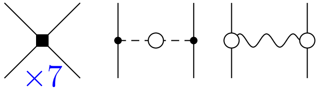
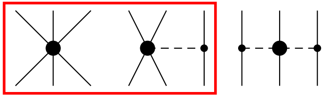
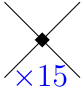
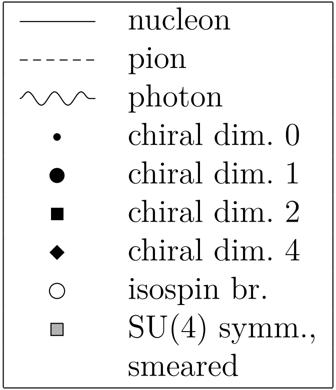
leading order (LO)		
next-to-LO (NLO)		LEC c_E LEC c_D
N^2LO		
N^3LO		



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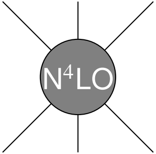
tuned to NN phase shifts, mixing angles & deuteron ground state (GS) energy; redundant for 3N; tuned to triton GS energy & half-life; rest well-known ($\pi \to W^{\pm}$, $N \to \pi N$, $\pi N \to \pi N$)

well-known e.g. from [P. Reinert et al. (2018)] and [M. Hoferichter et al. (2015)]

Few-nucleon observables

- considered sources of uncertainty:



truncation of chiral expansion
(error estimated based
on available lower orders)

Epelbaum-Krebs-Meißner approach [EKM (EPJA 2015)]

[EKM (PRL 2015)] [N. Li et al. (2018)] [E. Epelbaum (2019)]

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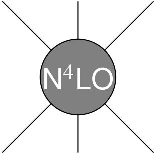

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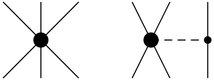

fitting of self-determined
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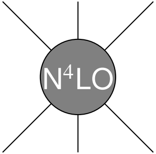

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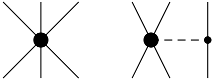

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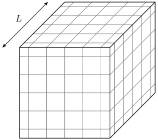

$(a = 2\ \mathrm{fm})$

energy extrap. for $L \to \infty$

[Ulf-G. Meißner et al. (2015)]

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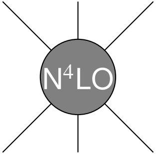
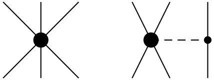


add truncation error and fitting errors in quadrature

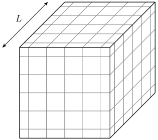
truncation of chiral expansion (error estimated based on available lower orders)

Epelbaum-Krebs-Meißner approach [EKM (EPJA 2015)]

[EKM (PRL 2015)] [N. Li et al. (2018)] [E. Epelbaum (2019)]



fitting of self-determined LECs c_E and c_D (error estimated based on bisection method)



$(a = 2 \text{ fm})$

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[Ulf-G. Meißner et al. (2015)]

(truncation error propagated via statistical sampling)

Few-nucleon observables

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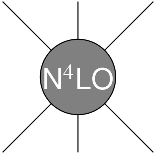

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truncation of chiral expansion (error estimated based on available lower orders)

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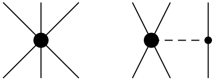
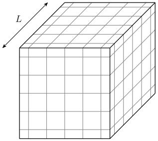


fitting of self-determined LECs c_E and c_D (error estimated based on bisection method)



$(a = 2\ \mathrm{fm})$

energy extrap. for $L \to \infty$

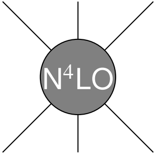
[Ulf-G. Meißner et al. (2015)]

(truncation error propagated via statistical sampling)

- lowest Hamiltonian eigenenergy from Lanczos alg. [C. Lanczos (1950)] [G. Stellin et al. (2018)]

Few-nucleon observables

- considered sources of uncertainty:



add truncation error and fitting errors in quadrature

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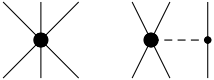

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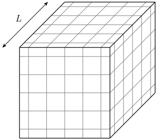

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[Ulf-G. Meißner et al. (2015)]

(truncation error propagated via statistical sampling)

- lowest Hamiltonian eigenenergy from Lanczos alg. [C. Lanczos (1950)] [G. Stellin et al. (2018)]

	$-E_{^3\mathrm{H}}$ [MeV]	$-E_{^3\mathrm{He}}$ [MeV]
experiment	$8.481795(2)$	$7.718040(2)$
	[M. Wang et al. (2017)]	
$A = 3$-fit	$8.48(7)$ fit	$7.73(7)$

Few-nucleon observables

- ground-state wave functions $\psi_{3\mathrm{H}}$, $\psi_{3\mathrm{He}}$ for $L = 18$ fm using Lanczos algorithm

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a few % too small (two-nucleon vector current may cure this [D. Möller (2024)])

	$-E_{3H}$ [MeV]	$-E_{3He}$ [MeV]	$R_{\text{ch},3H}$ [fm]	$R_{\text{ch},3He}$ [fm]
experiment	$8.481795(2)$	$7.718040(2)$	$1.7591(363)$	$1.9661(30)$
	[M. Wang et al. (2017)]		[I. Angeli, K. P. Marinova (2013)]	
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- half-life of triton beta decay: [A. Baroni et al. (2016)] [R. Schiavilla et al. (1998)] [S. Raman et al. (1978)]

$$t_{1/2} = \frac{1}{1 + \delta_{\mathrm{R}}} \frac{K/G_{\mathrm{V}}^2}{f_{\mathrm{V}} \langle \widehat{\mathbf{F}} \rangle^2 + f_{\mathrm{A}} g_{\mathrm{A}}^2 \langle \widehat{\mathbf{GT}} \rangle^2}$$

	$-E_{3\mathrm{H}}$ [MeV]	$-E_{3\mathrm{He}}$ [MeV]	$R_{\mathrm{ch},3\mathrm{H}}$ [fm]	$R_{\mathrm{ch},3\mathrm{He}}$ [fm]
experiment	$8.481795(2)$	$7.718040(2)$	$1.7591(363)$	$1.9661(30)$
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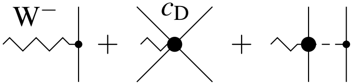

$$|| \psi_{3\mathrm{H}} \rangle + \mathcal{O}(\mathrm{N^3LO})$$

diagrams for nuclear axial current based on [H. Krebs et al. (2017)]

	$-E_{3\mathrm{H}}$ [MeV]	$-E_{3\mathrm{He}}$ [MeV]	$R_{\mathrm{ch,3H}}$ [fm]	$R_{\mathrm{ch,3He}}$ [fm]
experiment	$8.481795(2)$	$7.718040(2)$	$1.7591(363)$	$1.9661(30)$
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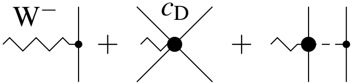

$+\mathcal{O}(\mathrm{N^3LO})$

diagrams for nuclear axial current based on [H. Krebs et al. (2017)]

	$-E_{3\mathrm{H}}$ [MeV]	$-E_{3\mathrm{He}}$ [MeV]	$R_{\mathrm{ch,3H}}$ [fm]	$R_{\mathrm{ch,3He}}$ [fm]	$t_{1/2}$ [yr]
experiment	$8.481795(2)$	$7.718040(2)$	$1.7591(363)$	$1.9661(30)$	$12.32(3)$
	[M. Wang et al. (2017)]		[I. Angeli, K. P. Marinova (2013)]		[J. J. Simpson (1987)]
$A = 3$-fit	$8.48(7)$ fit	$7.73(7)$	$1.695(10)$	$1.914(14)$	$12.31(10)$ fit

2. Wave function matching (WFM) benchmark

Wave function matching for improvement of perturbation theory using unitary transformations

[LB (chapter of PhD thesis in progress)]

Avoiding the sign problem

Monte Carlo (MC) simulations for $A > 3$

compute normal-ordered matrix element

$$\langle\psi| : e^{-L_t a_t \hat{H}} : |\psi\rangle$$

for L_t Euclidean time steps

of size a_t (cf. backup slide)

Avoiding the sign problem

Monte Carlo (MC) simulations for $A > 3$ ⟶ fermion sign problem

compute normal-ordered matrix element

$$\langle\psi| : e^{-L_t a_t \hat{H}} : |\psi\rangle$$

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of size a_t (cf. backup slide)

positive & negative

contributions cancel

for N[3]LO Hamiltonian $\hat{H}$

$\Rightarrow$ numerical inaccuracy

Avoiding the sign problem

Monte Carlo (MC) simulations for $A > 3$ → fermion sign problem

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contributions cancel

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$\Rightarrow$ numerical inaccuracy

↙

perturbation theory (PT)

using simple LO Hamiltonian $\hat{H}^{\mathrm{S}}$ instead (without severe sign problem)

$$\langle\psi_0|\hat{H}|\psi_0\rangle = \langle\psi_0^{\mathrm{S}}|\hat{H}^{\mathrm{S}}|\psi_0^{\mathrm{S}}\rangle + \langle\psi_0^{\mathrm{S}}|\hat{H} - \hat{H}^{\mathrm{S}}|\psi_0^{\mathrm{S}}\rangle + \mathcal{O}(\text{second order of PT})$$

for ground states $|\psi_0\rangle$, $|\psi_0^{\mathrm{S}}\rangle$ of $\hat{H}$, $\hat{H}^{\mathrm{S}}$

Avoiding the sign problem

Monte Carlo (MC) simulations for $A > 3$ → fermion sign problem

compute normal-ordered matrix element

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contributions cancel
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for ground states $|\psi_0\rangle$, $|\psi_0^{\mathrm{S}}\rangle$ of $\hat{H}$, $\hat{H}^{\mathrm{S}}$

but: slow convergence at first order

$$\langle\psi_0|\hat{H}|\psi_0\rangle \not\approx \langle\psi_0^{\mathrm{S}}|\hat{H}|\psi_0^{\mathrm{S}}\rangle$$

Avoiding the sign problem

Monte Carlo (MC) simulations for $A > 3$ ⟶ fermion sign problem

compute normal-ordered matrix element

$$\langle\psi| : e^{-L_t a_t \hat{H}} : |\psi\rangle$$

for L_t Euclidean time steps of size a_t (cf. backup slide)

positive & negative contributions cancel for N^{3}LO Hamiltonian $\hat{H}$

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using simple LO Hamiltonian $\hat{H}^{\mathrm{S}}$ instead (without severe sign problem)

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for ground states $|\psi_0\rangle$, $|\psi_0^{\mathrm{S}}\rangle$ of $\hat{H}$, $\hat{H}^{\mathrm{S}}$

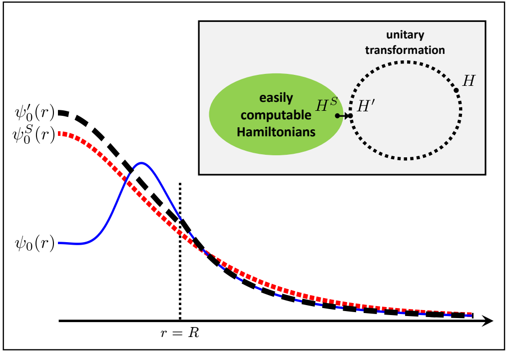
but: slow convergence at first order

$$\langle\psi_0|\hat{H}|\psi_0\rangle \not\approx \langle\psi_0^{\mathrm{S}}|\hat{H}|\psi_0^{\mathrm{S}}\rangle$$

$\Rightarrow$ wave function matching (WFM)

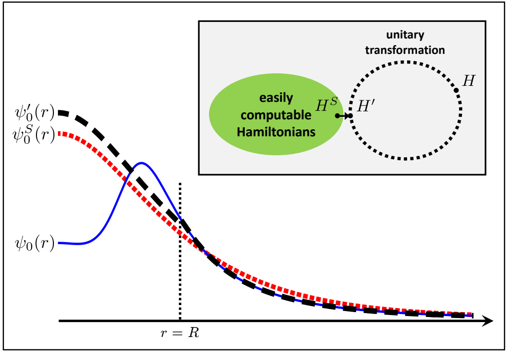
replace $\hat{H}$ by $\hat{H}'$ with $\langle\psi_0|\hat{H}|\psi_0\rangle \approx \langle\psi_0^{\mathrm{S}}|\hat{H}'|\psi_0^{\mathrm{S}}\rangle$

Avoiding the sign problem



[S. Elhatisari et al. (Nature 2024)]

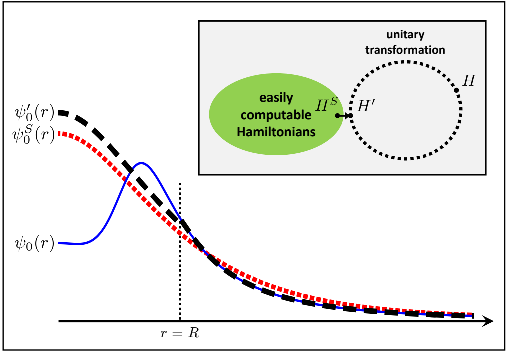
Avoiding the sign problem



[S. Elhatisari et al. (Nature 2024)]

- WFM: generate Hamiltonian
$$\hat{H}' = \hat{U}^\dagger \hat{H} \hat{U},$$
where unitary transformation $\hat{U}$ maps
$$|\psi_0^S\rangle \to |\psi_0\rangle \text{ (up to range } R)$$
while keeping phase shifts unchanged

Avoiding the sign problem



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  where unitary transformation $\hat{U}$ maps
  $$|\psi_0^{\rm S}\rangle \to |\psi_0\rangle \text{ (up to range } R)$$
  while keeping phase shifts unchanged

- H' has ground state
  $$|\psi_0'\rangle = \hat{U}^\dagger |\psi_0\rangle$$
  with
  $$\psi_0'(r \leq R) \propto \psi_0^{\rm S}(r \leq R),$$
  $$\psi_0'(r > R) = \psi_0(r > R)$$

Construction of unitary transformation (alternatives possible)

realistic Hamiltonian $\hat{H}$
eigenenergies E_n
eigenstates $|\psi_n\rangle$

simple Hamiltonian $\hat{H}^{\mathrm{S}}$
eigenenergies $E_{\mathrm{S},n}$
eigenstates $|\psi_n^{\mathrm{S}}\rangle$

$(n \in \{0, 1, \dots\})$

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eigenstates $|\psi_n^{\mathrm{S}}\rangle$

$(n \in \{0, 1, \ldots\})$

↓ take only normalized inner parts for $n = 0$ ↓

$|\psi_0\rangle_R$

$|\psi_0^{\mathrm{S}}\rangle_R$

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realistic Hamiltonian $\hat{H}$
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$|\psi_0\rangle_R$

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radial-coordinate states
$|r = 0\rangle, |r = a\rangle, \ldots$

[S. Elhatisari et al. (2015)] [B.-N. Lu et al. (2016)]

Construction of unitary transformation (alternatives possible)

realistic Hamiltonian $\hat{H}$
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[S. Elhatisari et al. (2015)] [B.-N. Lu et al. (2016)]

↓ Gram-Schmidt ↓ orthonormalization ↓

$$\{|\psi_0\rangle_R, |r = a\rangle_\perp, \ldots, |r = R\rangle_\perp\}, \{|\psi_0^{\mathrm{S}}\rangle_R, |r = a\rangle_\perp^{\mathrm{S}}, \ldots, |r = R\rangle_\perp^{\mathrm{S}}\}$$

Construction of unitary transformation (alternatives possible)

realistic Hamiltonian $\hat{H}$
eigenenergies E_n
eigenstates $|\psi_n\rangle$

simple Hamiltonian $\hat{H}^{\mathrm{S}}$
eigenenergies $E_{\mathrm{S},n}$
eigenstates $|\psi_n^{\mathrm{S}}\rangle$

$(n \in \{0, 1, \ldots\})$

take only normalized
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$|\psi_0\rangle_R$ $\qquad$ $|\psi_0^{\mathrm{S}}\rangle_R$

radial-coordinate states
$|r = 0\rangle, |r = a\rangle, \ldots$

[S. Elhatisari et al. (2015)] [B.-N. Lu et al. (2016)]

Gram-Schmidt $\quad$ orthonormalization

$$\{|\psi_0\rangle_R, |r = a\rangle_\perp, \ldots, |r = R\rangle_\perp\}, \{|\psi_0^{\mathrm{S}}\rangle_R, |r = a\rangle_\perp^{\mathrm{S}}, \ldots, |r = R\rangle_\perp^{\mathrm{S}}\}$$

unitary transformation $\hat{U}$

idea originated from [LB et al. (2022)]

with different $\hat{U}$ and purpose

(no action for $r > R$)

Benchmark check (using Lanczos algorithm)

- 3D benchmark: two scalar bosons with mass $m_{\mathrm{nucleon}} = 938.92\ \mathrm{MeV}$ [B. Borasoy et al. (2007)]

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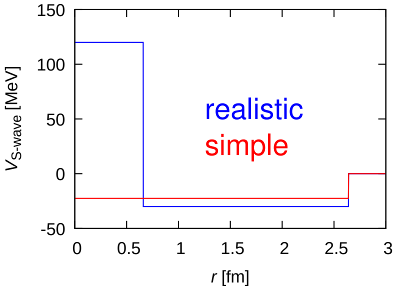

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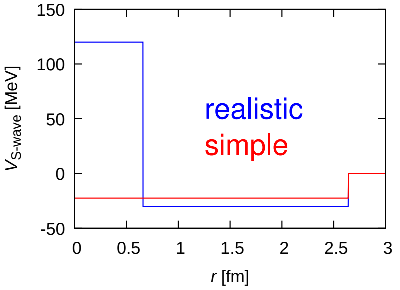

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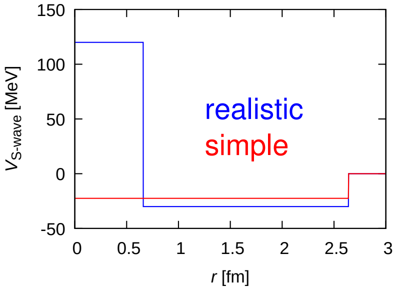
- center-of-mass system with S-wave projection [S. Elhatisari et al. (2015)] [B.-N. Lu et al. (2016)]



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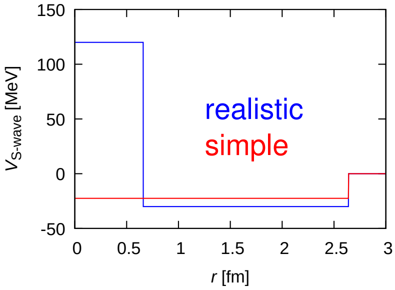
- WFM range: $R = \sqrt{2}a = 1.87\ \text{fm}$



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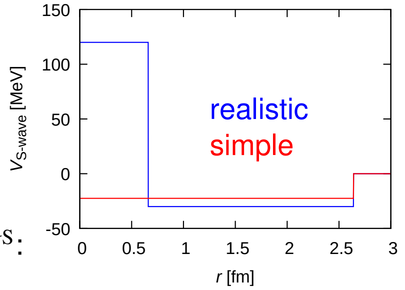
- WFM range: $R = \sqrt{2}a = 1.87\ \mathrm{fm}$
- test WFM with lowest eigenstates of $\hat{H}$ and $\hat{H}^S$:



n	$\langle \psi_n \vert \hat{H} \vert \psi_n \rangle$ [MeV]	$\langle \psi_n^S \vert \hat{H} \vert \psi_n^S \rangle$ [MeV]
0	-1.82870	-0.24118
1	0.50117	0.60504
2	1.91195	2.11690

- perturbation theory without WFM converges slowly

Benchmark check (using Lanczos algorithm)

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- lattice: $a = 1.32\ \text{fm}$, $L = 60a = 79.2\ \text{fm}$
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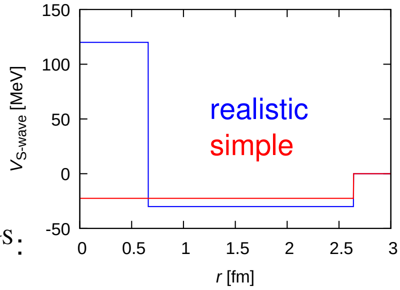

n	$\langle\psi_n\|\hat{H}\|\psi_n\rangle$ [MeV]	$\langle\psi_n^S\|\hat{H}\|\psi_n^S\rangle$ [MeV]	$\langle\psi_n^S\|\hat{H}'\|\psi_n^S\rangle$ [MeV]
0	-1.82870	-0.24118	-1.66531
1	0.50117	0.60504	0.49656
2	1.91195	2.11690	1.91403

- perturbation theory without WFM converges slowly
- single-state WFM moves perturbative energies much closer to realistic ones

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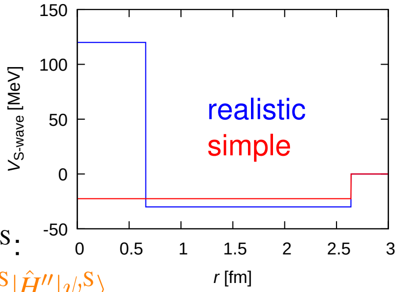

n	$\langle\psi_n\|\hat{H}\|\psi_n\rangle$ [MeV]	$\langle\psi_n^{\text{S}}\|\hat{H}\|\psi_n^{\text{S}}\rangle$ [MeV]	$\langle\psi_n^{\text{S}}\|\hat{H}'\|\psi_n^{\text{S}}\rangle$ [MeV]	$\langle\psi_n^{\text{S}}\|\hat{H}''\|\psi_n^{\text{S}}\rangle$ [MeV]
0	−1.82870	−0.24118	−1.66531	−1.66531
1	0.50117	0.60504	0.49656	0.49650
2	1.91195	2.11690	1.91403	1.91396

$\{|\psi_0\rangle_R, |\psi_1\rangle_{R\perp}, \ldots\}$

$\uparrow \hat{U}$

$\{|\psi_0^{\text{S}}\rangle_R, |\psi_1^{\text{S}}\rangle_{R\perp}, \ldots\}$

- perturbation theory without WFM converges slowly
- single-state WFM moves perturbative energies much closer to realistic ones
- only small improvement or even disimprovement by two-state WFM

3. WFM potential perturbatively for $A \geq 2$

Wavefunction matching for solving quantum many-body problems

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Serdar Elhatisari[1,2], Lukas Bovermann[3], Yuan-Zhuo Ma[4,5], Evgeny Epelbaum[3], Dillon Frame[6,7], Fabian Hildenbrand[6,7], Myungkuk Kim[8], Youngman Kim[8], Hermann Krebs[3], Timo A. Lähde[6,7], Dean Lee[4]✉, Ning Li[9], Bing-Nan Lu[10], Ulf-G. Meißner[2,6,7,11], Gautam Rupak[12], Shihang Shen[6,7], Young-Ho Song[13] & Gianluca Stellin[14]

[S. Elhatisari et al. (Nature 2024)]

Many-nucleon Hamiltonian ($\neq$ part 1)

$a = 1.32$ fm

WFM applied to lowest state in each partial wave of 2NF ($R = 3.72$ fm)

$\hat{U}$-induced short-range (3)NF [LB et al. (2022)] compensated by LEC fit

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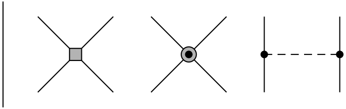
$\hat{H}^{\mathrm{S}}_{\mathrm{LO}}$



(basic features correct **[B.-N. Lu et al. (2019)]**)

isospin-dependent

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diagrams based on [E. Epelbaum et al. (2009)]; technical differences compared to part 1 on backup slide

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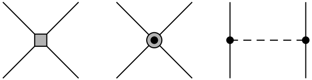
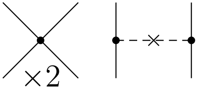
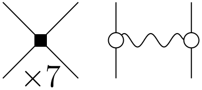
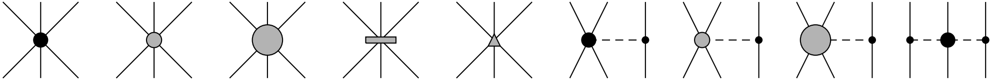
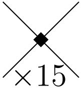
$\hat{H}^{\text{S}}_{\text{LO}}$		(basic features correct **[B.-N. Lu et al. (2019)]**)
$\hat{H}_{\text{LO}}$		
$\hat{H}_{\text{NLO}}$		
$\hat{H}_{\text{N2LO}}$		
$\hat{H}_{\text{N3LO}}$		WFM applied to lowest state in each partial wave of 2NF ($R = 3.72\ \text{fm}$) $\hat{U}$-induced short-range (3)NF **[LB et al. (2022)]** compensated by LEC fit

⊙	isospin-dependent
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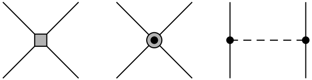
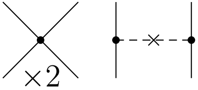
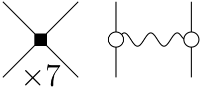
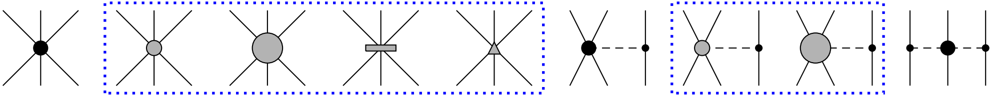
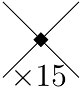
$\hat{H}^{\mathrm{S}}_{\mathrm{LO}}$		(basic features correct [B.-N. Lu et al. (2019)])
$\hat{H}_{\mathrm{LO}}$		⊙ isospin-dependent $\times$ with counterterm and larger cutoff
$\hat{H}_{\mathrm{NLO}}$		six additional 3N contact interactions
$\hat{H}_{\mathrm{N2LO}}$		
$\hat{H}_{\mathrm{N3LO}}$		WFM applied to lowest state in each partial wave of 2NF ($R = 3.72$ fm) $\hat{U}$-induced short-range (3)NF [LB et al. (2022)] compensated by LEC fit

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Why six additional terms?

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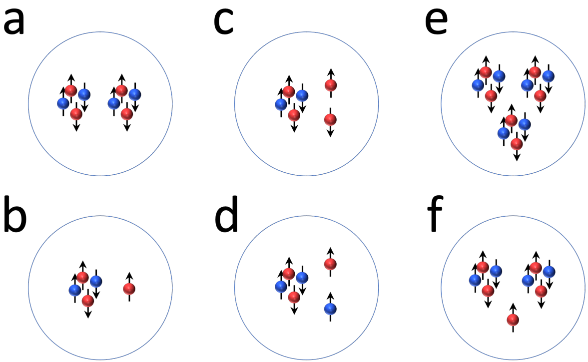

cluster EFT for α and N

[C. A. Bertulani et al. (2002)] [R. Higa et al. (2008)]

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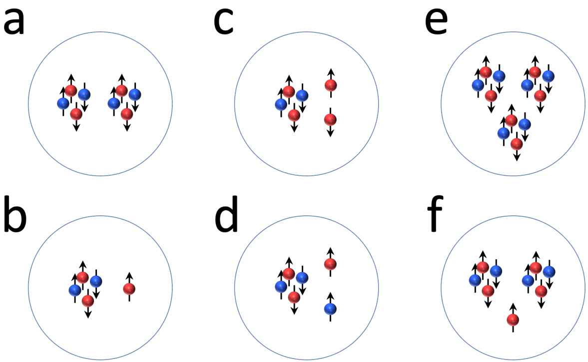

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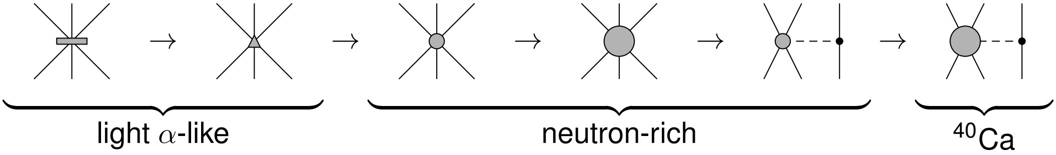
$\Rightarrow$ two-cluster & three-cluster force suggest up to 6 additional 3NF contacts

$\Rightarrow$ fit these to GS energies of selected nuclei

$\Rightarrow$ significantly reduce deviation of E & R_{ch} from experiment

Why *these* six additional terms?

tune additional 3NF terms to GS energies step by step:



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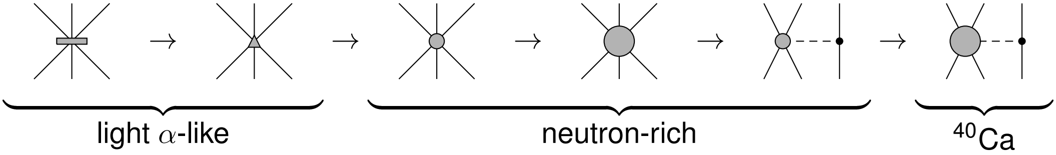
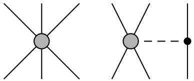
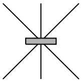


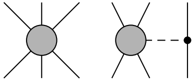
The contacts differ in the regularization (smearing to neighboring lattice sites):



spherical with small range



3N neighboring on a line



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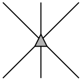
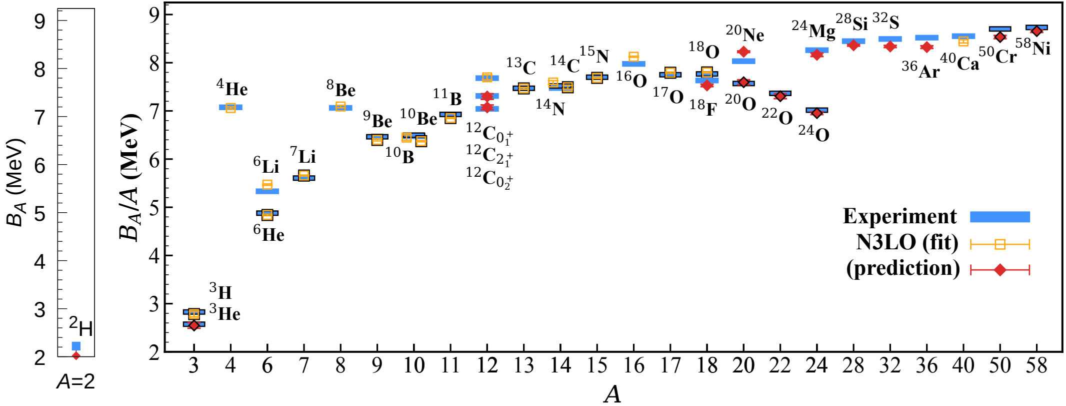


3N as equilateral triangle

cf. prolate/oblate configurations of carbon-12 [S. Shen et al. (2023)]

Many-nucleon observables

bound state energies with WFM (MC methods on backup slide):

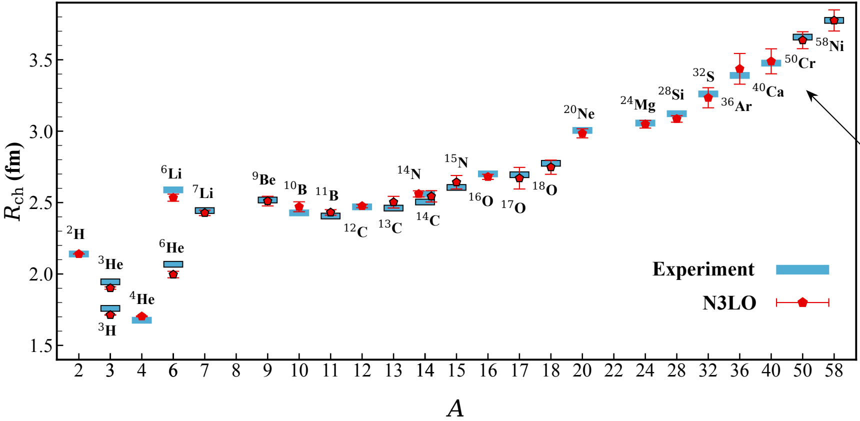


experimental data roughly agrees with [M. Wang et al. (2017)] and [J. H. Kelley et al. (2017)]

good predictions e.g. for excited ^{12}C states [F. Hoyle (1954)] and oxygen dripline (computational error bars from MC, $L \to \infty$ and $L_t \to \infty$)

Many-nucleon observables

charge radii with WFM (MC methods on backup slide):



errors reducible with more computations

experimental data roughly agrees with [I. Angeli, K. P. Marinova (2013)]

good predictions for all shown nuclei, no fit to radii
(computational error bars from MC, $L \to \infty$ and $L_t \to \infty$)

Comparison of few-nucleon observables

	$-E_{3H}$ [MeV]	$-E_{3He}$ [MeV]	$R_{ch,3H}$ [fm]	$R_{ch,3He}$ [fm]	$t_{1/2}$ [yr]
experiment	$8.481795(2)$	$7.718040(2)$	$1.7591(363)$	$1.9661(30)$	$12.32(3)$
	[M. Wang et al. (2017)]		[I. Angeli, K. P. Marinova (2013)]		[J. J. Simpson (1987)]
$A = 3$-fit	$8.48(7)$ fit	$7.73(7)$	$1.695(10)$	$1.914(14)$	$12.31(10)$ fit
$A \geq 3$-fit PT	$8.35(18)$ fit	$7.64(17)$	$1.713(9)$	$1.901(28)$	

Comparison of few-nucleon observables

- previous computational uncertainty
  - Monte Carlo error
  - errors of extrapolations $L \to \infty$ and $L_t \to \infty$

  added in quadrature to chiral-EFT uncertainty
  - experimental, fitting and truncation error for 2NF
  - fitting error for 3NF
- no error propagation from $R^2_{\text{ch,p}}$, $R^2_{\text{ch,n}}$ and $R^2_{\text{Darwin-Foldy}}$
- more (energy) error sources $\overset{?}{\Rightarrow}$ larger uncertainties (compared to part 1)

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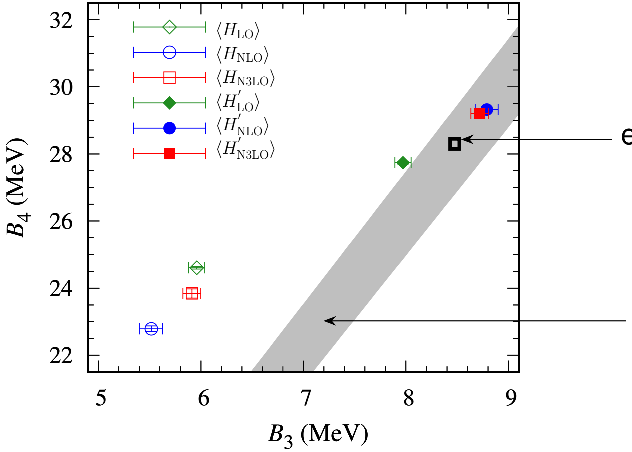
Effect of WFM

clear improvement by WFM:



experiment **roughly [M. Wang et al. (2017)]**

Tjon band: correlation between GS energies of ^{3}H and ^{4}He

[J. A. Tjon (1975)] [L. Platter et al. (2005)]

(using only 2NF for focus here)

4. WFM potential non-perturbatively for $A = 3$

The triton lifetime from nuclear lattice effective field theory

Serdar Elhatisari [a,b,c], Fabian Hildenbrand [d,*], Ulf-G. Meißner [c,d,e]

[S. Elhatisari et al. (PLB 2024)]

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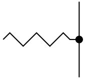

$$+ \mathcal{O}(\mathrm{N^2LO}) \; || \psi_{3\mathrm{H}} \rangle$$

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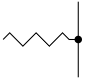

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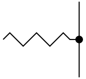

- error sources:
  - extrapolation $L \to \infty$
  - variation of 3NF at constant GS energies (for half-life) [D. Gazit et al. (2009)]
  - uncertainty of K/G_{V}^2 (for half-life)
- neglected truncation error $\overset{?}{\Rightarrow}$ too large deviations from experiment

	$-E_{3\mathrm{H}}$ [MeV]	$-E_{3\mathrm{He}}$ [MeV]	$R_{\mathrm{ch},3\mathrm{H}}$ [fm]	$R_{\mathrm{ch},3\mathrm{He}}$ [fm]	$t_{1/2}$ [yr]
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Summary and outlook

two nuclear-interaction models with different ranges of fitting & application:

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Non-perturbative three-nucleon simulation using chiral lattice EFT

Lukas Bovermann,[a,*] Evgeny Epelbaum,[a] Hermann Krebs[a] and Dean Lee[b]

[LB et al. (arXiv 2024)]

suitable for few-nucleon problems, e.g.

- 3N charge radii at N^3LO

  lattice version of [D. Möller (2024)]

- nucleon-deuteron phase shifts using adiabatic projection method

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[S. Elhatisari et al. (Nature 2024)]

suitable for many-nucleon problems, e.g.

- beta decays in heavier nuclei

  outlook of [S. Elhatisari et al. (PLB 2024)]

- $\alpha\alpha$ scattering [S. Elhatisari et al. (2015)]
- nuclear resonances

  [in progress by A. Sarkar, C. Wang]

Thank you for your attention!

Backup: Monte Carlo methods

- bound state energies: [D. Lee (2009)] [B. Borasoy et al. (2006)]
  - evolve Hamiltonian $\hat{H}^{\mathrm{S}}$ over L_t Euclidean time steps of size a_t
  - consider normal-ordered matrix element $\langle\psi| : e^{-L_t a_t \hat{H}^{\mathrm{S}}/2} \hat{H}' e^{-L_t a_t \hat{H}^{\mathrm{S}}/2} : |\psi\rangle$, where $|\psi\rangle$ must have non-zero overlap with desired ground/excited state
  - apply MC for path integral over pion fields and auxiliary Hubbard-Stratonovich fields [J. Hubbard (1959)] [R. L. Stratonovich (1958)]
  - divide matrix element by $\langle\psi| : e^{-L_t a_t \hat{H}^{\mathrm{S}}} : |\psi\rangle$ to get eigenenergy of Hamiltonian $\hat{H}'$
- charge radii: [S. Elhatisari et al. (2017)] [D. K. Frame (2019)]
  - insert "pinhole screen" at middle time in $\langle\psi| : e^{-(L_t-1)a_t \hat{H}^{\mathrm{S}}/2} e^{-a_t \hat{H}'} e^{-(L_t-1)a_t \hat{H}^{\mathrm{S}}/2} : |\psi\rangle$ to track positions and (iso)spins of nucleons
  - perform MC importance sampling for pinholes
  - calculate expectation value of A-body density operator and thus point-proton radius
- MC error from jackknife analysis [B. Efron, C. Stein (1981)] for different seeds of random-number generator
- PT error negligible [S. Elhatisari et al. (Nature 2024)]

Backup: Differences of WFM Hamiltonians compared to part 1

- exact kinetic-energy term (both Hamiltonians)
- Galilean-invariance restoration up to higher order (realistic Hamiltonian)
- two-nucleon contact interactions in simple Hamiltonian roughly adjusted to overall behavior of GS energies [B.-N. Lu et al. (2019)] and slightly optimized for simulations of heavier nuclei
- different non-local smearing parameter [B.-N. Lu et al. (2019)] [B. N. Lu et al. (2020)] (simple Hamiltonian)
- channel-specific two-nucleon contact interactions with infinite-range Gaussian regulator and without fit to deuteron GS energy (realistic Hamiltonian)
- one-pion exchange with different regulator cutoff (both Hamiltonians)
- slightly different LEC values (both Hamiltonians)

[S. Elhatisari et al. (Nature 2024)] [S. Elhatisari et al. (PLB 2024)]