

Ab initio nuclear theory on the lattice

Ulf-G. Meißner, Univ. Bonn & FZ Jülich

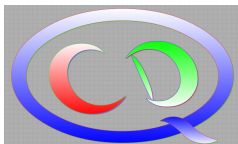
supported by DFG, SFB/TR-110

by CAS, PIFI

by DFG, SFB 1639

by ERC, EXOTIC

by NRW-FAIR



Contents

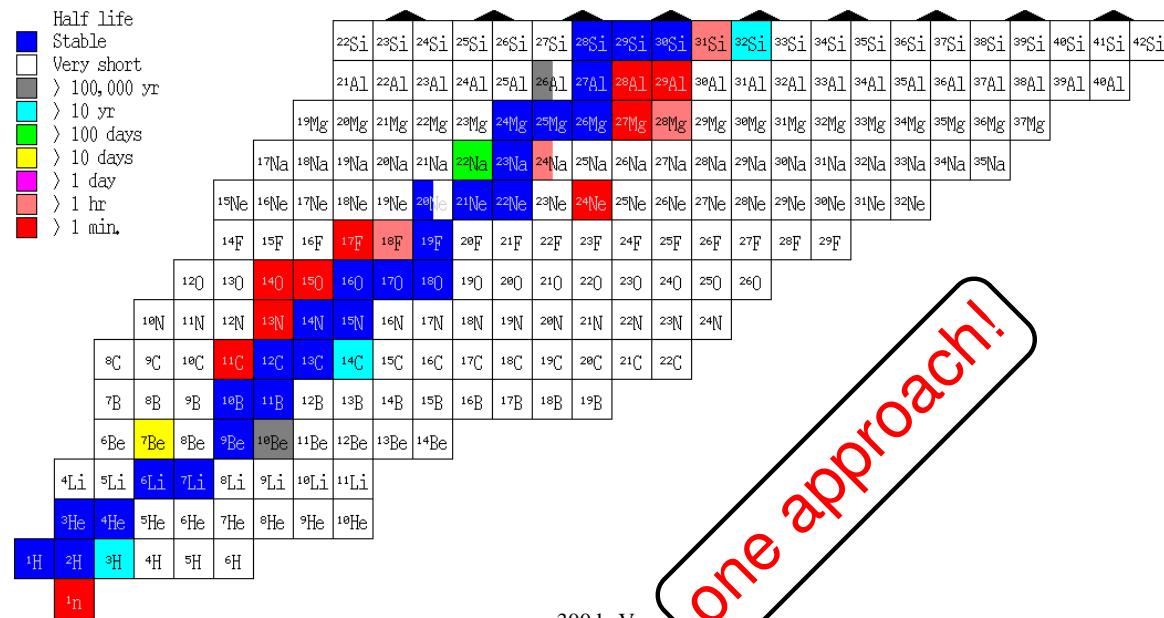
- Very brief Introduction
- Chiral EFT on a lattice
- Chiral interactions at N³LO
 - Foundations
 - Applications to nuclear structure
 - Applications to scattering
- Summary & outlook

Very brief Introduction

Our goal: Ab initio nuclear structure & reactions

• Nuclear structure:

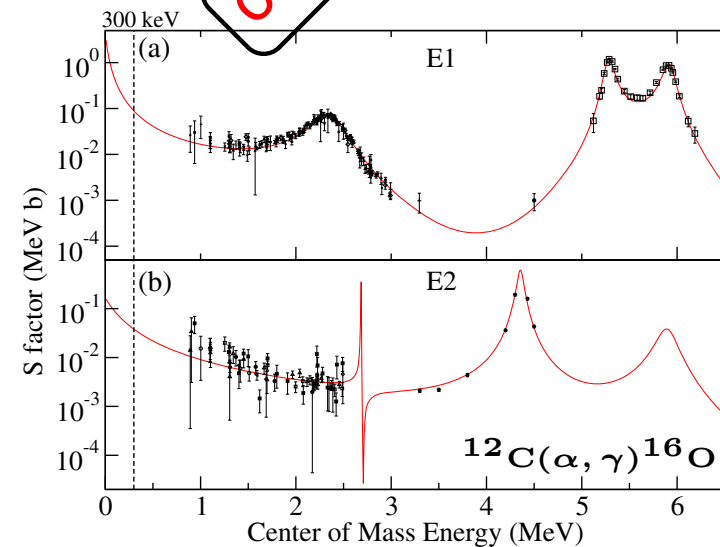
- ★ limits of stability
- ★ 3-nucleon forces
- ★ alpha-clustering
- ★ EoS & neutron stars
- ⋮



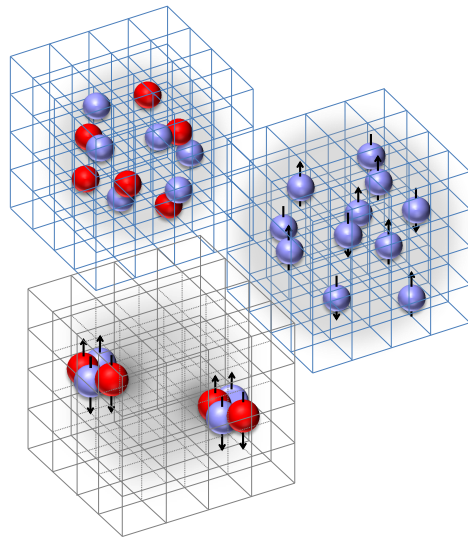
• Nuclear reactions, nuclear astrophysics:

- ★ alpha-particle scattering
- ★ triple-alpha reaction
- ★ alpha-capture on carbon
- ⋮

de Boer et al, Rev. Mod. Phys. **89** (2017) 035007



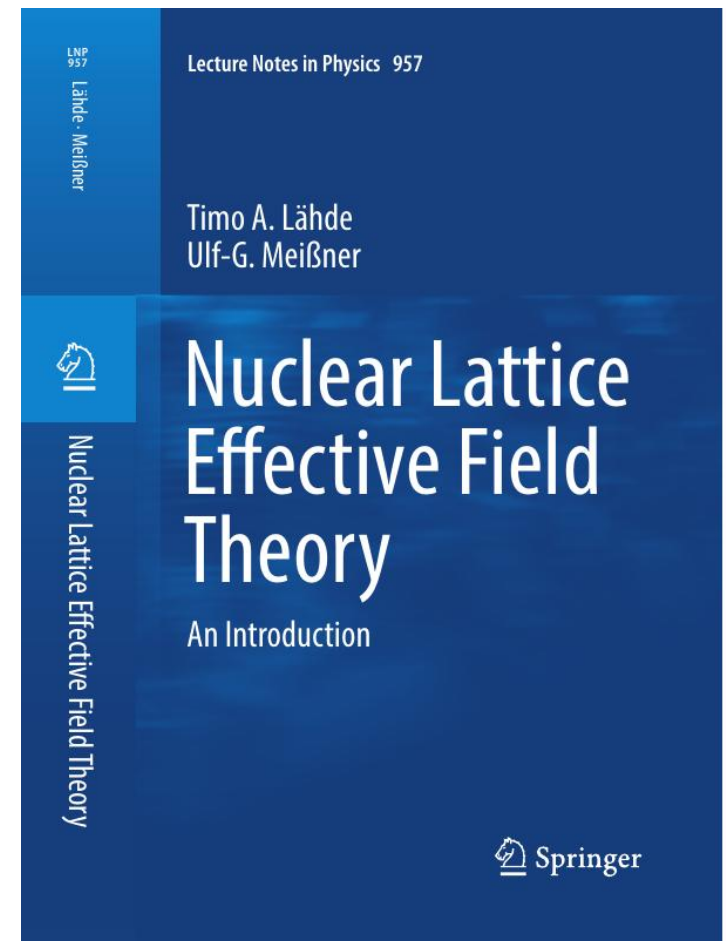
Chiral EFT on a lattice



T. Lähde & UGM

Nuclear Lattice Effective Field Theory - An Introduction

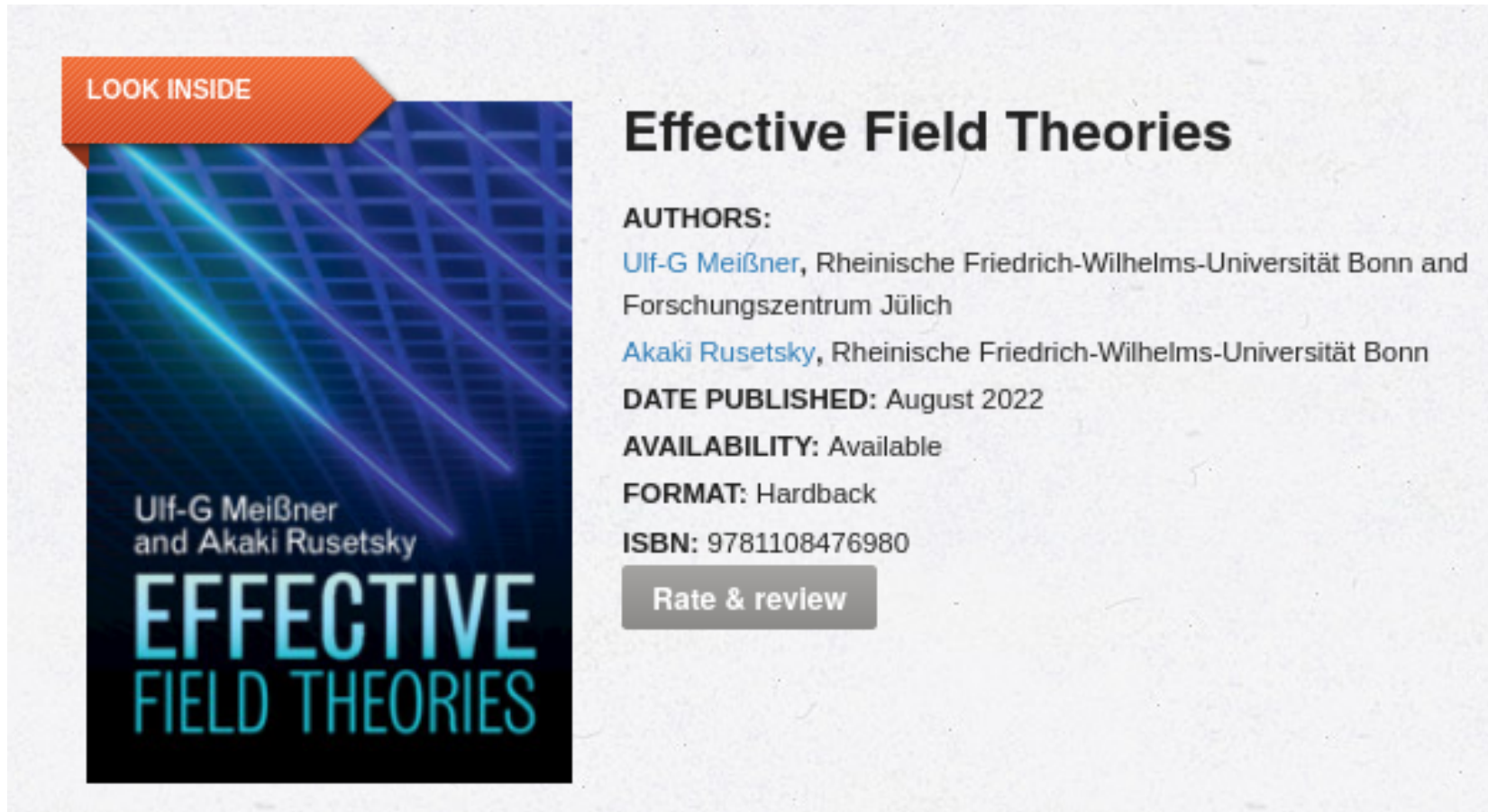
Springer Lecture Notes in Physics **957** (2019) 1 - 396



More on EFTs

6

- Much more details on EFTs in light quark physics:



<https://www.cambridge.org/de/academic/subjects/physics/theoretical-physics-and-mathematical-physics/effective-field-theories>

Nuclear lattice effective field theory (NLEFT)

7

Frank, Brockmann (1992), Koonin, Müller, Seki, van Kolck (2000), Lee, Schäfer (2004), . . .
Borasoy, Krebs, Lee, UGM, Nucl. Phys. **A768** (2006) 179; Borasoy, Epelbaum, Krebs, Lee, UGM, Eur. Phys. J. **A31** (2007) 105

- *new method* to tackle the nuclear many-body problem

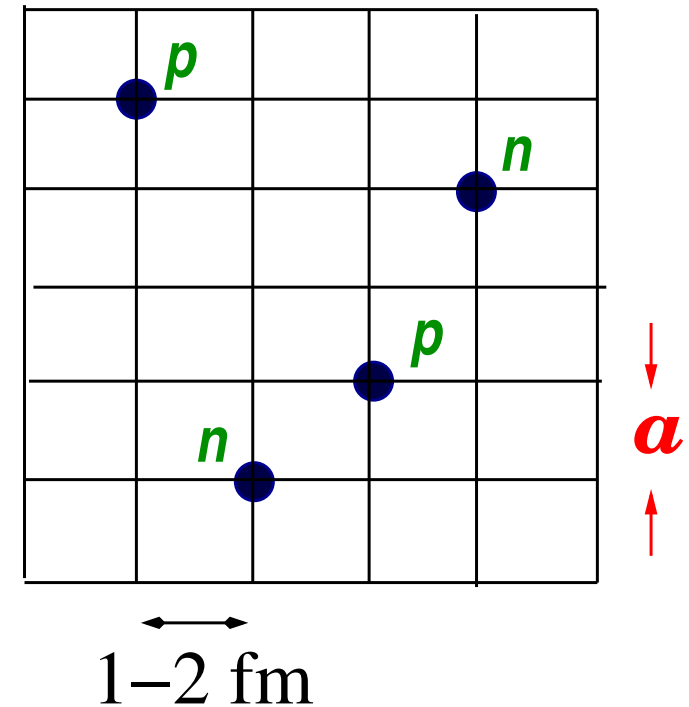
- discretize space-time $V = L_s \times L_s \times L_s \times L_t$:
nucleons are point-like particles on the sites

- discretized chiral potential w/ pion exchanges
and contact interactions + Coulomb

→ see Epelbaum, Hammer, UGM, Rev. Mod. Phys. **81** (2009) 1773

- typical lattice parameters

$$p_{\max} = \frac{\pi}{a} \simeq 315 - 630 \text{ MeV [UV cutoff]}$$



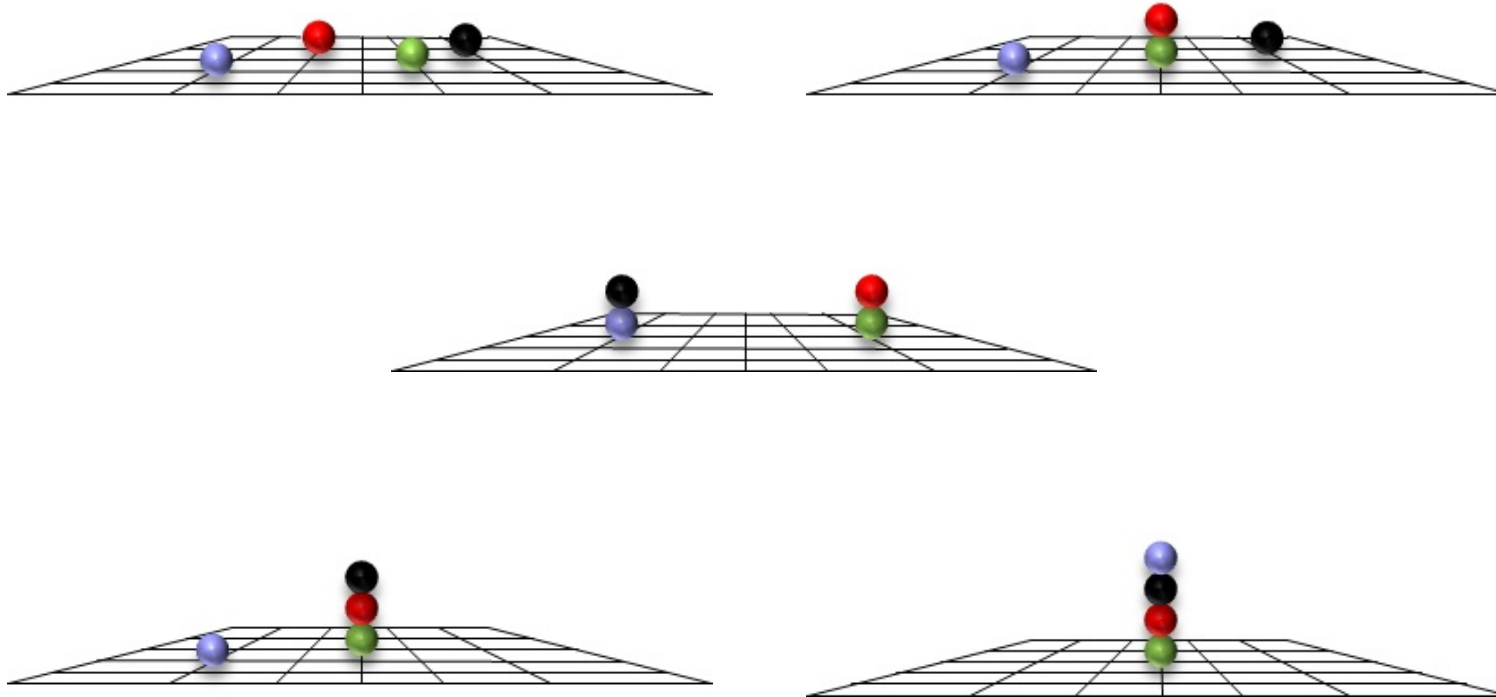
- strong suppression of sign oscillations due to approximate Wigner SU(4) symmetry

E. Wigner, Phys. Rev. **51** (1937) 106; T. Mehen et al., Phys. Rev. Lett. **83** (1999) 931; J. W. Chen et al., Phys. Rev. Lett. **93** (2004) 242302

- physics independent of the lattice spacing for $a = 1 \dots 2 \text{ fm}$

Alarcon, Du, Klein, Lähde, Lee, Li, Lu, Luu, UGM, EPJA **53** (2017) 83; Klein, Elhatisari, Lähde, Lee, UGM, EPJA **54** (2018) 121

Configurations

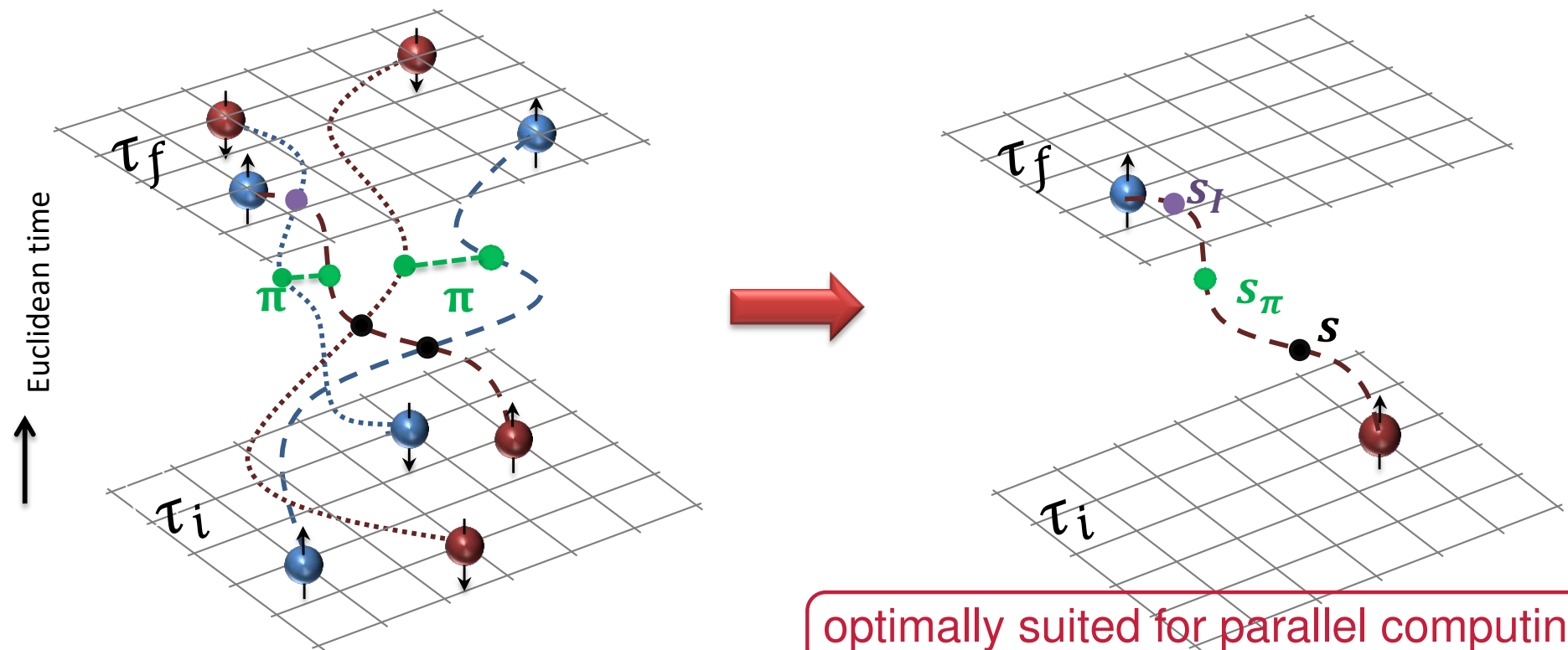


- ⇒ *all possible* configurations are sampled
- ⇒ preparation of *all possible* initial/final states
- ⇒ *clustering* emerges *naturally*

Auxiliary field method

- Represent interactions by auxiliary fields (Gaussian quadrature):

$$\exp \left[-\frac{C}{2} (N^\dagger N)^2 \right] = \sqrt{\frac{1}{2\pi}} \int ds \exp \left[-\frac{s^2}{2} + \sqrt{C} s (N^\dagger N) \right]$$



Computational equipment

- Present = JUWELS (modular system) + JUPITER + ...



Chiral Interactions at N³LO: Foundations

Towards precision calculations of heavy nuclei

- Groundbreaking work (Hoyle state, α - α scattering, ...) done at N2LO

↪ precision limited, need to go to N3LO

- Two step procedure:

1) Further improve the LO action

↪ minimize the sign oscillations

↪ minimize the higher-body forces

↪ done ✓

2) Work out the corrections to N3LO

↪ first on the level of the NN interaction ✓ see also Wu et al., 2503.18017

↪ new important technique: **wave function matching** ✓

↪ second for the spectra/radii/... of nuclei (first results) ✓

↪ third for nuclear reactions/astrophysics (first results) ✓

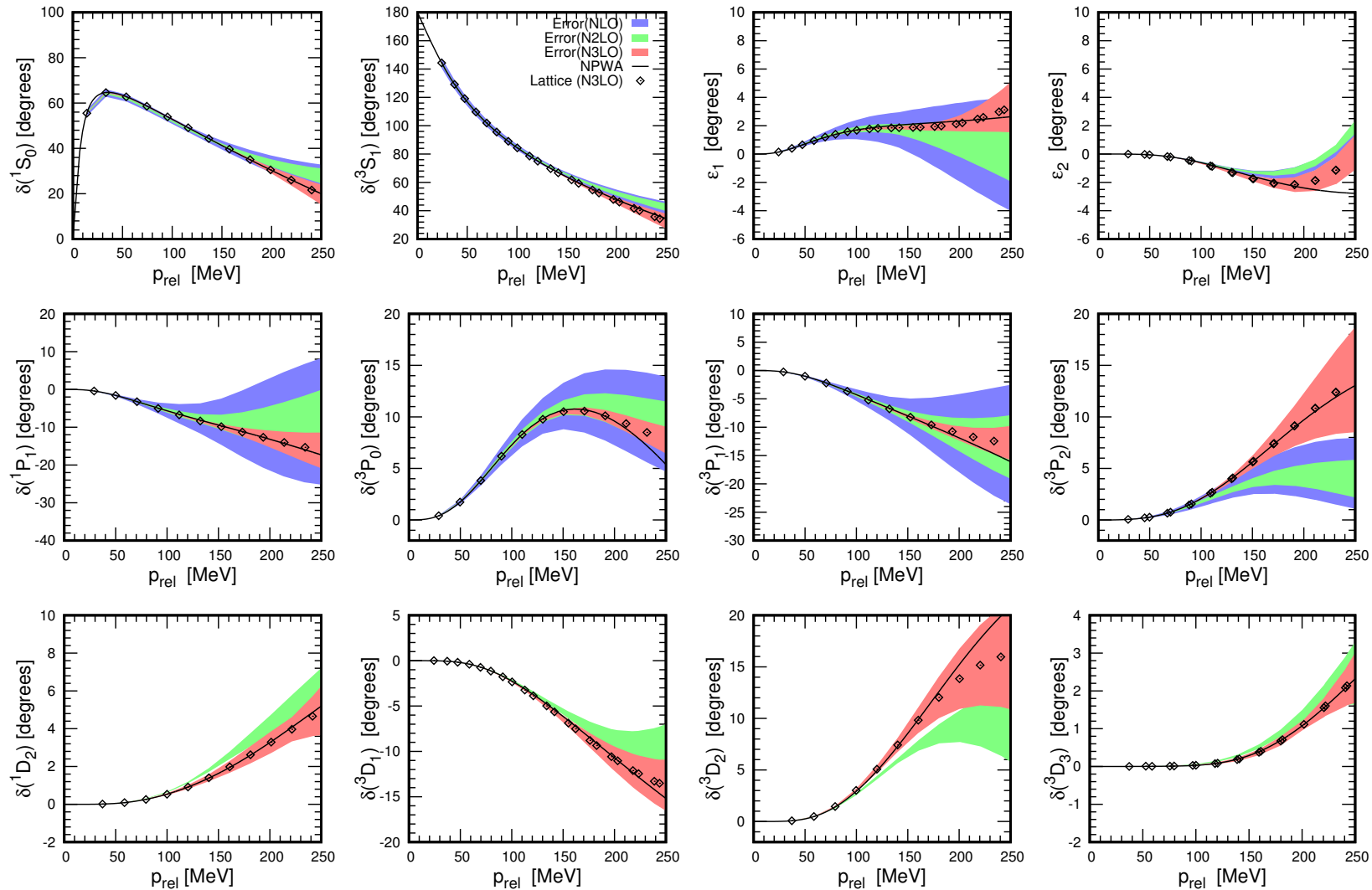
NN interaction at N3LO

13

Li et al., Phys. Rev. C **98** (2018) 044002; Phys. Rev. C **99** (2019) 064001

- np phase shifts including uncertainties for $a = 1.32$ fm (cf. Nijmegen PWA)

NLO
N2LO
N3LO



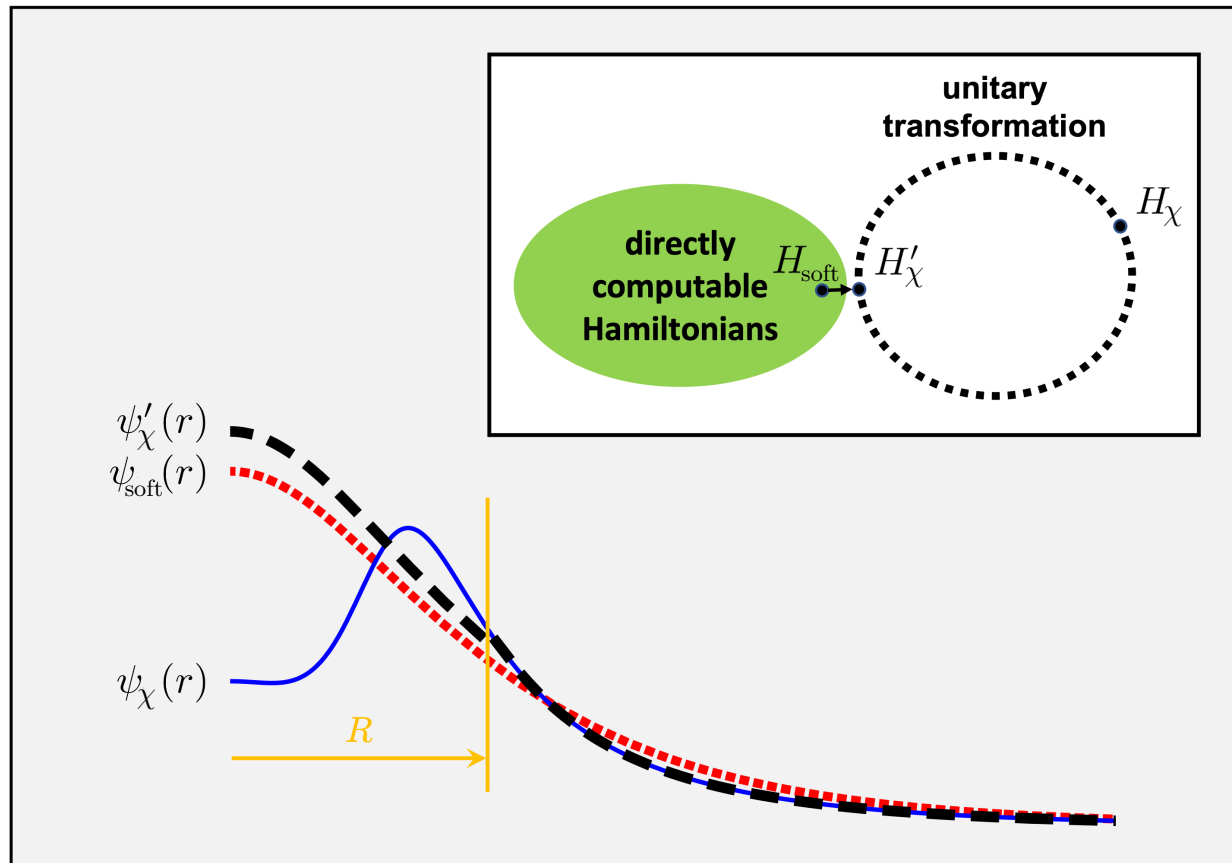
uncertainty estimates à la Epelbaum, Krebs, UGM,
Eur. Phys. J. A **51** (2015) 53

Wave function matching

14

Elhatisari et al., Nature **630** (2024) 59

- Graphical representation of w.f. matching



- W.F. matching is a “Hamiltonian translator”:
eigenenergies from H_1 but w.f. from $H_2 = U^\dagger H_1 U$

- The time-honored Lüscher approach:

Lüscher, Commun. Math. Phys. **105** (1986) 153; Nucl. Phys. B **354** (1991) 531

Phase shifts from the volume dependence of the energy levels

↪ works in many cases, problems w/ partial-wave mixing and cluster-cluster scattering

- Spherical wall technique:
impose spherical b.c.'s on the lattice

Carlson et al., Nucl. Phys. A **424** (1984) 47; Borasoy et al., Eur. Phys. J. A **34** (2007) 185

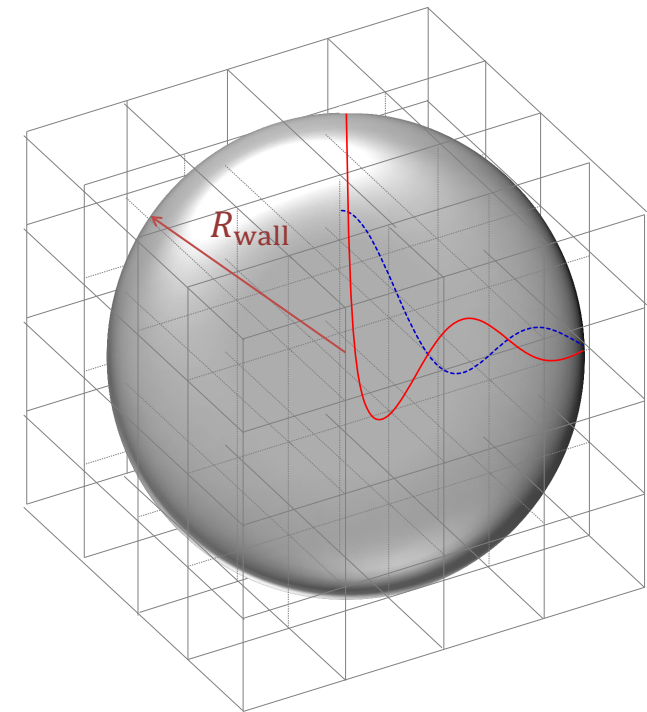
↪ not too small lattices, partial-wave mixing under control

- Improved spherical wall method:

Lu, Lähde, Lee, UGM, Phys. Lett. B **760** (2016) 309

- perform angular momentum projection
- impose an auxiliary potential behind R_{wall}

↪ much improved precision



Scattering: Methods II

16

- Adiabatic projection method :

Rupak, Lee, Phys. Rev. Lett. **111** (2013) 032502; Pine, Lee, Rupak, Eur. Phys. J. A **49** (2013) 151; Elhatisari et al., Eur. Phys. J. A **52** (2016) 174;

- Construct a low-energy effective theory for clusters
- Use initial states parameterized by the relative separation between clusters

$$|\vec{R}\rangle = \sum_{\vec{r}} |\vec{r} + \vec{R}\rangle \otimes \vec{r}$$

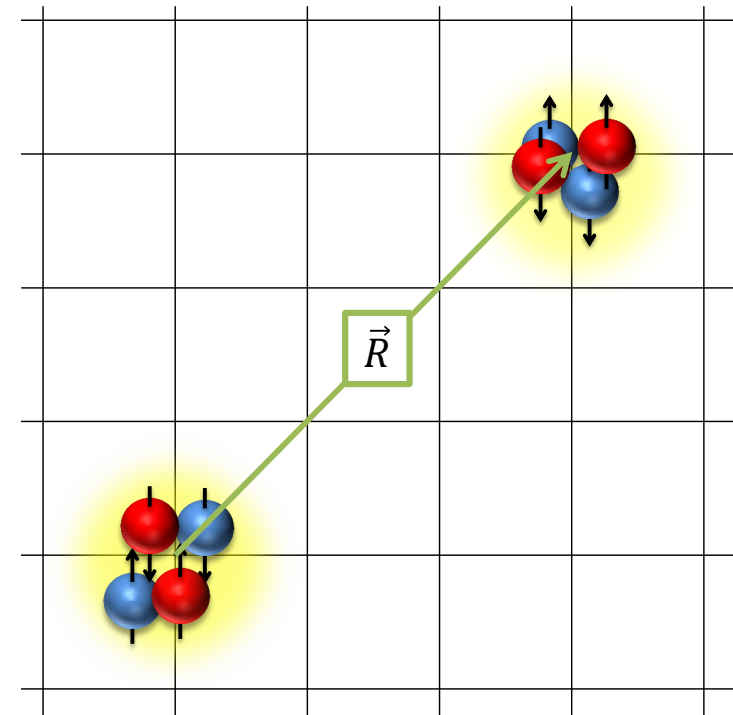
- project them in Euclidean time
with the chiral EFT Hamiltonian H

$$|\vec{R}\rangle_{\tau} = \exp(-H\tau)|\vec{R}\rangle$$

→ “dressed cluster states” (polarization, deformation, Pauli)

- Adiabatic Hamiltonian (requires norm matrices)

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



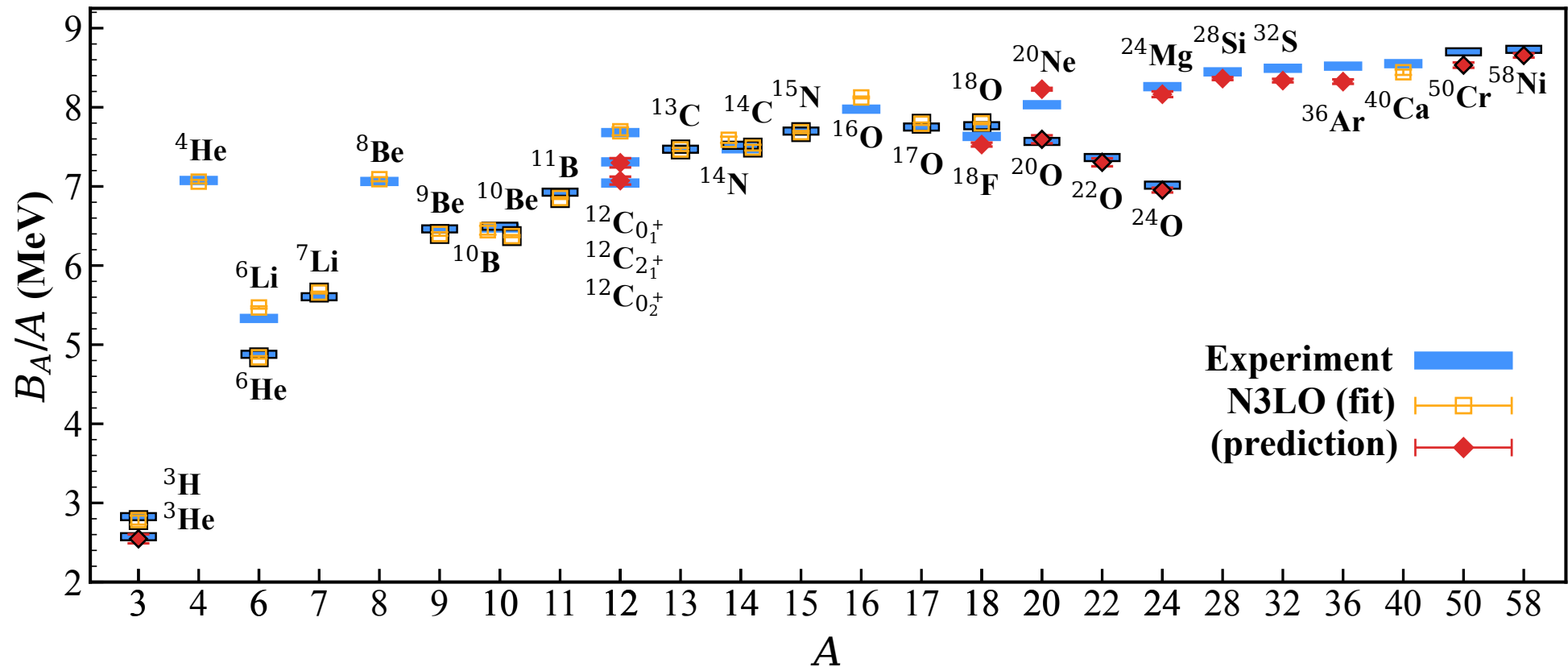
Chiral Interactions at N³LO: Applications to nuclear structure

Binding Energies at N3LO

18

- Binding energies of nuclei for $a = 1.32$ fm: Determining the 3NF LECs

Elhatisari et al., Nature **630** (2024) 59



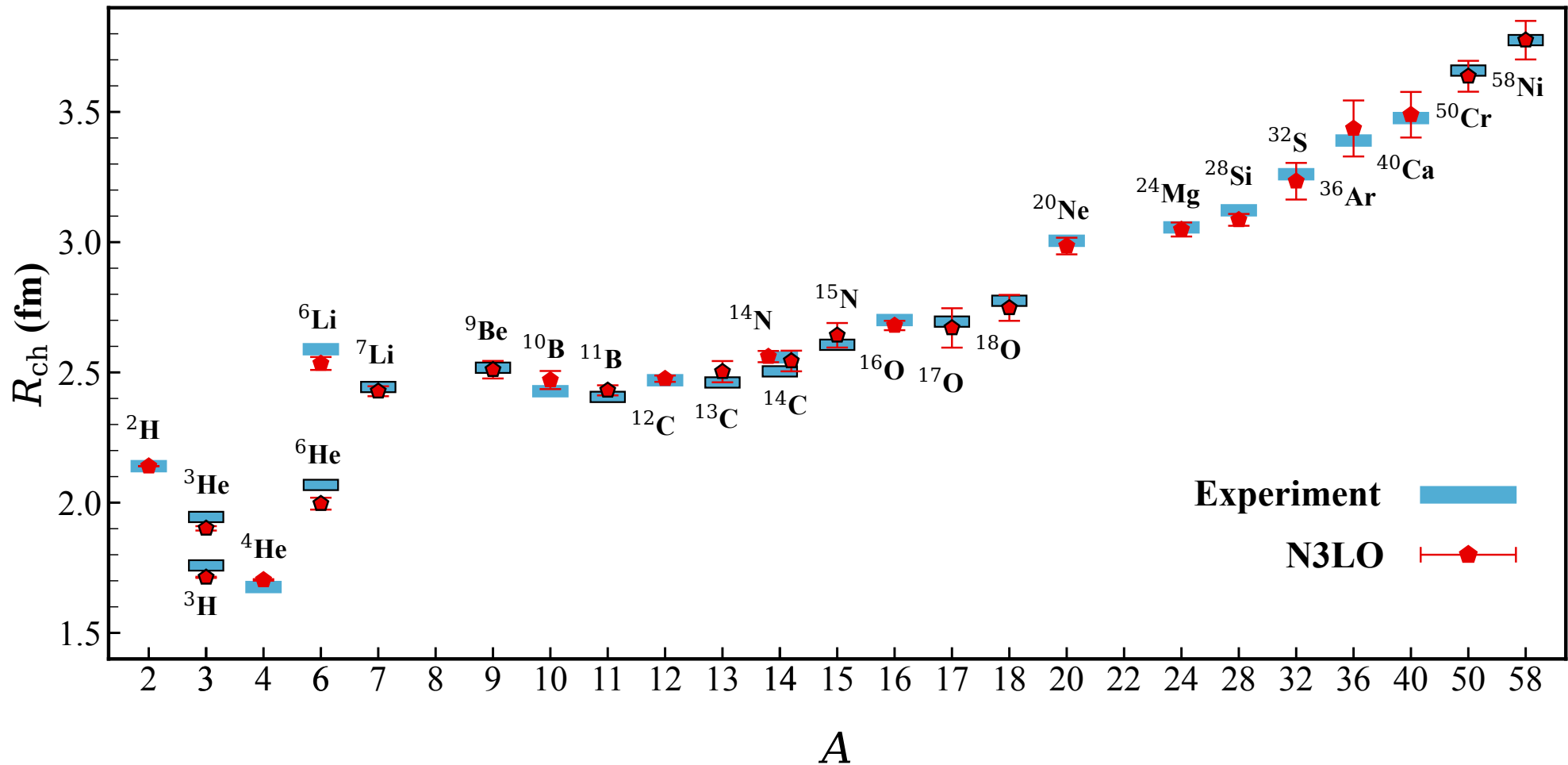
→ excellent starting point for precision studies

Prediction: Charge radii at N3LO

19

Elhatisari et al., Nature **630** (2024) 59

- Charge radii ($a = 1.32$ fm, statistical errors can be reduced)



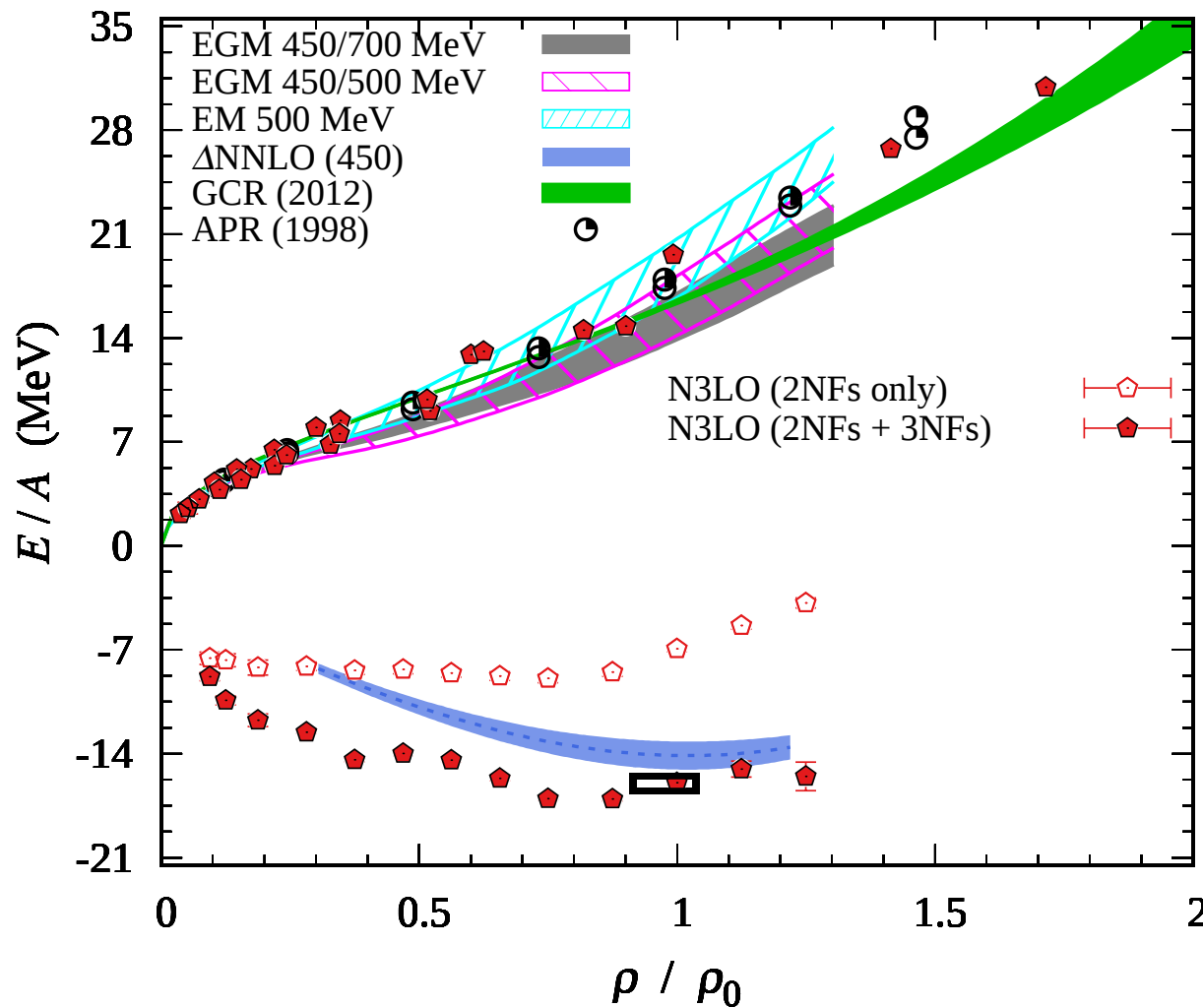
↪ no radius problem!

Prediction: Neutron & nuclear matter at N3LO

20

Elhatisari et al., Nature **630** (2024) 59

- EoS of pure neutron matter & nuclear matter ($a = 1.32$ fm)



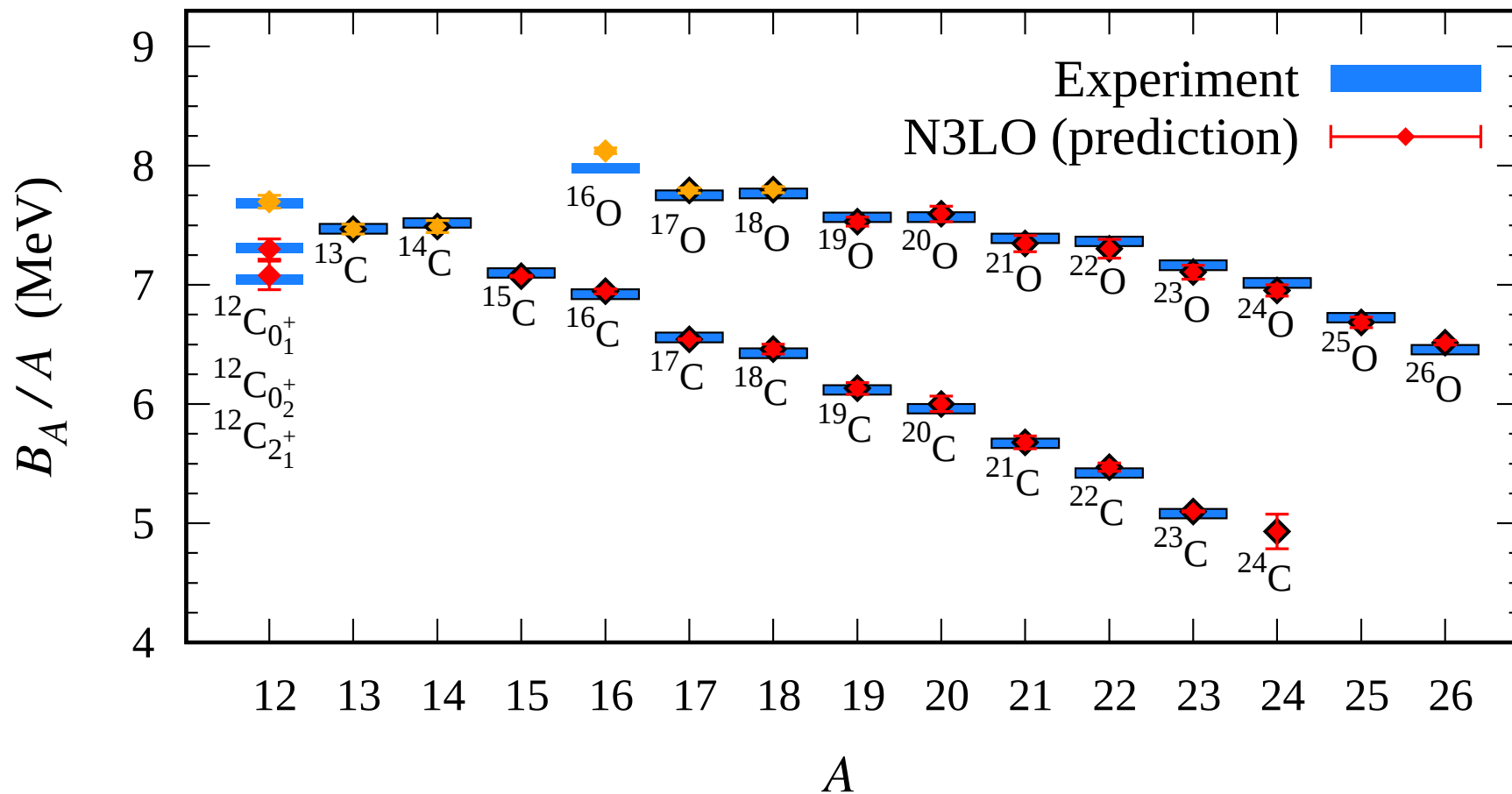
→ can be improved using twisted b.c.'s

Prediction: Isotope chains of carbon & oxygen

21

Song et al., 2502.18722 [nucl-th]

- Towards the neutron drip-line in carbon and oxygen:



↪ 3NFs of utmost importance for the n-rich isotopes!

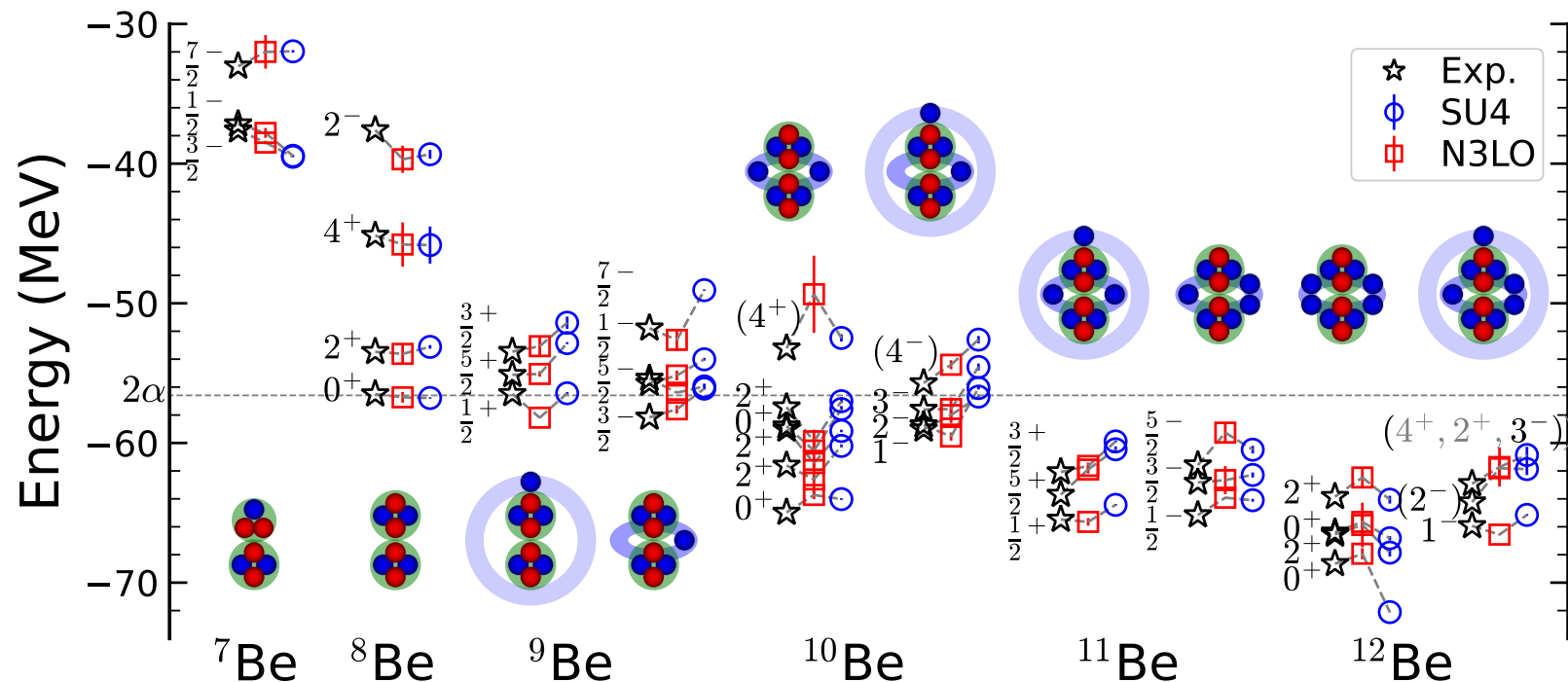
↪ universal features of neutron correlations

Prediction: Be isotopes

22

Shen et al., Phys. Rev. Lett. **134** (2025) 162503

- Systematic study of the Be isotopes & their em transitions:



↪ new method to quantify nuclear shapes

↪ clusters, halos, molecular orbitals in **one shot**

Prediction: Triton β -decay at N3LO

23

Elhatisari, Hildenbrand, UGM, Phys. Lett. B **859** (2024) 139086

- Master formula: $(1 + \delta_R) t_{1/2} f_V = \frac{K/G_V^2}{\langle \mathbf{F} \rangle^2 + \frac{f_A}{f_V} g_A^2 \langle \mathbf{GT} \rangle^2}$
- Experiment: $\langle \mathbf{F} \rangle = \sum_{n=1}^3 \langle {}^3\text{He} \| \tau_{n,+} \| {}^3\text{H} \rangle = 0.9998$ [theory!]
- $\langle \mathbf{GT} \rangle = \sum_{n=1}^3 \langle {}^3\text{He} \| \sigma_n \tau_{n,+} \| {}^3\text{H} \rangle = 1.6474(23)$

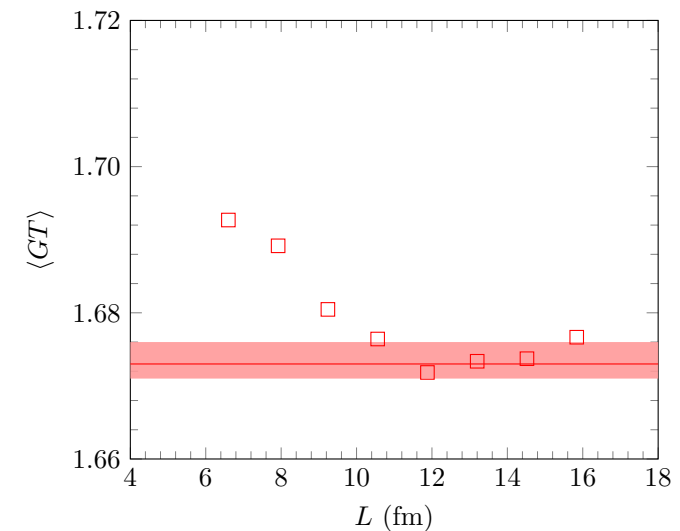
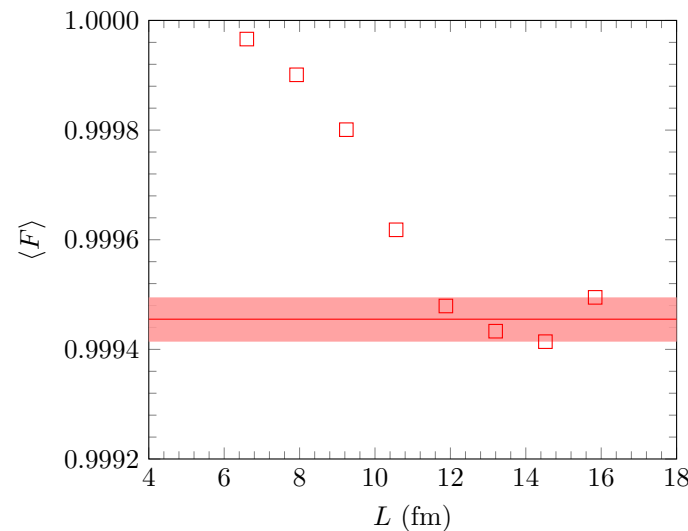
NLEFT:

$$\langle \mathbf{F} \rangle_{\text{N3LO}} = 0.99949(11)$$

$$\langle \mathbf{GT} \rangle_{\text{N3LO}} = 1.6743(58)$$

↪ Important first step

↪ Larger nuclei underway...



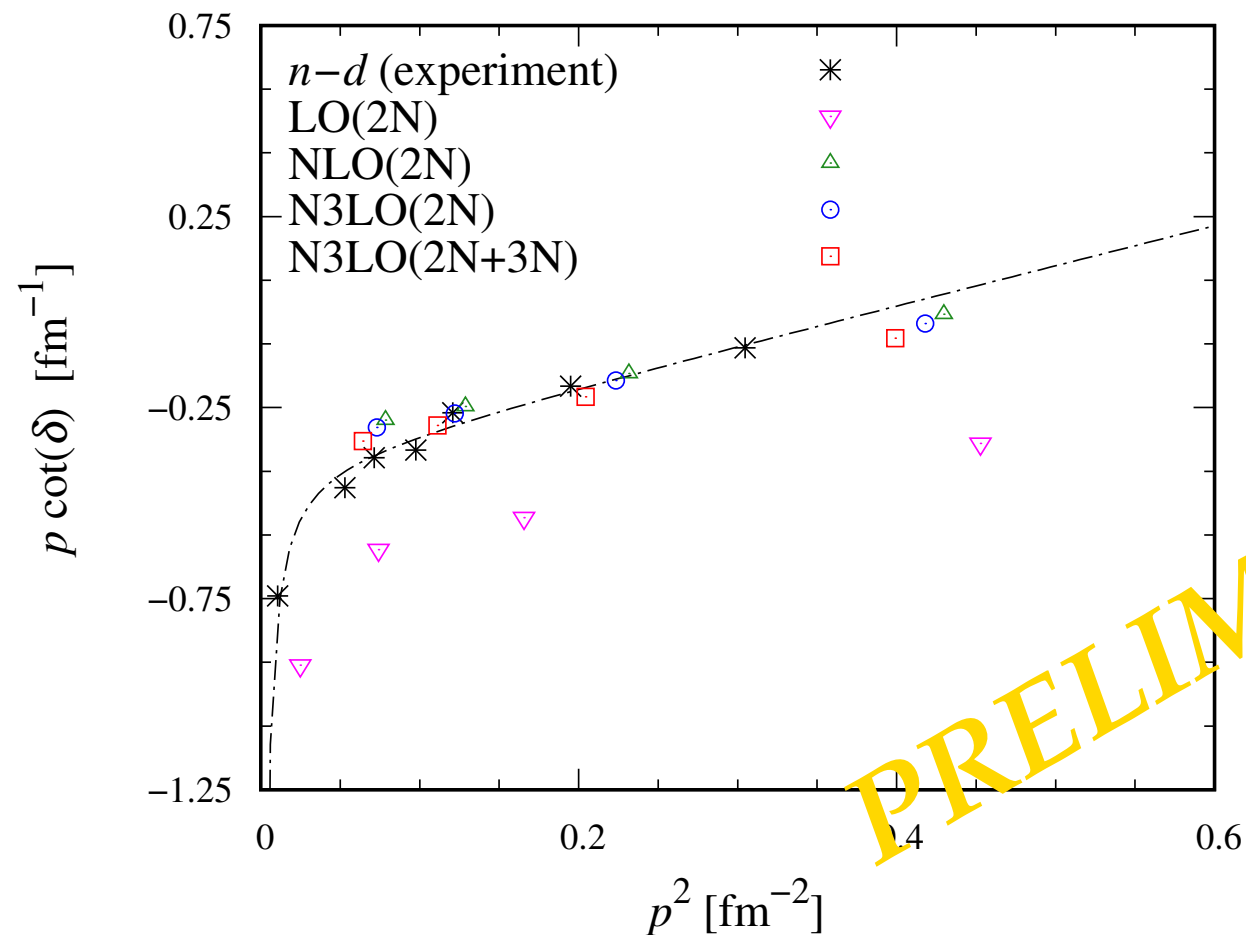
Chiral Interactions at N³LO: Applications to scattering

Scattering: Neutron-deuteron scattering at N3LO

25

Elhatisari, Hildenbrand, UGM, in progress

- Use Lüscher's method to calculate spin doublet n - d scattering



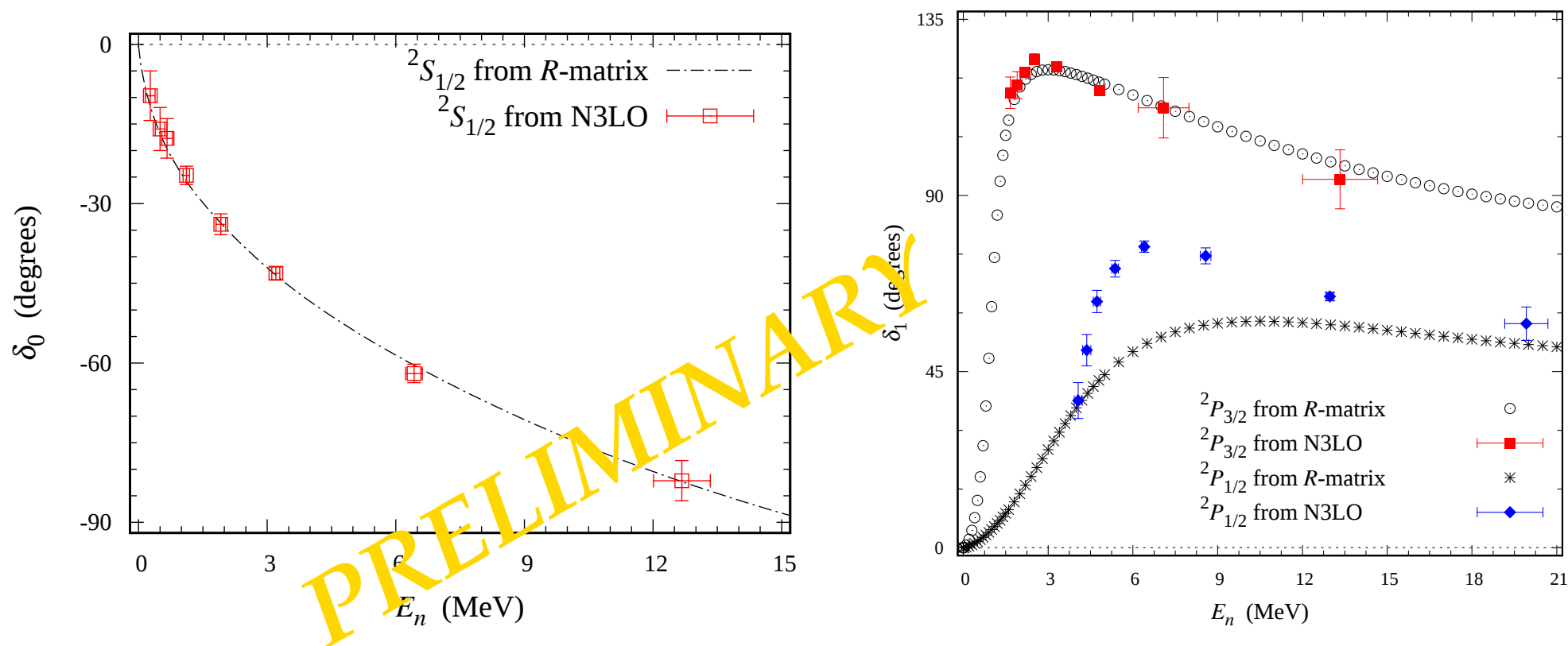
↪ shows good convergence

Scattering: Neutron-alpha scattering at N3LO

26

Elhatisari, Hildenbrand, UGM, in progress

- Use Lüscher's method to calculate n - α scattering



- R-matrix results from G. Hale, private communication
↪ Some fine-tuning of three-body forces for $^2P_{1/2}$ needed

Scattering: Alpha-carbon scattering at N3LO

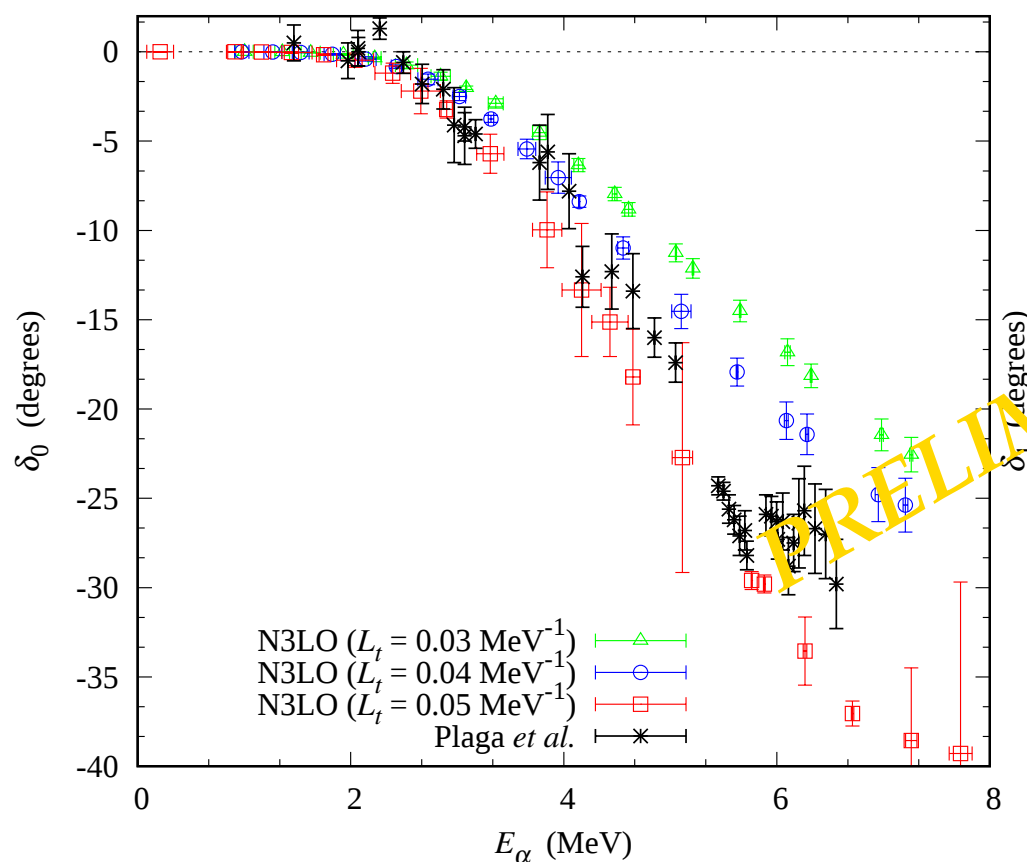
27

Elhatisari, Hildenbrand, UGM, ... NLEFT, in progress

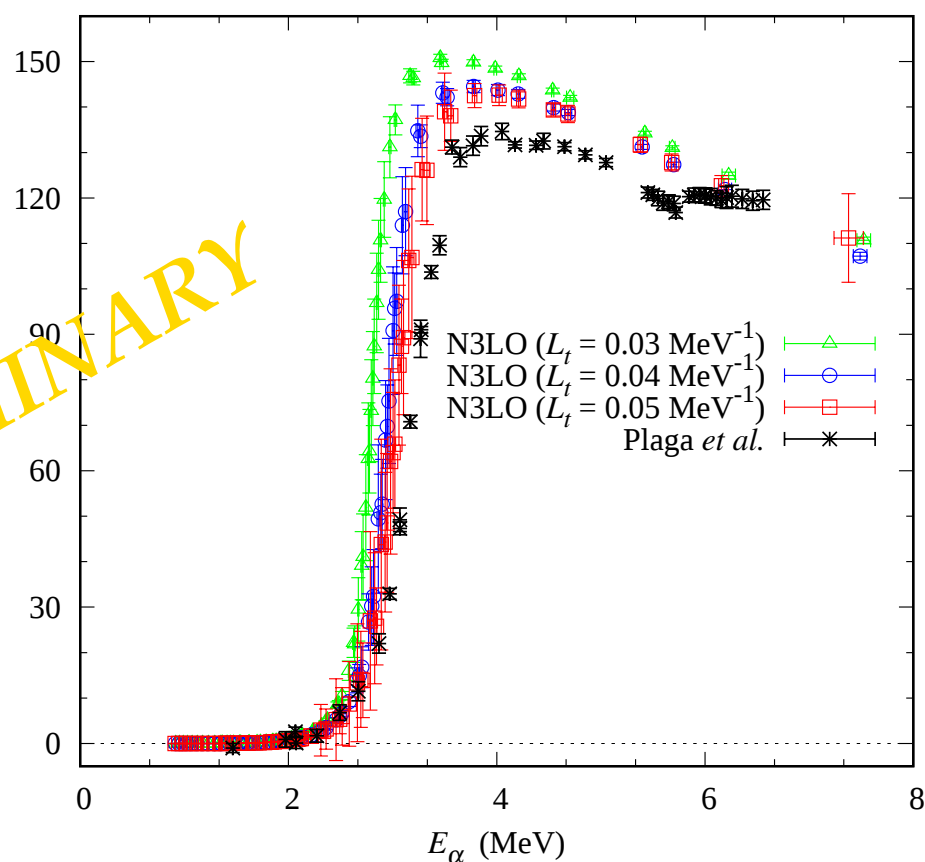
- Use the APM, first step for the holy grail of nuclear astrophysics $^{12}\text{C}(\alpha, \gamma)^{16}\text{O}$

↪ different Euclidean times & different initial states

• S-wave



• P-wave



Plaga *et al.*, Nucl. Phys. A **465** (1987) 291

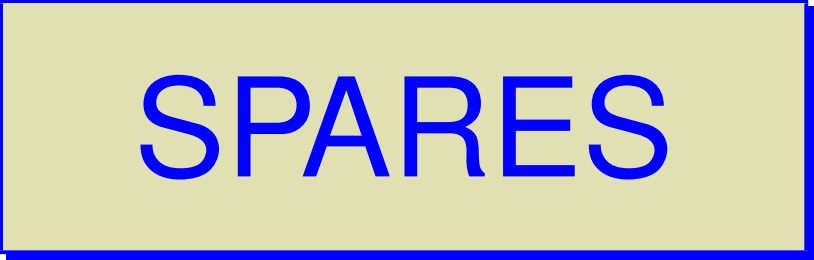
clear resonance signal!

Summary & outlook

- Nuclear lattice simulations: a new quantum many-body approach
 - based on the successful continuum nuclear chiral EFT
 - a number of highly visible results already obtained
 - Recent developments
 - NN(N) interaction at N³LO w/ wave function matching
 - ↔ first promising results for nuclear structure, matter and scattering
 - ↔ hypernuclei are under investigation

Hildenbrand et al., Eur. Phys. J. A **60** (2024) 215
 - ↔ first results for neutron stars (including hyperons)

Tong et al., Sci. Bull. **70** (2025) 825; Astrophys. J. **982** (2025) 164
- ↔ stay tuned!



SPARES

Transfer matrix method

- Correlation-function for A nucleons: $Z_A(\tau) = \langle \Psi_A | \exp(-\tau H) | \Psi_A \rangle$

with Ψ_A a Slater determinant for A free nucleons
[or a more sophisticated (correlated) initial/final state]

- Transient energy

$$E_A(\tau) = -\frac{d}{d\tau} \ln Z_A(\tau)$$

→ ground state: $E_A^0 = \lim_{\tau \rightarrow \infty} E_A(\tau)$

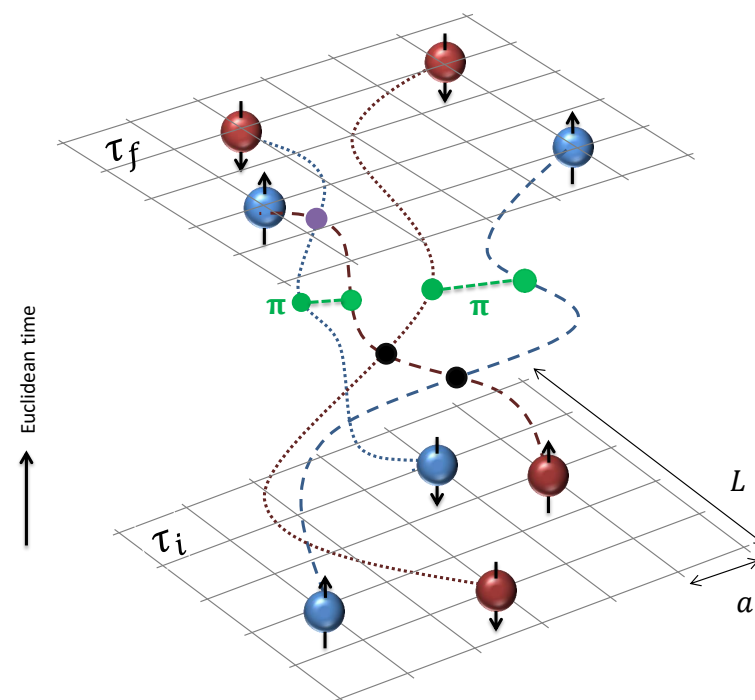
- Exp. value of any normal-ordered operator $\mathcal{O}$

$$Z_A^{\mathcal{O}} = \langle \Psi_A | \exp(-\tau H/2) \mathcal{O} \exp(-\tau H/2) | \Psi_A \rangle$$

$$\lim_{\tau \rightarrow \infty} \frac{Z_A^{\mathcal{O}}(\tau)}{Z_A(\tau)} = \langle \Psi_A | \mathcal{O} | \Psi_A \rangle$$

- Excited states: $Z_A(\tau) \rightarrow Z_A^{ij}(\tau)$, diagonalize, e.g. $0_1^+, 0_2^+, 0_3^+, \dots$ in ^{12}C

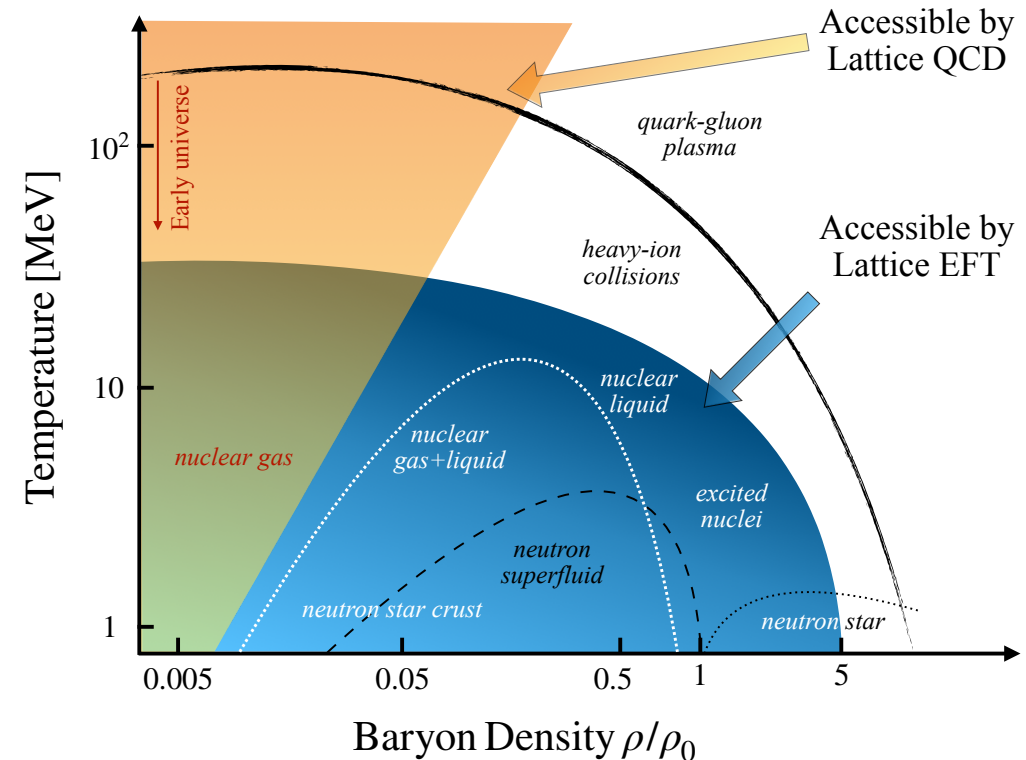
Euclidean time



Comparison to lattice QCD

31

LQCD (quarks & gluons)	NLEFT (nucleons & pions)
relativistic fermions	non-relativistic fermions
renormalizable th'y	EFT
continuum limit	no continuum limit
(un)physical masses	physical masses
Coulomb - difficult	Coulomb - easy
high T/small ρ	small T/nuclear densities
sign problem severe	sign problem moderate



- For nuclear physics, NLEFT is the far better methodology!

Computational equipment

- Present = JUWELS (modular system) + FRONTIER + ...



The minimal nuclear interaction: Extension to hyper-nuclei

The minimal interaction with strangeness I

34

Tong, Elhatisari, UGM, Sci. Bull. **70** (2025) 825

- Baryon-baryon interaction (consider nucleons and Λ 's plus non-local smearing):

$$V_{\Lambda N} = c_{N\Lambda} \sum_{\vec{n}} \tilde{\rho}(\vec{n}) \tilde{\xi}(\vec{n}) + c_{\Lambda\Lambda} \frac{1}{2} \sum_{\vec{n}} [\tilde{\xi}(\vec{n})]^2$$

$$\tilde{\rho}(\vec{n}) = \sum_{i,j=0,1} \tilde{a}_{i,j}^\dagger(\vec{n}) \tilde{a}_{i,j}(\vec{n}) + s_L \sum_{|\vec{n}-\vec{n}'|^2=1} \sum_{i,j=0,1} \tilde{a}_{i,j}^\dagger(\vec{n}') \tilde{a}_{i,j}(\vec{n}')$$

$$\tilde{\xi}(\vec{n}) = \sum_{i=0,1} \tilde{b}_i^\dagger(\vec{n}) \tilde{b}_i(\vec{n}) + s_L \sum_{|\vec{n}-\vec{n}'|^2=1} \sum_{i=0,1} \tilde{b}_i^\dagger(\vec{n}') \tilde{b}_i(\vec{n}')$$

- Three-baryon forces (consider nucleons and Λ 's, no non-local smearing):

Petschauer, Kaiser, Haidenbauer, UGM, Weise, Phys. Rev. C **93** (2016) 014001

$$V_{NN\Lambda} = c_{NN\Lambda} \frac{1}{2} \sum_{\vec{n}} [\rho(\vec{n})]^2 \xi(\vec{n}), \quad V_{N\Lambda\Lambda} = c_{N\Lambda\Lambda} \frac{1}{2} \sum_{\vec{n}} \rho(\vec{n}) [\xi(\vec{n})]^2$$

↪ must determine 4 LECs! [smearing parameters from the nucleon sector]

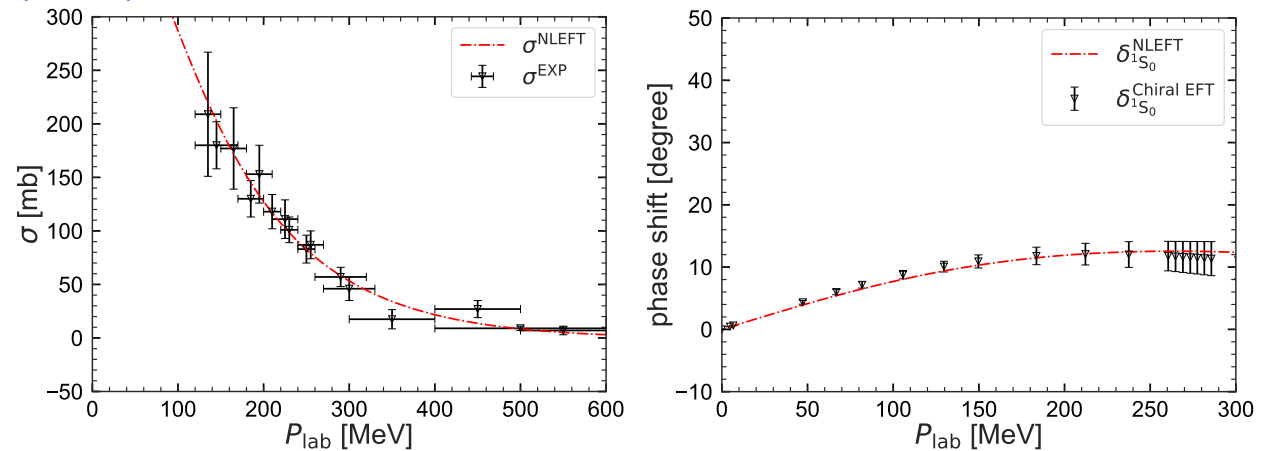
↪ first time that the $\Lambda\Lambda N$ three-body force is included

The minimal interaction with strangeness II

35

Tong, Elhatisari, UGM, Sci. Bull. **70** (2025) 825

- Two-body LECs from scattering data (ΛN) & chiral EFT phase shift ($\Lambda\Lambda$)



- Three-body LECs from the separation energies of Λ and $\Lambda\Lambda$ hyper-nuclei:

$$B_{\Lambda}({}^A_{\Lambda}Z) = E({}^{A-1}Z) - E({}^A_{\Lambda}Z)$$

$$B_{\Lambda\Lambda}({}^A_{\Lambda\Lambda}Z) = E({}^{A-2}Z) - E({}^A_{\Lambda\Lambda}Z)$$

Nucleus	NLEFT [MeV]	Exp. [MeV]
${}^5_{\Lambda}\text{He}$	3.10(9)	3.10(3)
${}^9_{\Lambda}\text{Be}$	6.64(13)	6.61(7)
${}^{13}_{\Lambda}\text{C}$	11.71(14)	11.80(16)
${}^6_{\Lambda\Lambda}\text{He}$	6.96(9)	6.91(16)
${}^{10}_{\Lambda\Lambda}\text{Be}$	14.35(13)	14.70(40)

↪ this defines our EoS of hyper-nuclear matter called **HMN(I)**

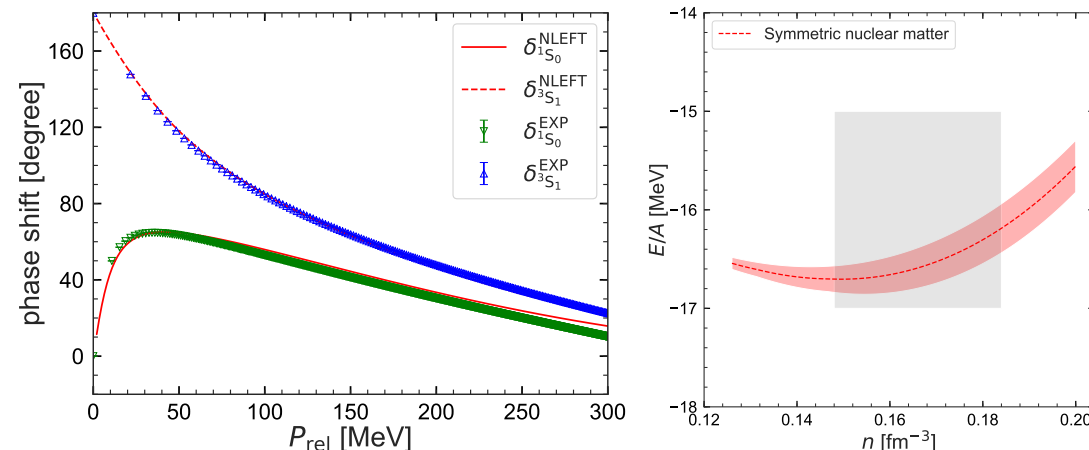
The minimal nuclear interaction: EoS & neutron star properties

Pure neutron matter

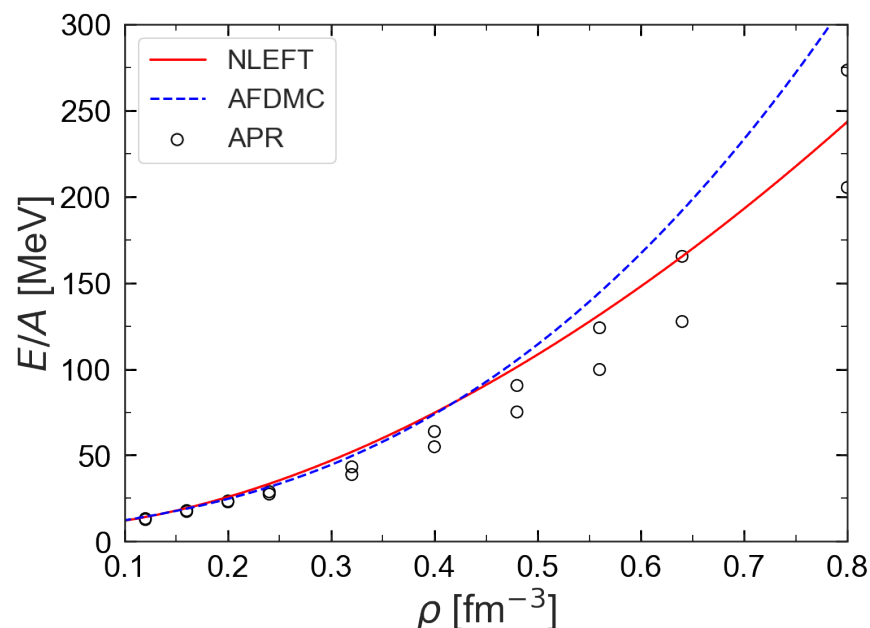
37

Tong, Elhatisari, UGM, Sci. Bull. **70** (2025) 825

- Input: S-wave phase shifts (2N)
& symmetric nuclear matter (3N)
- Note: extension of the minimal interaction (leading SU(4) breaking)



⇒ Output: Pure neutron matter (PNM) EoS



— comparable to the renowned APR EoS

Akmal, Pandharipande, Ravenhall, Phys. Rev. C **58** (1998) 1804

— less stiff than the recent AFDMC one

Gandolfi et al., Eur. Phys. J. A **50** (2014) 10

→ work out consequences for
neutron stars based on this PNM EoS

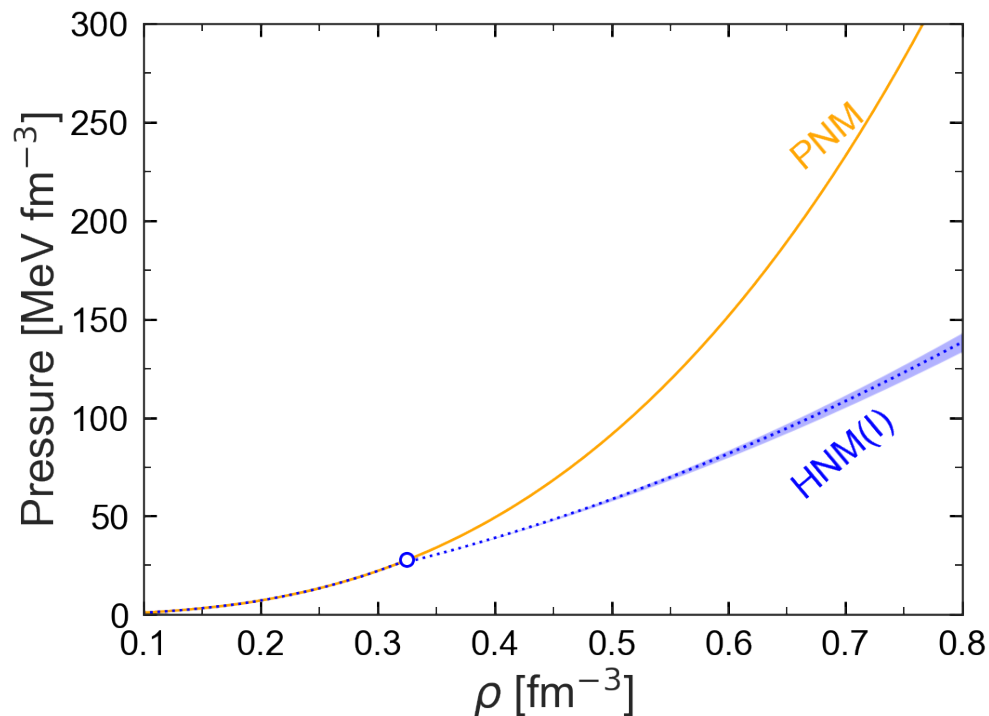
Neutron star properties

38

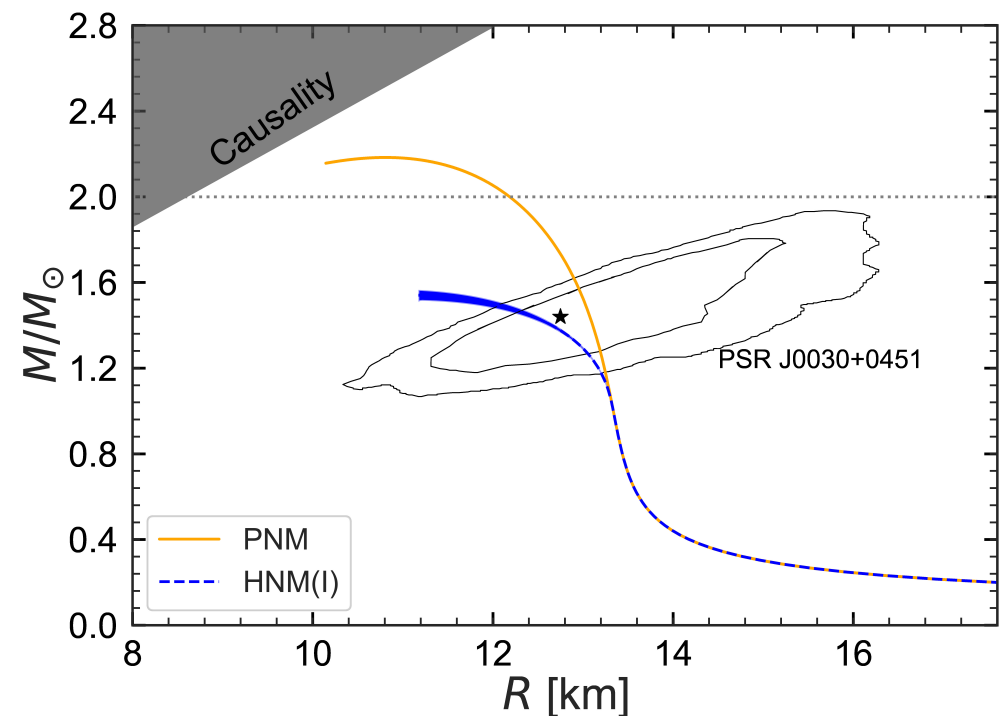
Tong, Elhatisari, UGM, Sci. Bull. **70** (2025) 825

- Now solve the TOV equations for the PNM and HNM(I) EoSs:

- EoS (PNM and HNM(I))



- Mass-radius relation



- Maximum neutron star mass: $M_{\max} = 2.18(1) M_\odot$ for PNM

$$M_{\max} = 1.54(2) M_\odot \text{ for HNM(I)} \rightarrow \text{need repulsion}$$

EoS of hyper-neutron matter

39

Tong, Elhatisari, UGM, Sci. Bull. **70** (2025) 825; Astrophys. J. **982** (2025) 164

- Not surprisingly, we need more repulsion [as in the pure neutron matter case]

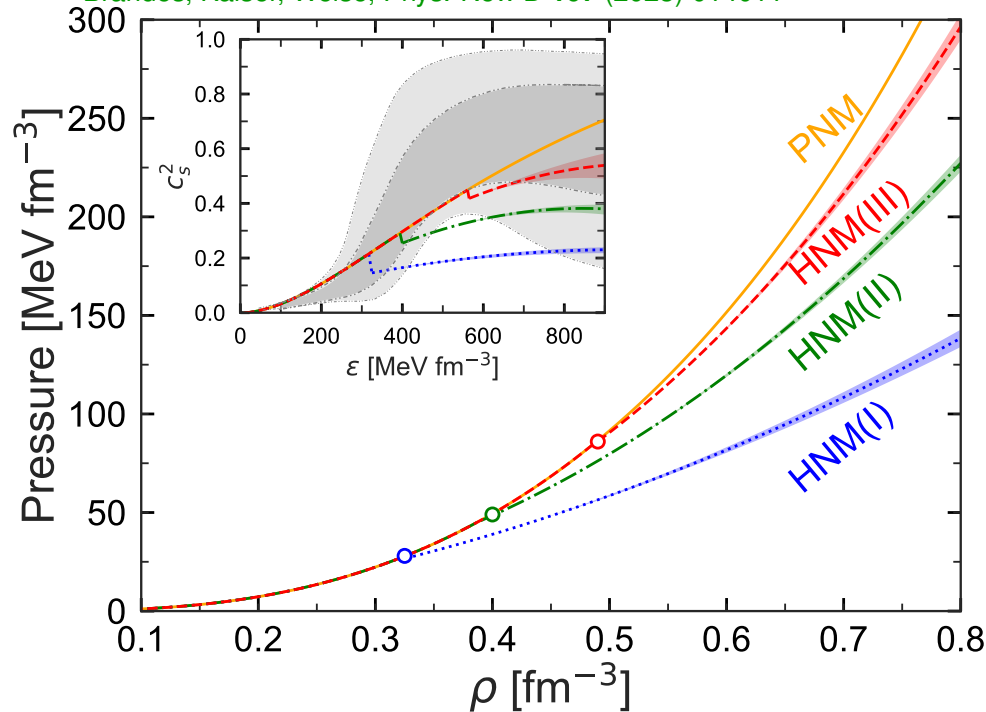
↪ this will move the threshold of $\mu_\Lambda = \mu_n$ up

↪ take $M_{\max}$ as data point: $M_{\max} = 1.9M_\odot$ for HNM(II)

$M_{\max} = 2.1M_\odot$ for HNM(III)

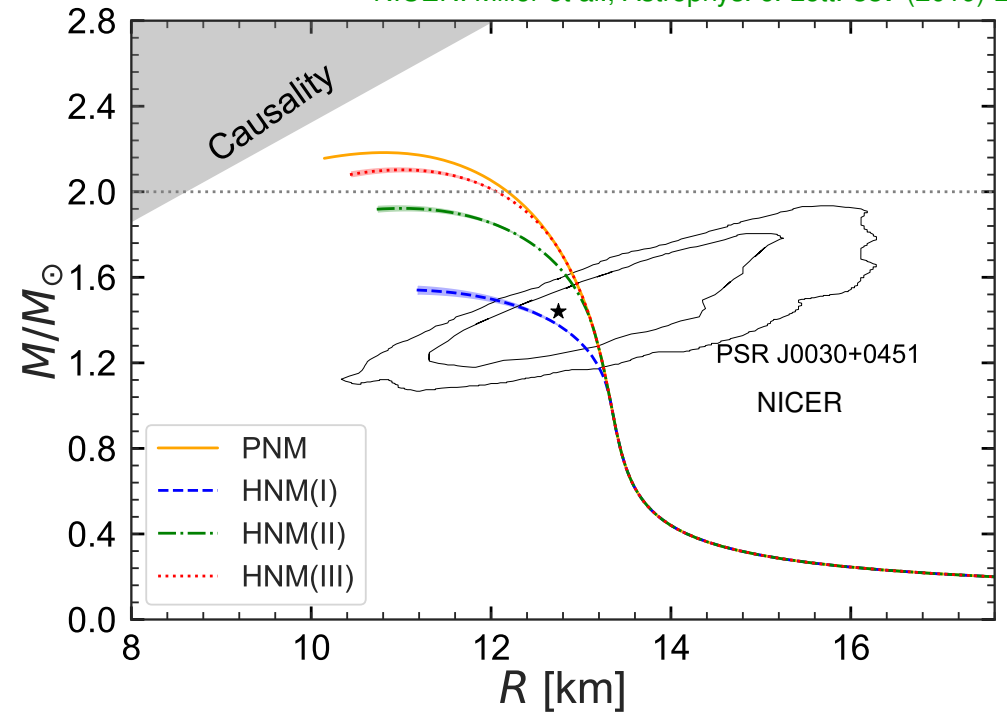
- EoS & speed of sound

Brandes, Kaiser, Weise, Phys. Rev. D **107** (2023) 014011



- Mass-radius relation

NICER: Miller et al., Astrophys. J. Lett. **887** (2019) L24



- Just two teasers for finite T calculations

PHYSICAL REVIEW LETTERS **125**, 192502 (2020)

Ab Initio Nuclear Thermodynamics

Bing-Nan Lu¹, Ning Li¹, Serdar Elhatisari², Dean Lee¹, Joaquín E. Drut³, Timo A. Lähde⁴,
Evgeny Epelbaum⁵ and Ulf-G. Meißner^{6,4,7}

¹Facility for Rare Isotope Beams and Department of Physics and Astronomy, Michigan State University,
East Lansing, Michigan 48824, USA

²Faculty of Engineering, Karamanoglu Mehmetbey University, Karaman 70100, Turkey

³Department of Physics and Astronomy, University of North Carolina, Chapel Hill, North Carolina 27599-3255, USA

⁴Institute for Advanced Simulation, Institut für Kernphysik, and Jülich Center for Hadron Physics,
Forschungszentrum Jülich, D-52425 Jülich, Germany

⁵Ruhr-Universität Bochum, Fakultät für Physik und Astronomie, Institut für Theoretische Physik II, D-44780 Bochum, Germany

⁶Helmholtz-Institut für Strahlen- und Kernphysik and Bethe Center for Theoretical Physics, Universität Bonn, D-53115 Bonn, Germany

⁷Tbilisi State University, 0186 Tbilisi, Georgia

 (Received 11 April 2020; revised 6 August 2020; accepted 29 September 2020; published 3 November 2020)

We propose a new Monte Carlo method called the pinhole trace algorithm for *ab initio* calculations of the thermodynamics of nuclear systems. For typical simulations of interest, the computational speedup relative to conventional grand-canonical ensemble calculations can be as large as a factor of one thousand. Using a leading-order effective interaction that reproduces the properties of many atomic nuclei and neutron matter to a few percent accuracy, we determine the location of the critical point and the liquid-vapor coexistence line for symmetric nuclear matter with equal numbers of protons and neutrons. We also present the first *ab initio* study of the density and temperature dependence of nuclear clustering.

- new pinhole trace algorithm

↪ liquid-vapor phase transition

↪ location of the critical point

- new light cluster distillation method

↪ abundances of dimers, trimers, tetramers

↪ benchmark for virial calculations

Phys. Lett. B 850 (2024) 138463



Contents lists available at ScienceDirect

Physics Letters B

journal homepage: www.elsevier.com/locate/physletb



Letter

Ab initio study of nuclear clustering in hot dilute nuclear matter

Zhengxue Ren^{a,b,c,*}, Serdar Elhatisari^{c,b}, Timo A. Lähde^{a,d}, Dean Lee^c, Ulf-G. Meißner^{b,a,f}

^a Institut für Kernphysik, Institute for Advanced Simulation and Jülich Center for Hadron Physics, Forschungszentrum Jülich, D-52425 Jülich, Germany

^b Helmholtz-Institut für Strahlen- und Kernphysik und Bethe Center for Theoretical Physics, Universität Bonn, D-53115 Bonn, Germany

^c Faculty of Natural Sciences and Engineering, Gaziantep Islam Science and Technology University, Gaziantep 27010, Turkey

^d Center for Advanced Simulation and Analytics (CASA), Forschungszentrum Jülich, D-52425 Jülich, Germany

^e Facility for Rare Isotope Beams and Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824, USA

^f Tbilisi State University, 0186 Tbilisi, Georgia

ARTICLE INFO

Editor: A. Schwenk

ABSTRACT

We present a systematic *ab initio* study of clustering in hot dilute nuclear matter using nuclear lattice effective field theory with an SU(4)-symmetric interaction. We introduce a method called light-cluster distillation to determine the abundances of dimers, trimers, and alpha clusters as a function of density and temperature. Our lattice results are compared with an ideal gas model composed of free nucleons and clusters. Excellent agreement is found at very low density, while deviations from ideal gas abundances appear at increasing density due to cluster-nucleon and cluster-cluster interactions. In addition to determining the composition of hot dilute nuclear matter as a function of density and temperature, the lattice calculations also serve as benchmarks for virial expansion calculations, statistical models, and transport models of fragmentation and clustering in nucleus-nucleus collisions.

