Ab initio nuclear theory on the lattice

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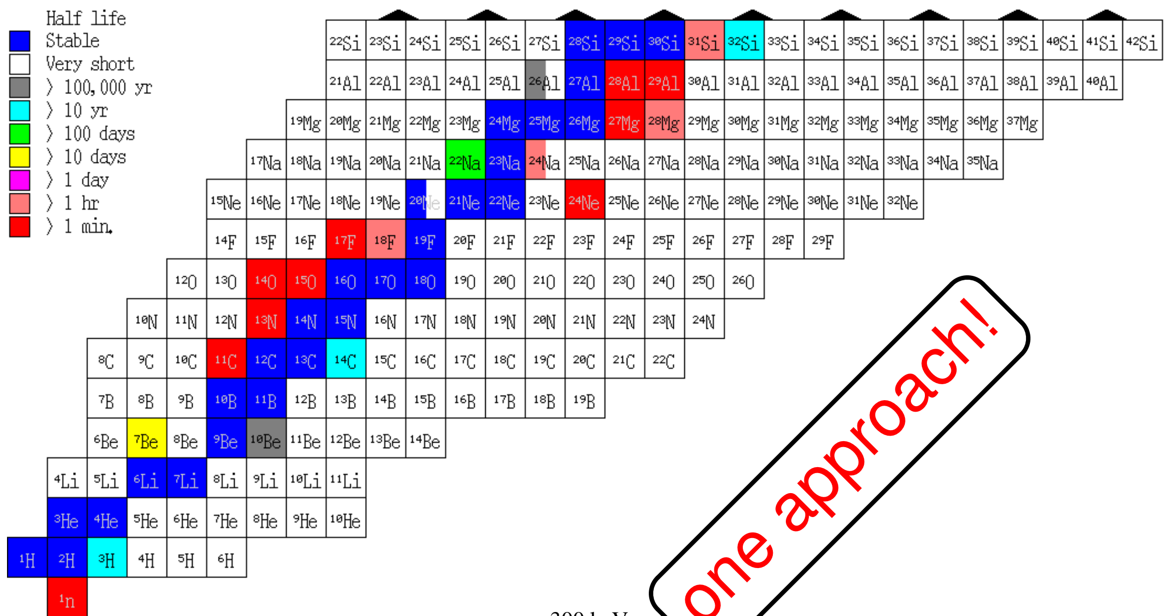
Contents

Very brief Introduction

Our goal: Ab initio nuclear structure & reactions

- Nuclear structure:
  - ⋆ limits of stability
  - ⋆ 3-nucleon forces
  - ⋆ alpha-clustering
  - ⋆ EoS & neutron stars
  - ⋮



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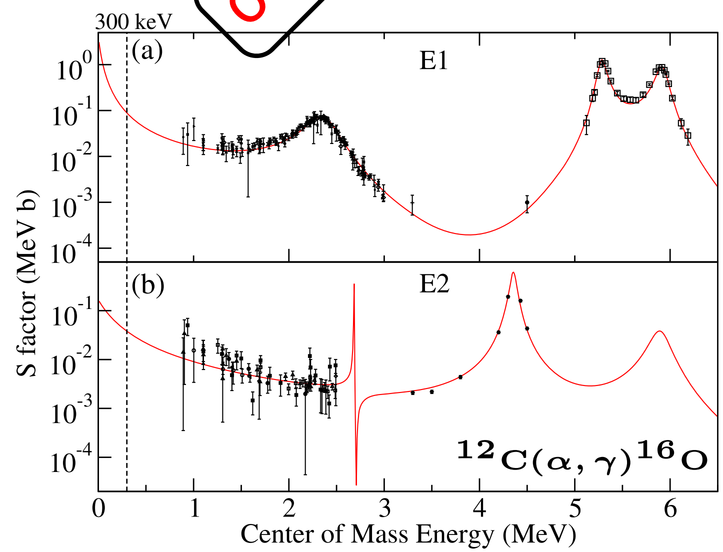
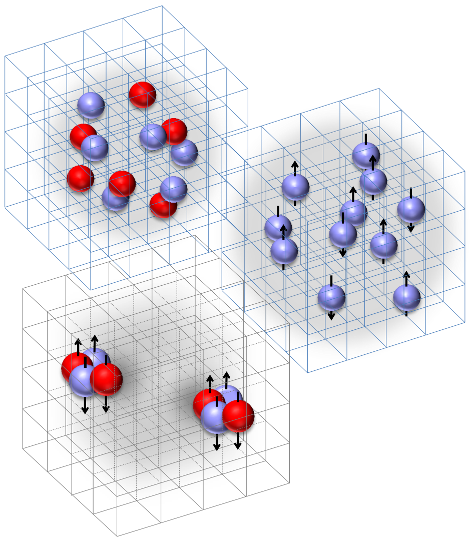
one approach!

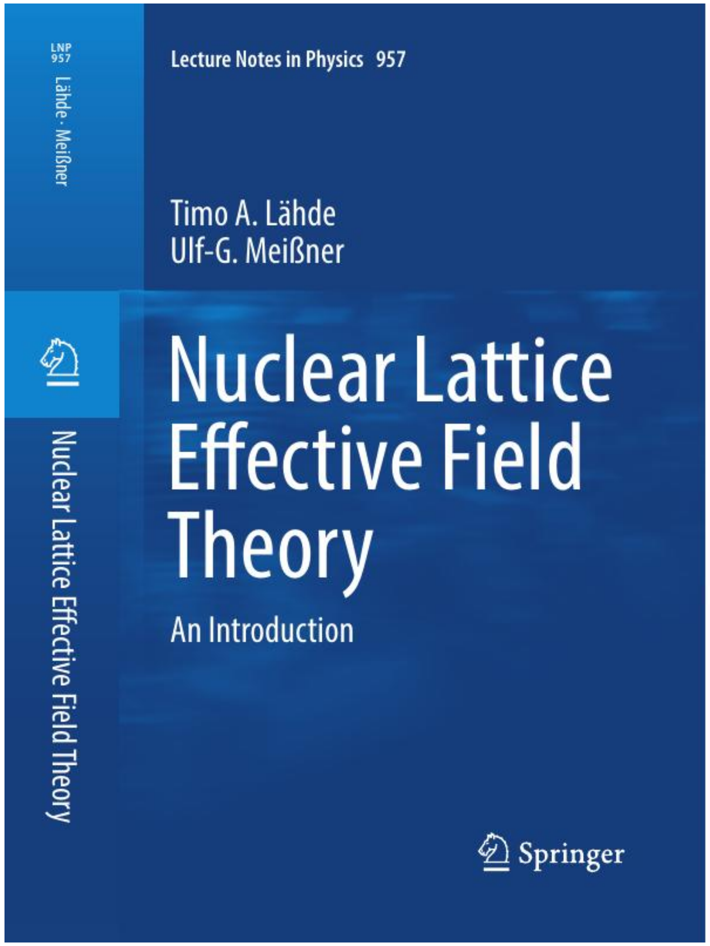
- Nuclear reactions, nuclear astrophysics:
  - ⋆ alpha-particle scattering
  - ⋆ triple-alpha reaction
  - ⋆ alpha-capture on carbon
  - ⋮



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

- Much more details on EFTs in light quark physics:

Effective Field Theories

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Nuclear lattice effective field theory (NLEFT)

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

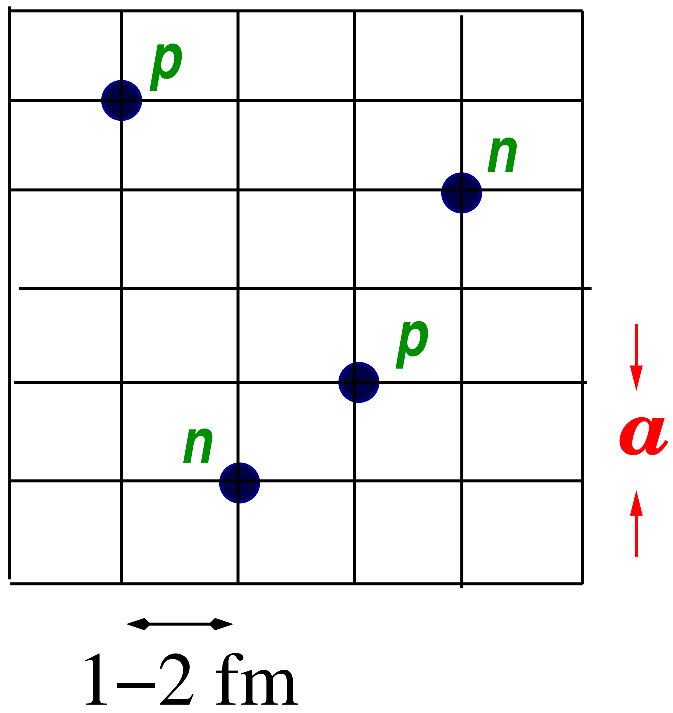
- discretize space-time $V = L_s \times L_s \times L_s \times L_t$: nucleons are point-like particles on the sites

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

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

- typical lattice parameters

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



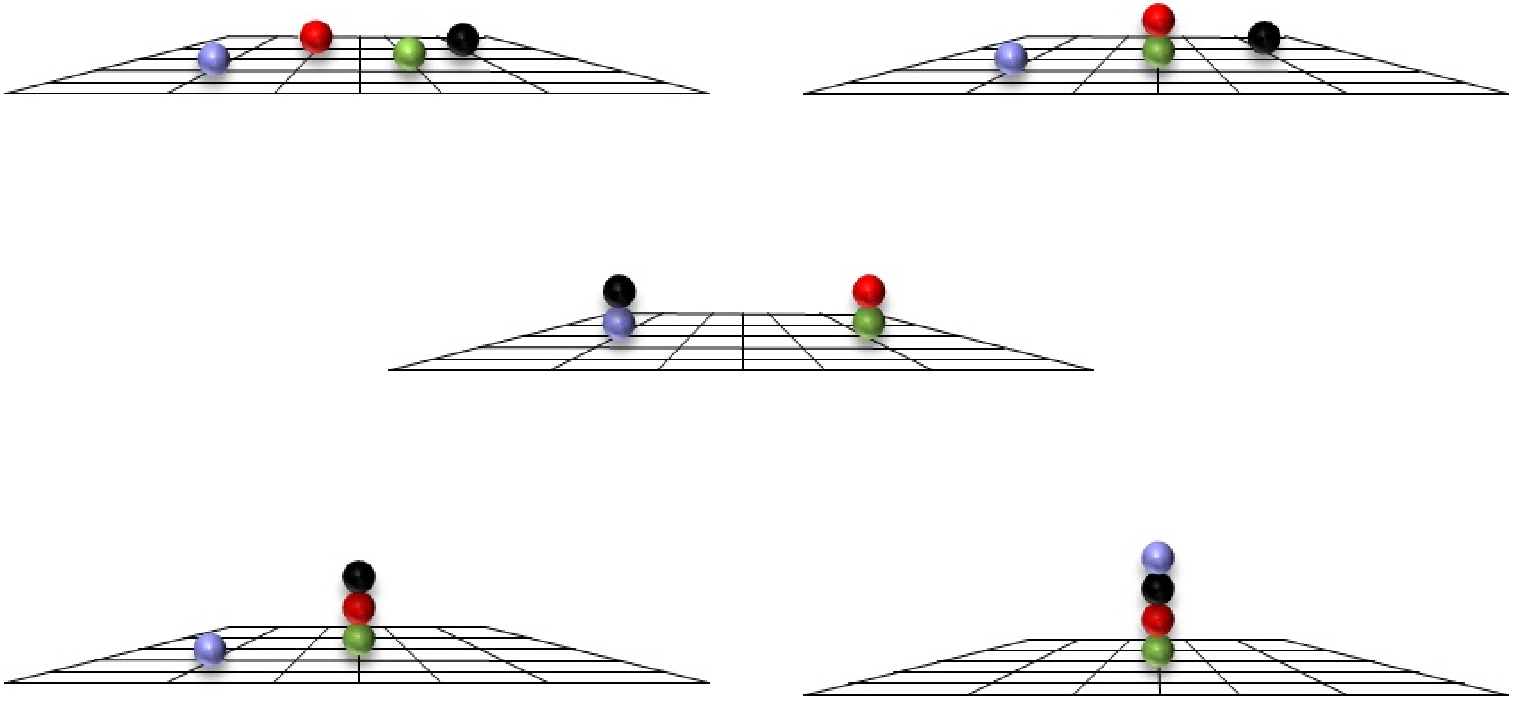
- strong suppression of sign oscillations due to approximate Wigner SU(4) symmetry

  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 $a = 1 \ldots 2$ 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

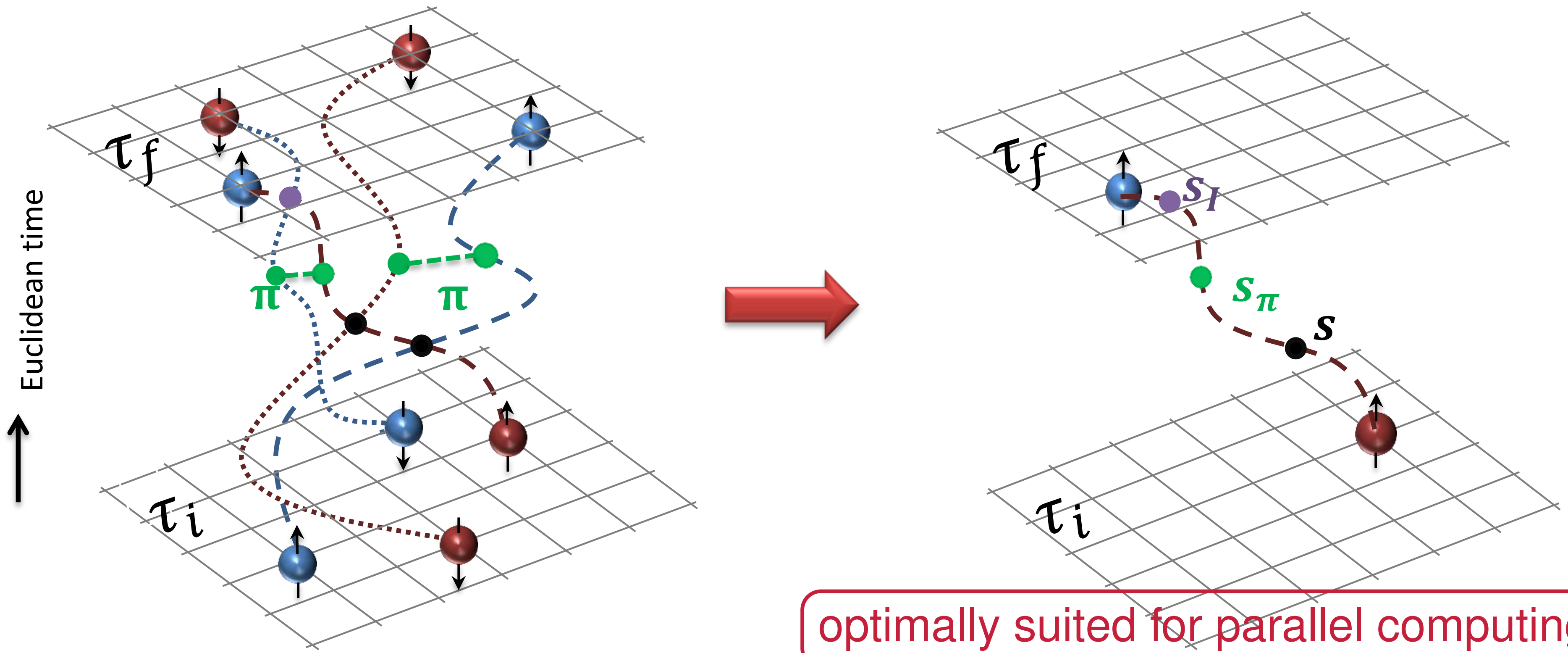
⇒ preparation of *all possible* initial/final states

⇒ *clustering* emerges *naturally*

Auxiliary field method

- Represent interactions by auxiliary fields (Gaussian quadrature):

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



optimally suited for parallel computing!

Computational equipment

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

87 Pflops $\rightarrow$ Exascale

Chiral Interactions at N3LO: Foundations

Towards precision calculations of heavy nuclei

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

  $\hookrightarrow$ precision limited, need to go to N3LO

- Two step procedure:

  1) Further improve the LO action

  $\hookrightarrow$ minimize the sign oscillations

  $\hookrightarrow$ minimize the higher-body forces

  $\hookrightarrow$ done $\surd$ see also Wu et al., 2503.18017

  2) Work out the corrections to N3LO

  $\hookrightarrow$ first on the level of the NN interaction $\surd$

  $\hookrightarrow$ new important technique: **wave function matching** $\surd$

  $\hookrightarrow$ second for the spectra/radii/... of nuclei (first results) $\surd$

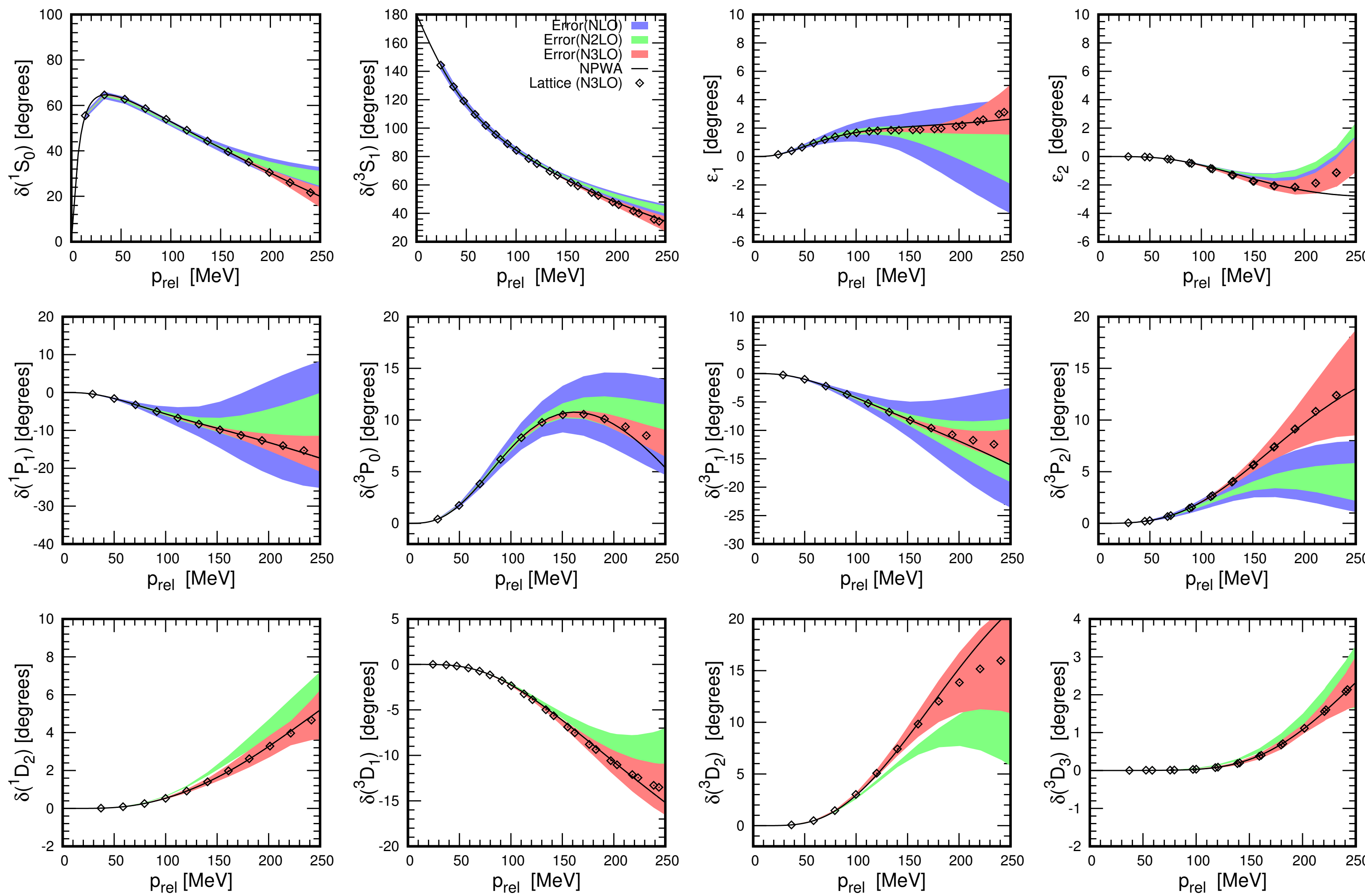
  $\hookrightarrow$ third for nuclear reactions/astrophysics (first results) $\surd$

NN interaction at N3LO

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

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

NLO
N2LO
N3LO

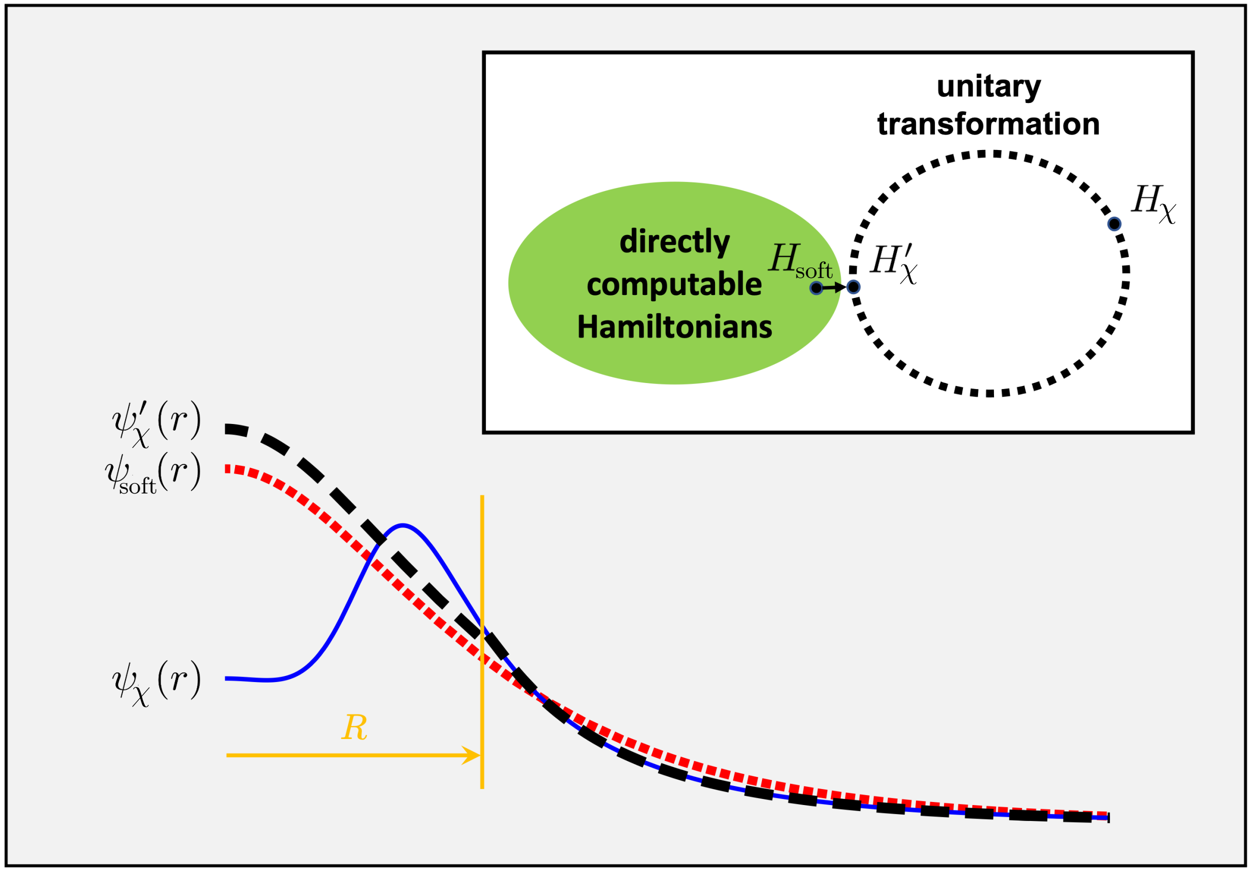


uncertainty estimates á la Epelbaum, Krebs, UGM,
Eur. Phys. J. A **51** (2015) 53

Wave function matching

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

- Graphical representation of w.f. matching



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

Scattering: Methods I

- 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

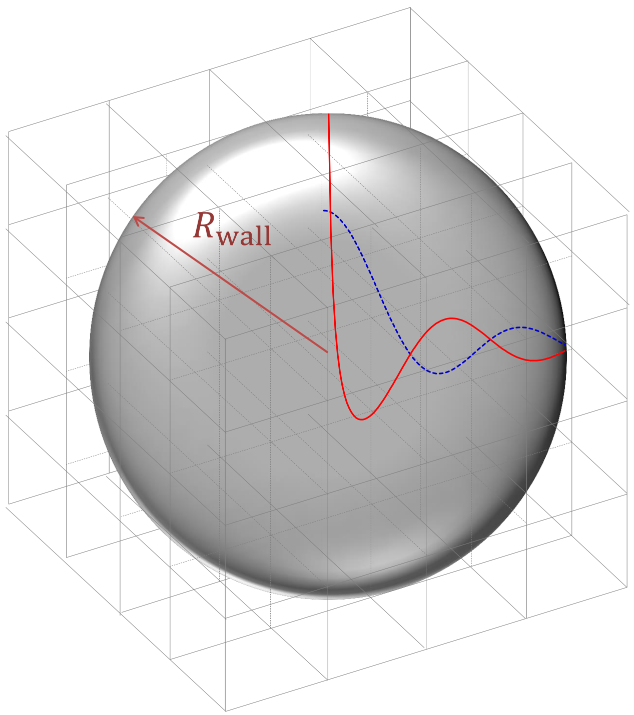
$\hookrightarrow$ works in many cases, problems w/ partial-wave mixing and cluster-cluster scattering

- 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

$\hookrightarrow$ 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}

  $\hookrightarrow$ much improved precision

Scattering: Methods II

- 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

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

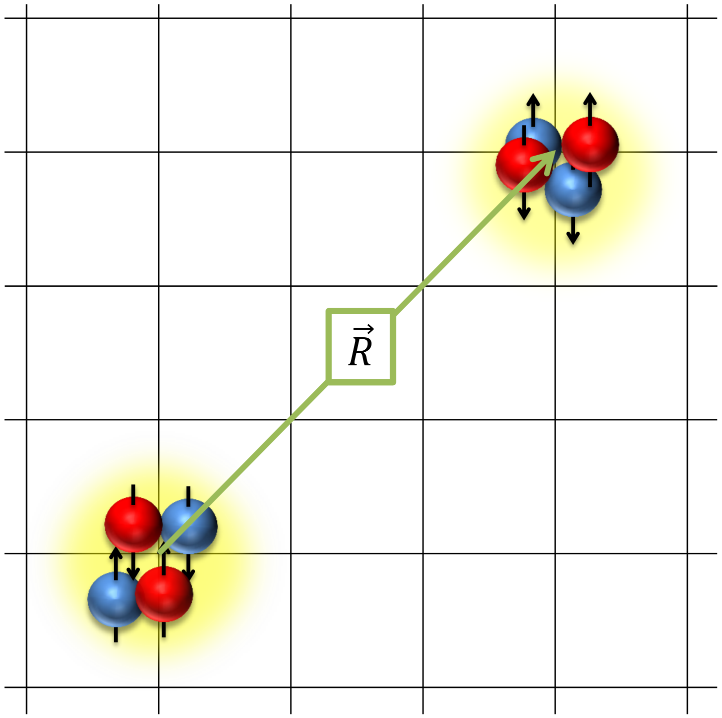
- project them in Euclidean time with the chiral EFT Hamiltonian H

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

$\rightarrow$ "dressed cluster states" (polarization, deformation, Pauli)

- Adiabatic Hamiltonian (requires norm matrices)

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

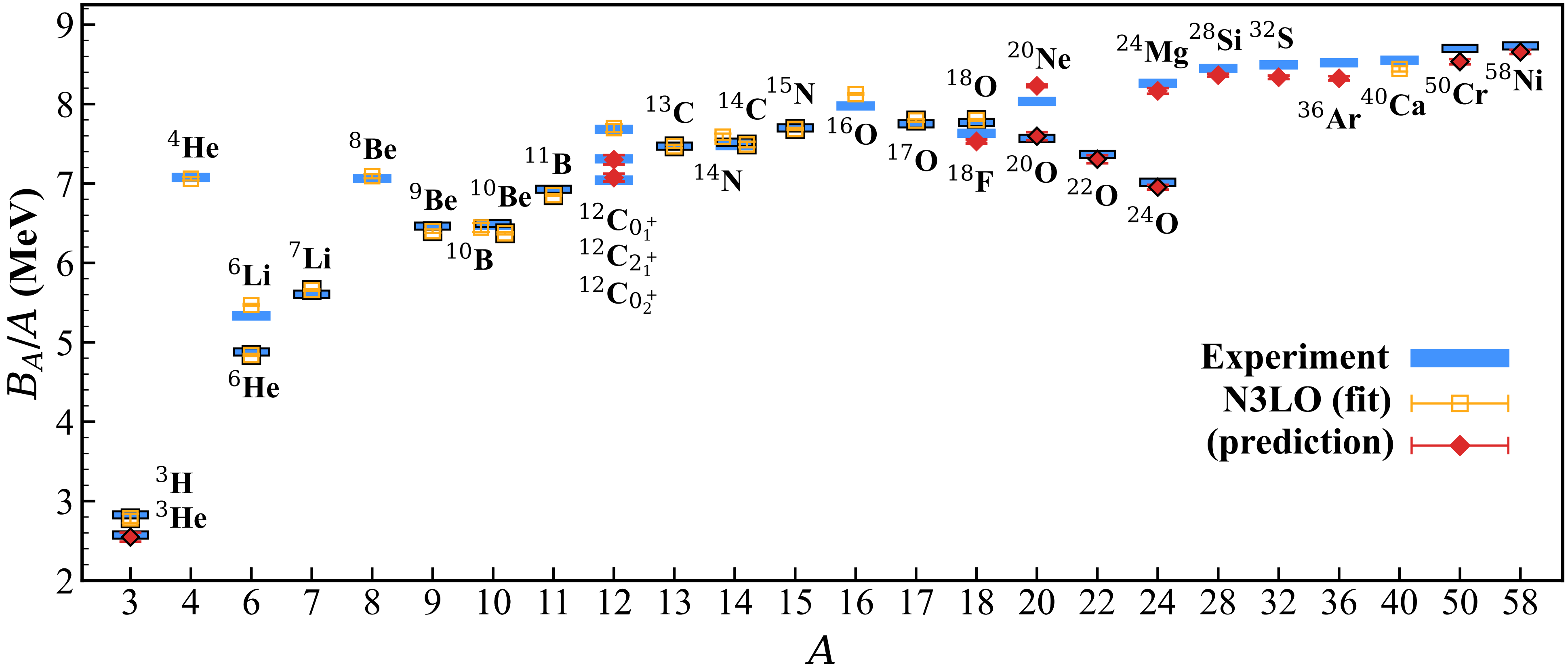


Chiral Interactions at N3LO: Applications to nuclear structure

Binding Energies at N3LO

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

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

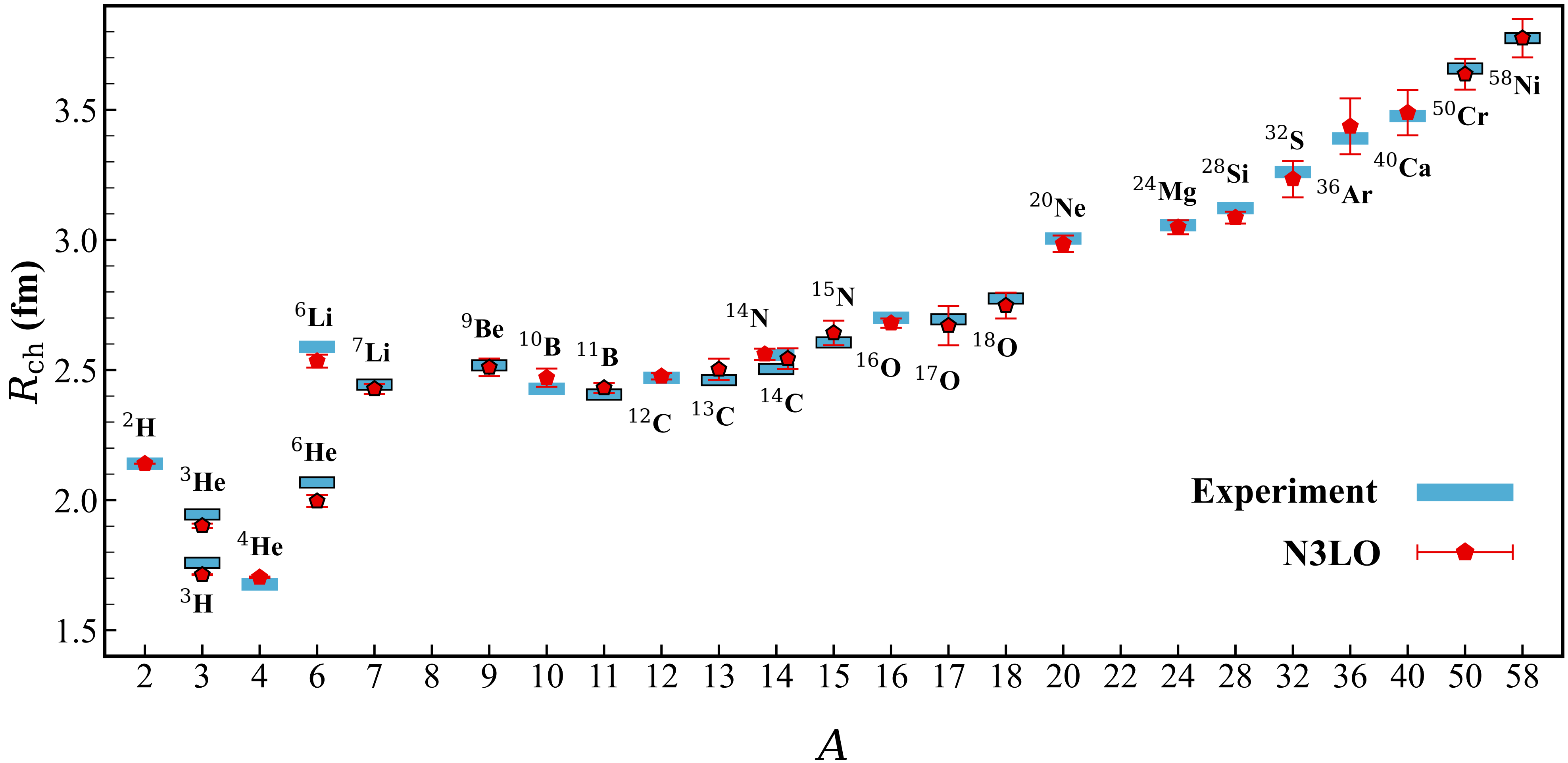


$\rightarrow$ excellent starting point for precision studies

Prediction: Charge radii at N3LO

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

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

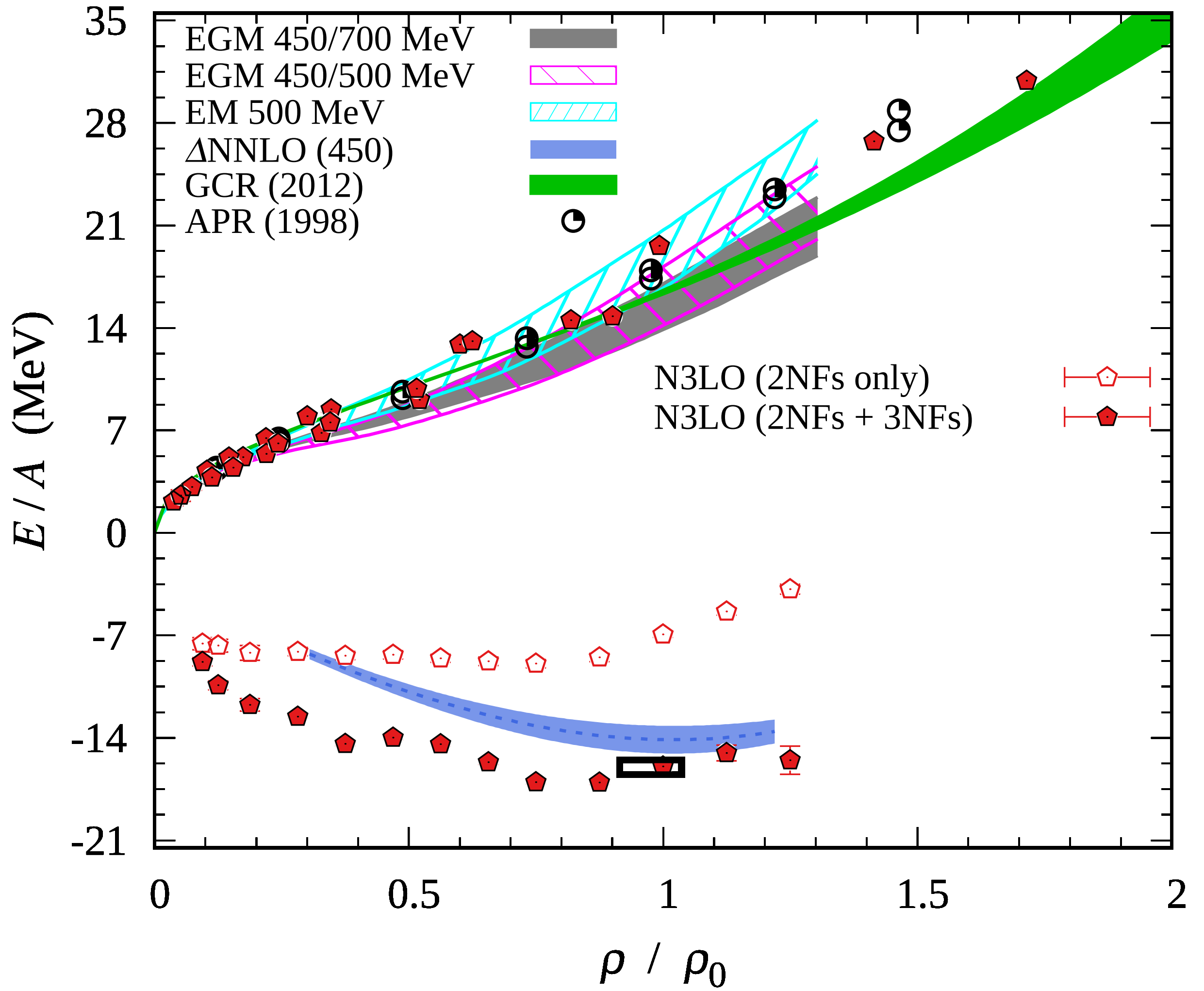


$\hookrightarrow$ no radius problem!

Prediction: Neutron & nuclear matter at N3LO

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

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

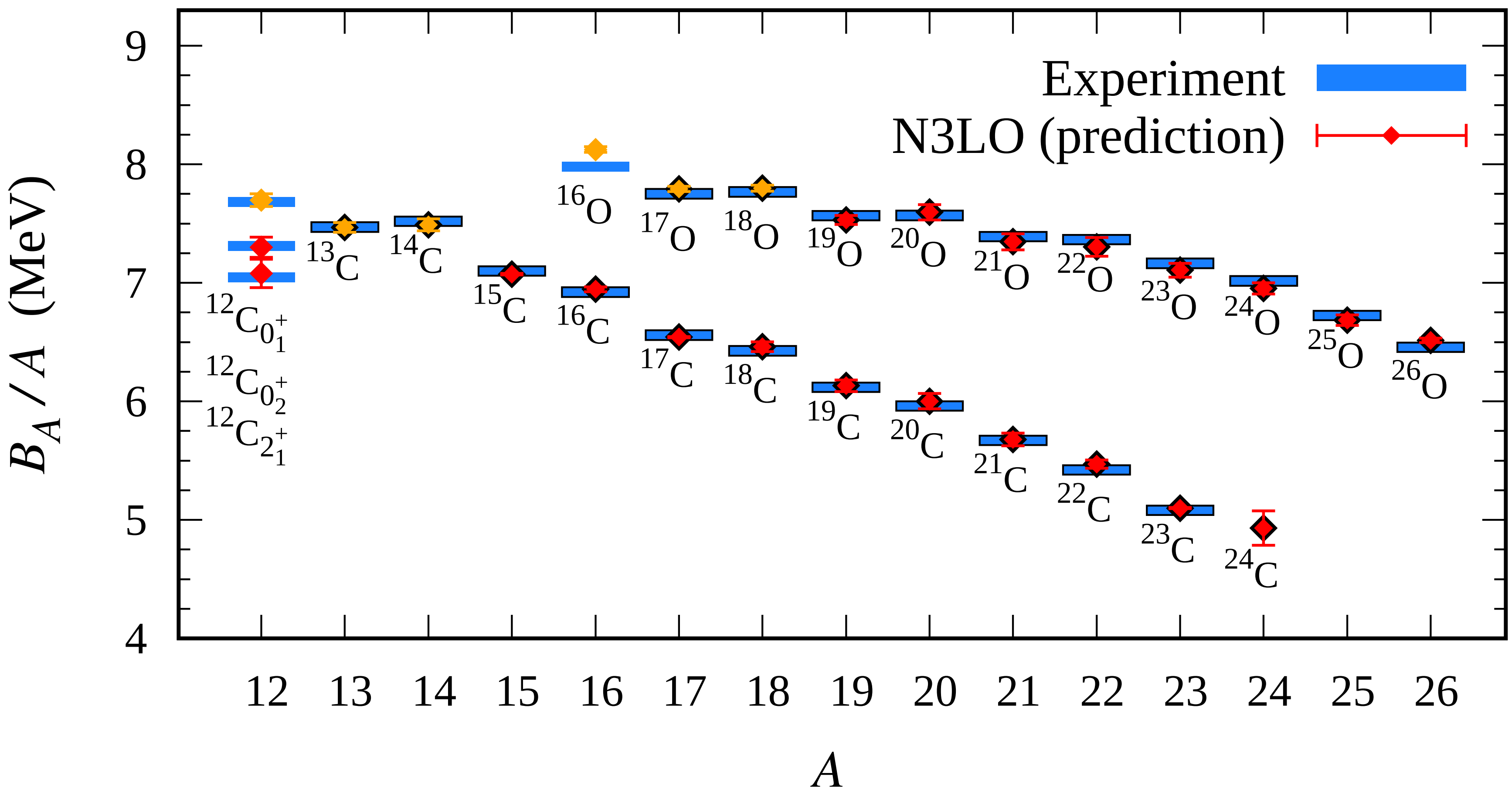


$\hookrightarrow$ can be improved using twisted b.c.'s

Prediction: Isotope chains of carbon & oxyen

Song et al., 2502.18722 [nucl-th]

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



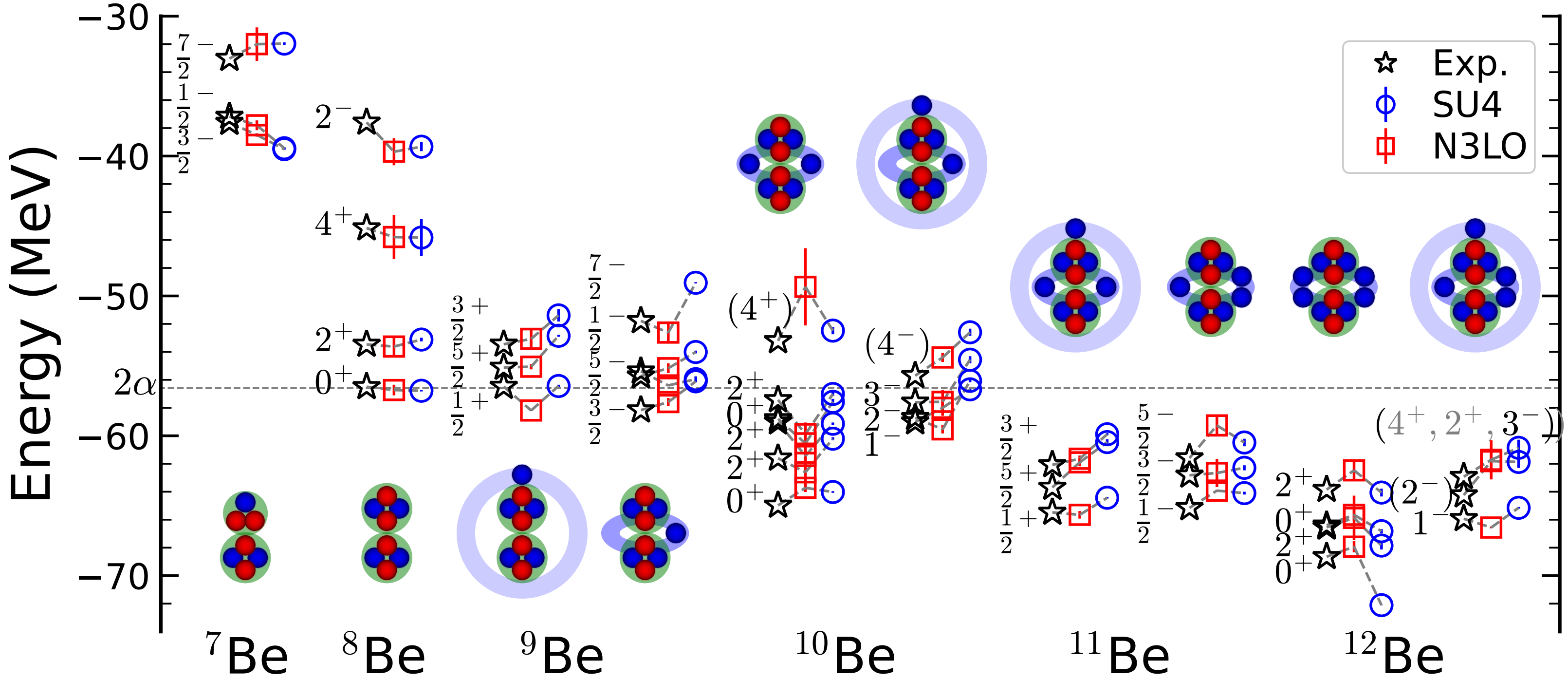
$\hookrightarrow$ 3NFs of utmost importance for the n-rich isotopes!

$\hookrightarrow$ universal features of neutron correlations

Prediction: Be isotopes

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

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

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

- Experiment: $\langle \mathbf{F}\rangle = \sum_{n=1}^{3} \langle {}^3\mathrm{He}\|\tau_{n,+}\|{}^3\mathrm{H}\rangle = 0.9998$ [theory!]

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

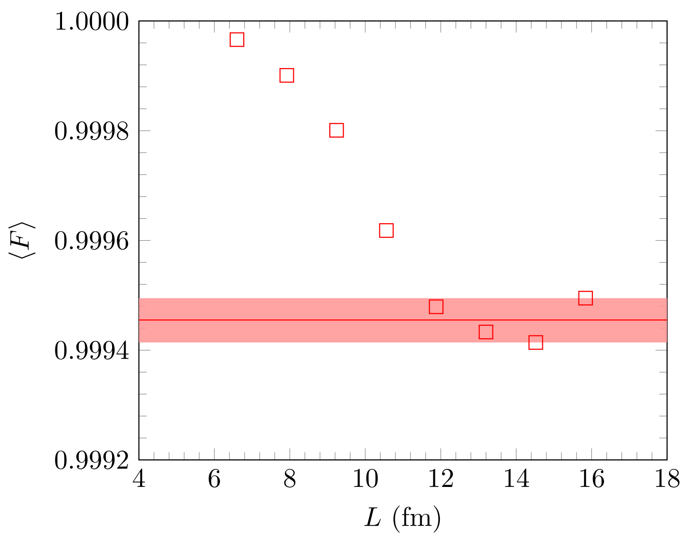
- NLEFT:

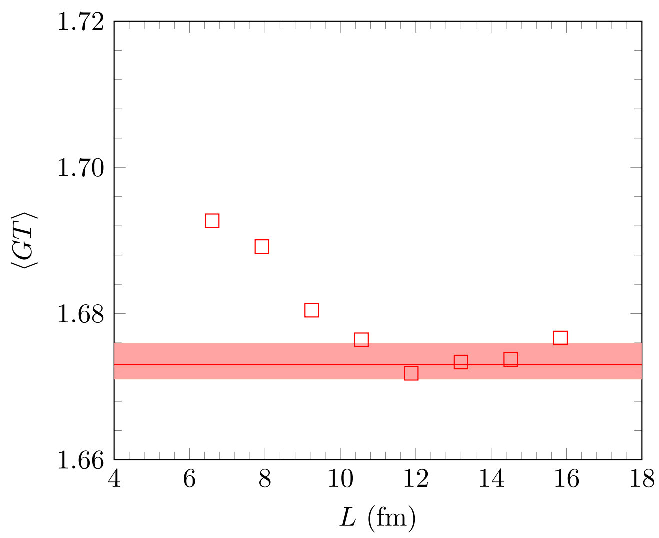
$$\langle \mathbf{F}\rangle_{\mathrm{N3LO}} = 0.99949(11)$$

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

$\hookrightarrow$ Important first step

$\hookrightarrow$ Larger nuclei underway...



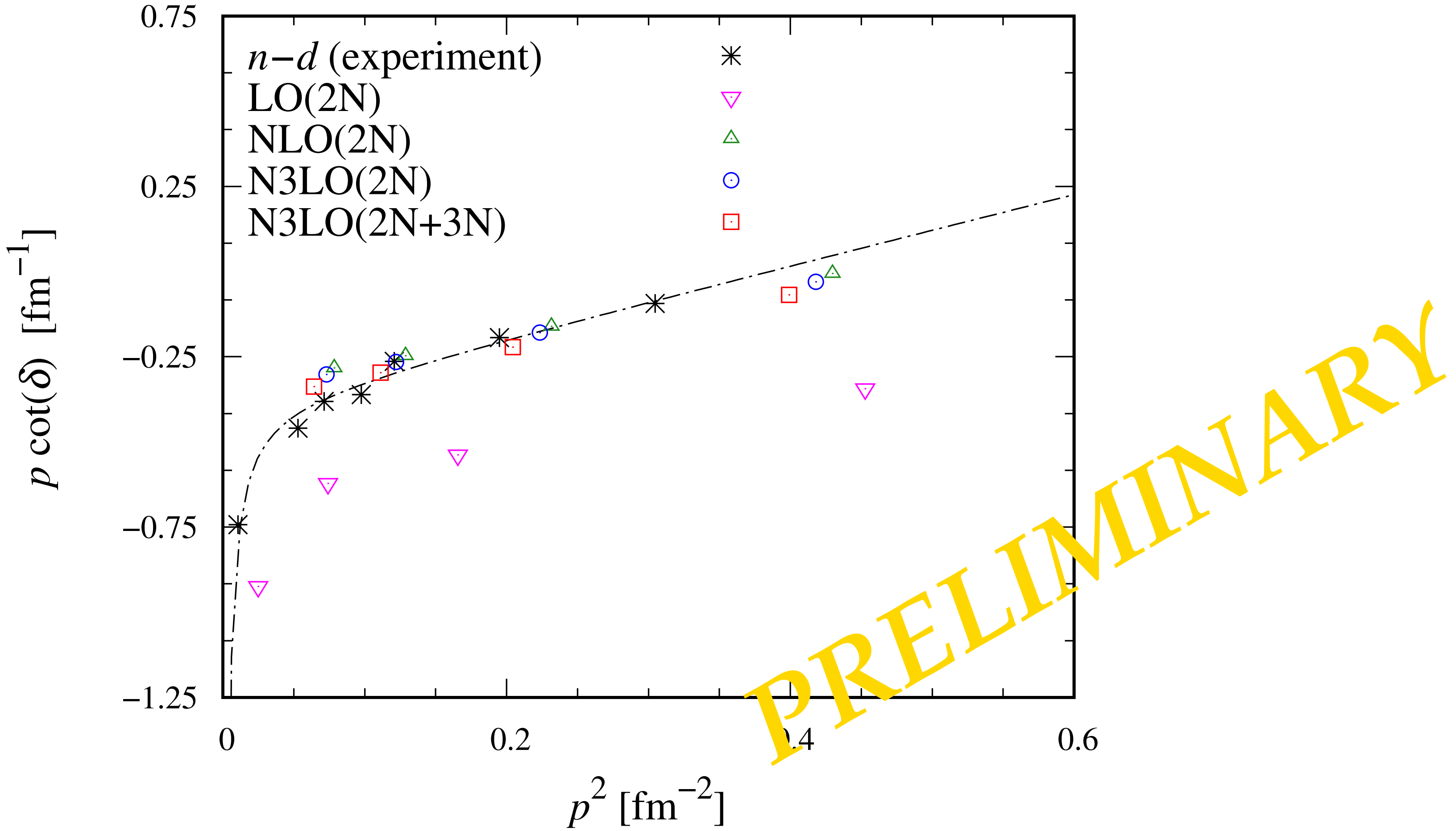


Chiral Interactions at N3LO: Applications to scattering

Scattering: Neutron-deuteron scattering at N3LO

Elhatisari, Hildenbrand, UGM, in progress

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

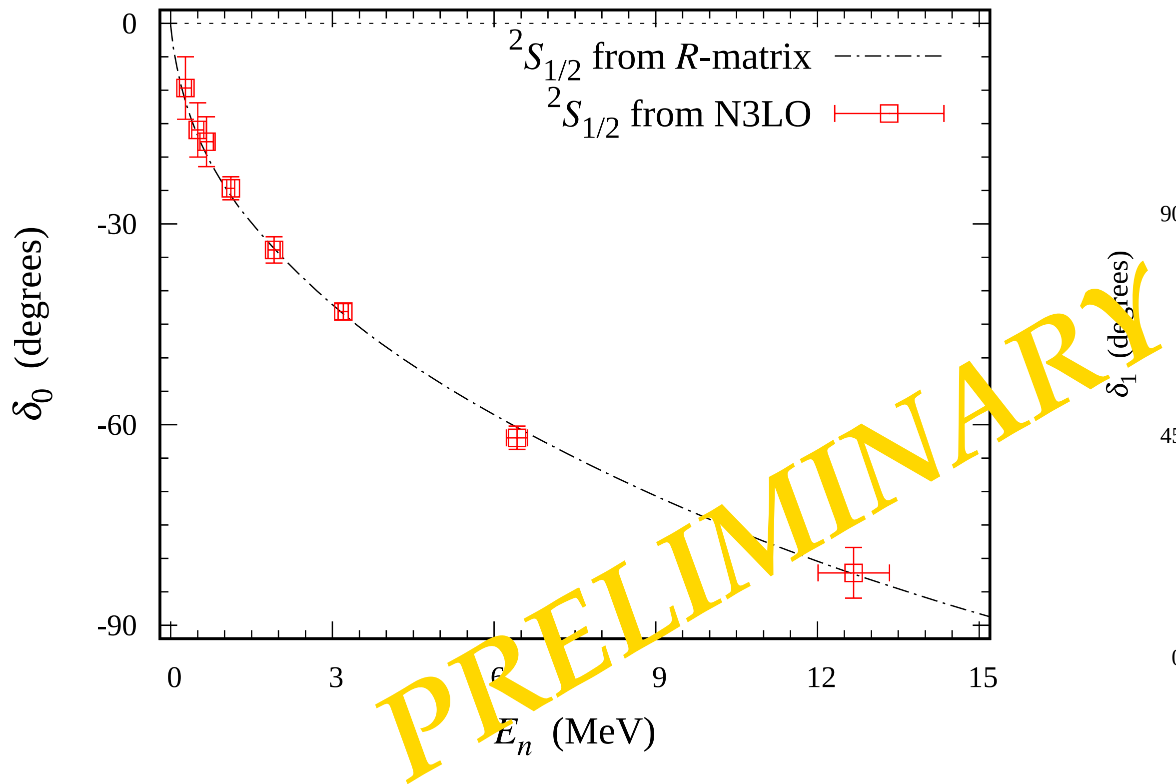


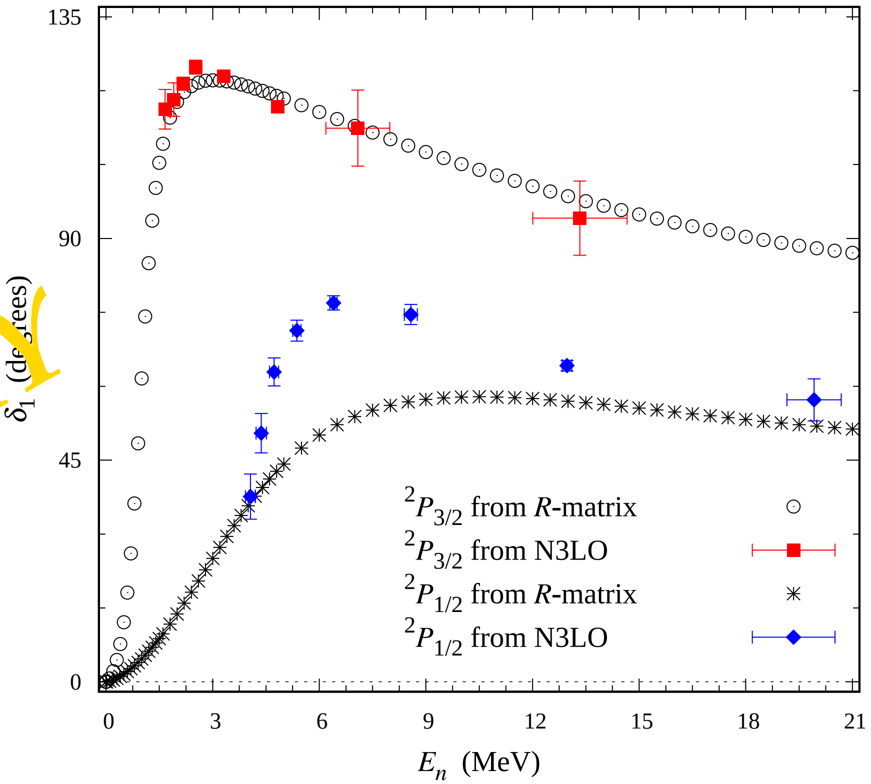
$\hookrightarrow$ shows good convergence

Scattering: Neutron-alpha scattering at N3LO

Elhatisari, Hildenbrand, UGM, in progress

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





- R-matrix results from G. Hale, private communication

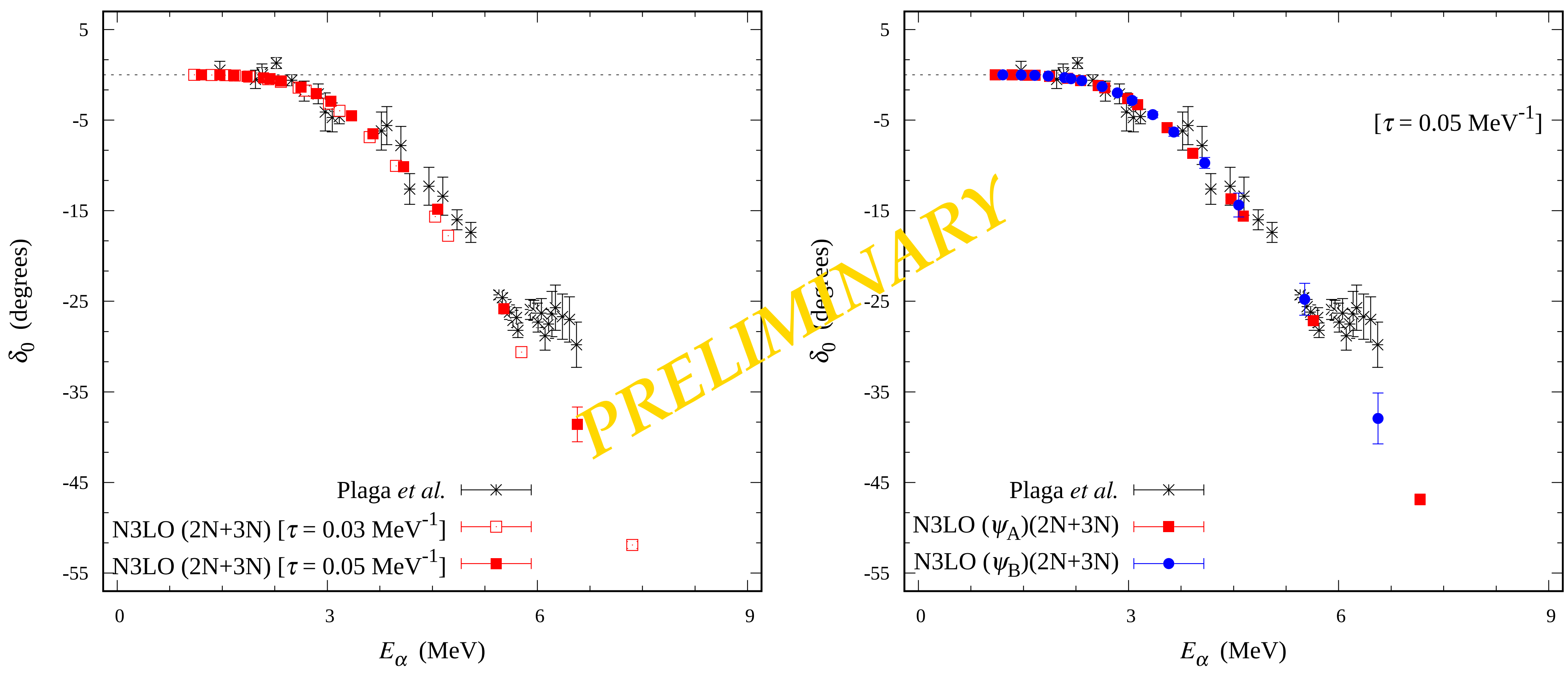
$\hookrightarrow$ Some fine-tuning of three-body forces for $^2P_{1/2}$ needed

Scattering: Alpha-carbon scattering at N3LO

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

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

  $\hookrightarrow$ different Euclidean times & different initial states



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

$\psi_A \sim {}^{16}\text{O}\,,\ \ \psi_B \sim {}^{12}\text{C} + {}^{4}\text{He}$

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
    - ↪ hyper-nuclei are under investigation

Hildenbrand et al., Eur. Phys. J. A **60** (2024) 215

    - ↪ first results for neutron stars

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

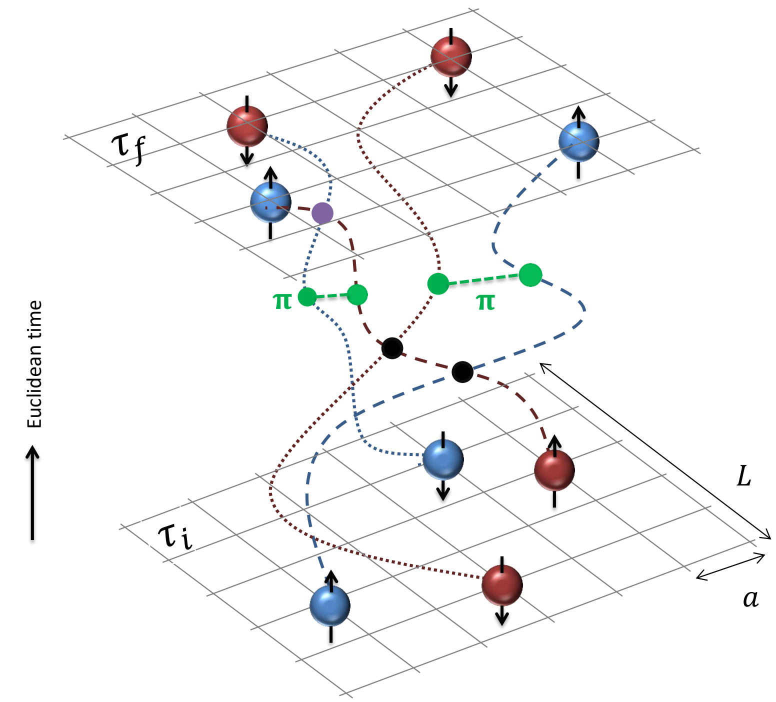
  [or a more sophisticated (correlated) initial/final state]

Euclidean time

- Transient energy

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

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



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

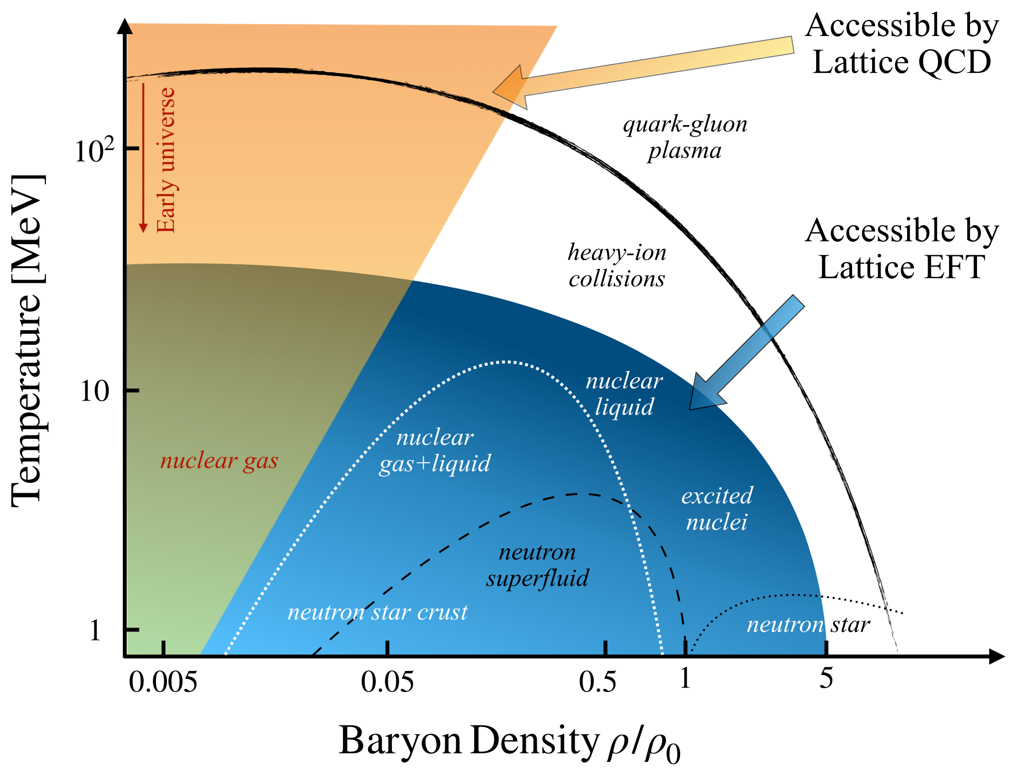
$$Z_A^{\mathcal{O}} = \langle \Psi_A | \exp(-\tau H/2)\, \mathcal{O}\, \exp(-\tau H/2)\, | \Psi_A \rangle$$

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

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

Comparison to lattice QCD

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

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

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

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

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

$$\tilde{\xi}(\vec{n}) = \sum_{i=0,1} \tilde{b}^\dagger_{i}(\vec{n})\, \tilde{b}_{i}(\vec{n}) + s_{\rm L} \sum_{|\vec{n}-\vec{n}'|^2=1} \sum_{i=0,1} \tilde{b}^\dagger_{i}(\vec{n}')\, \tilde{b}_{i}(\vec{n}')$$

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

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

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

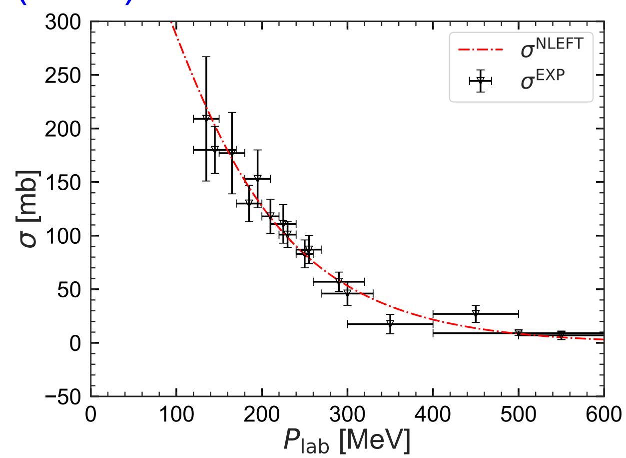
$\hookrightarrow$ must determine 4 LECs! [smearing parameters from the nucleon sector]

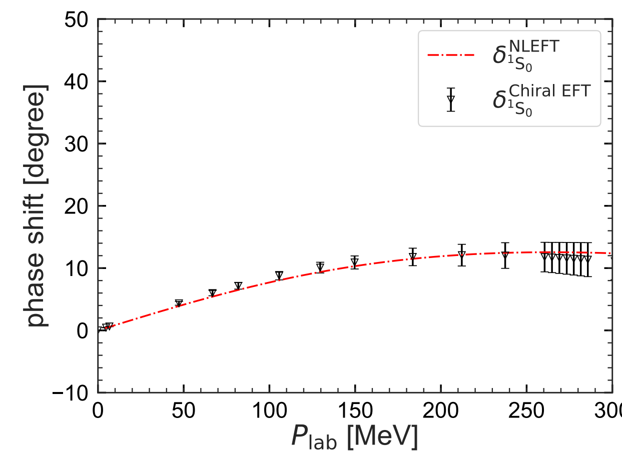
$\hookrightarrow$ first time that the $\Lambda\Lambda N$ three-body force is included

The minimal interaction with strangeness II

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

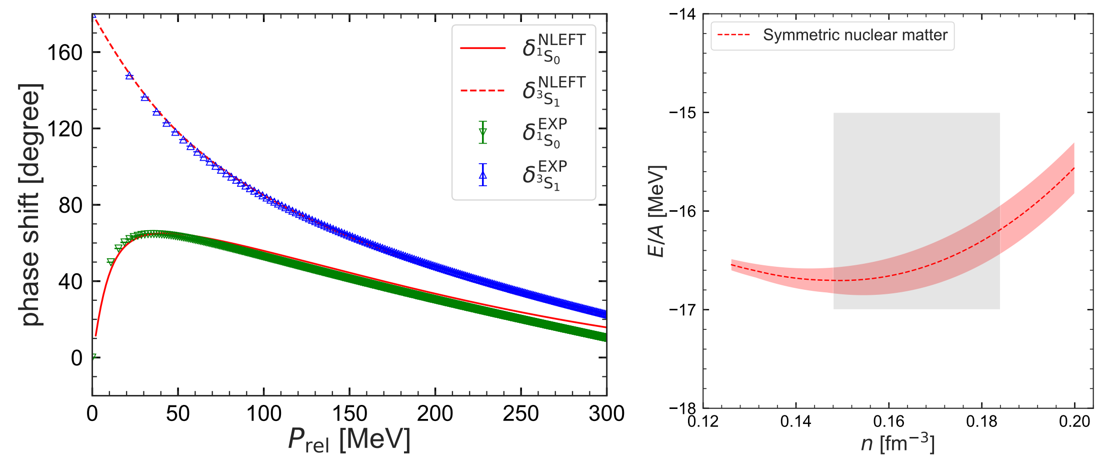
$\hookrightarrow$ this defines our EoS of hyper-nuclear matter called **HMN(I)**

The minimal nuclear interaction: EoS & neutron star properties

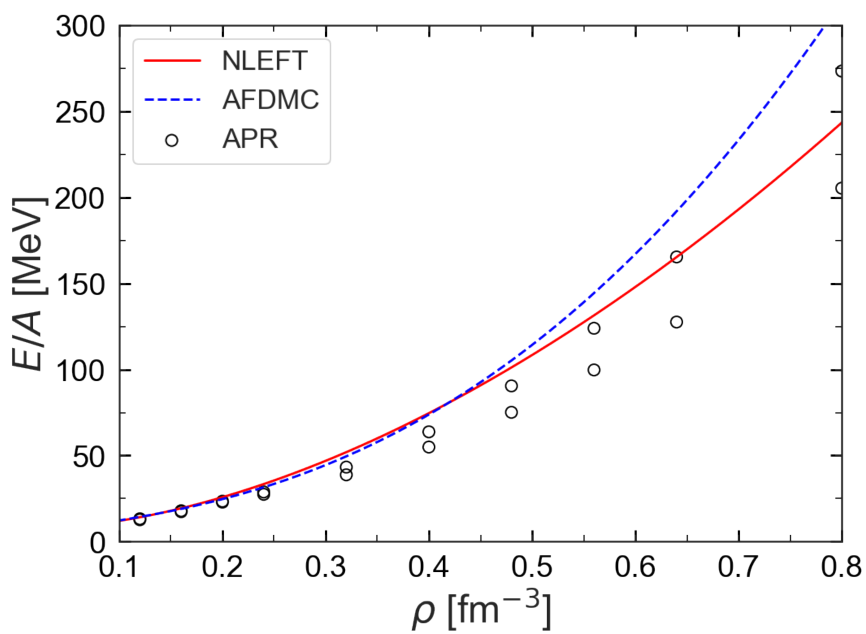
Pure neutron matter

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

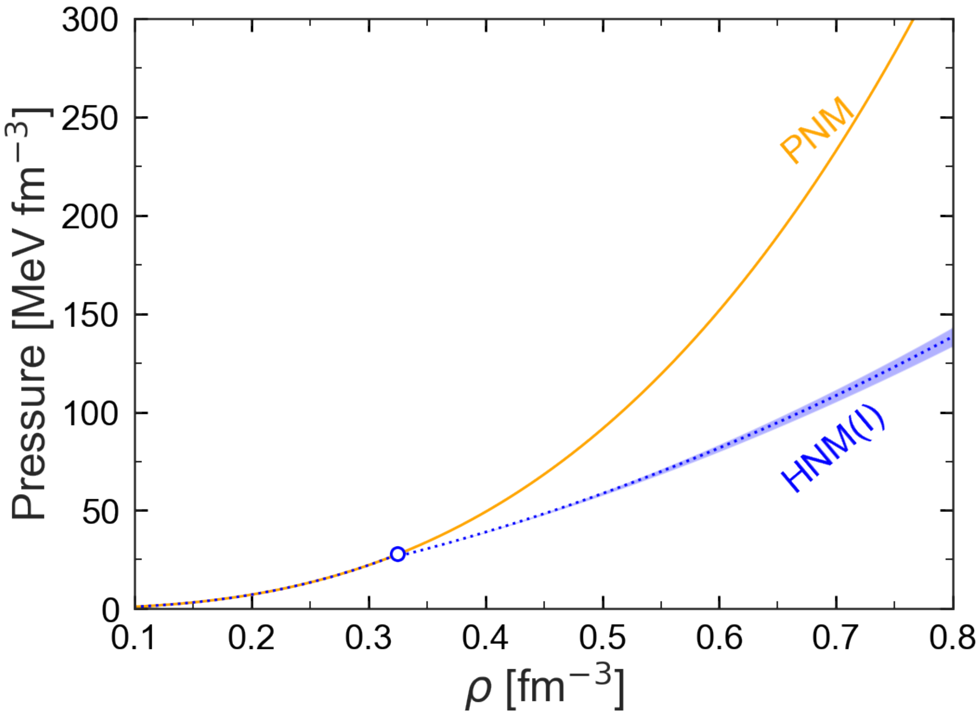
→ work out consequences for
neutron stars based on this PNM EoS

Neutron star properties

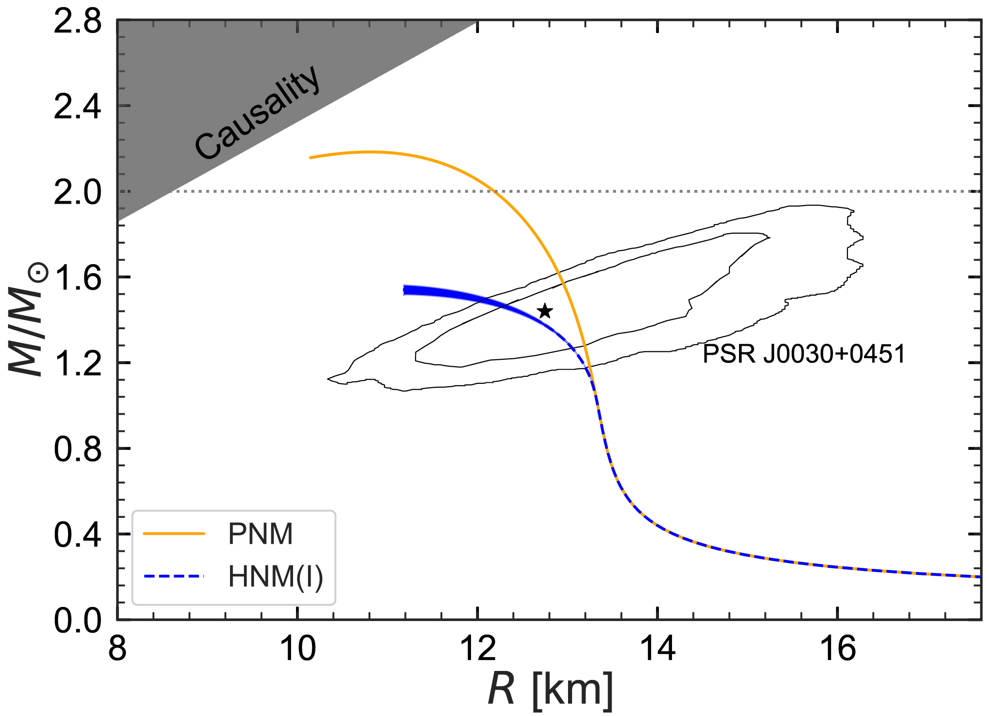
Tong, Elhatisari, UGM, Sci. Bull. **70** (2025) 825

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

  - EoS (PNM and HMN(I))



  - Mass-radius relation



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

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

EoS of hyper-neutron matter

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]

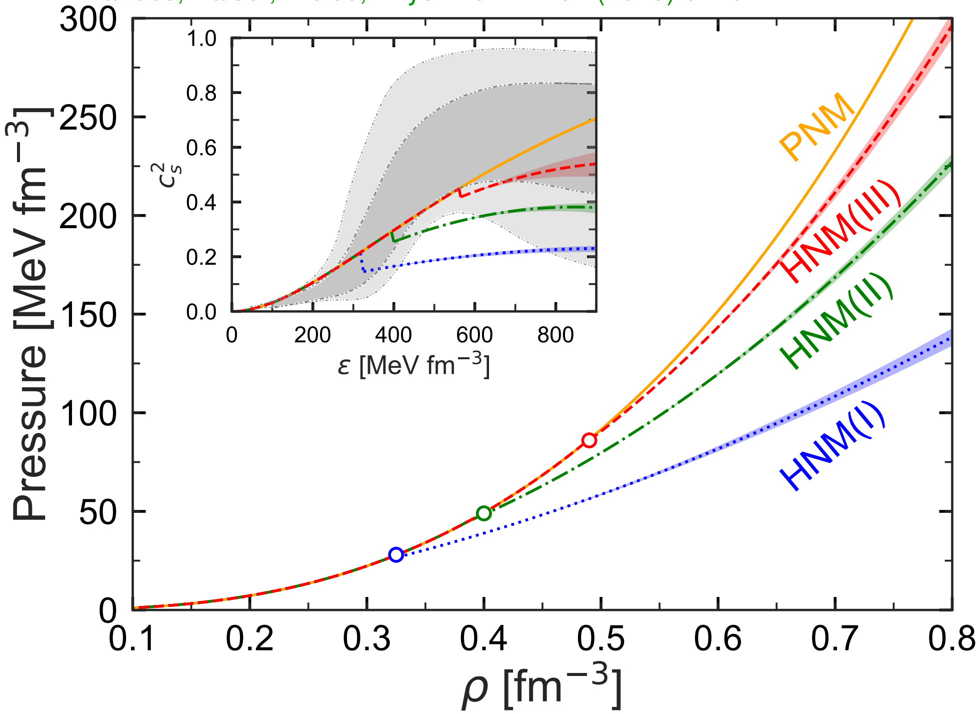
  $\hookrightarrow$ this will move the threshold of $\mu_\Lambda = \mu_n$ up

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

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

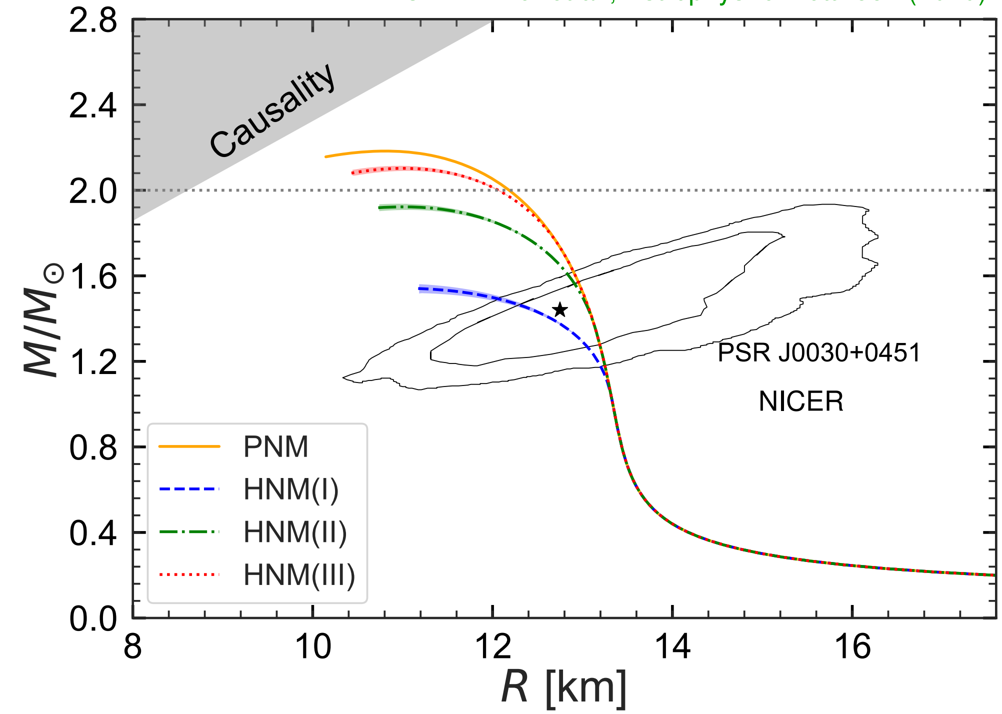
- EoS & speed of sound

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



- Mass-radius relation

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



Finite temperature physics

- Just two teasers for finite T calculations

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

Ab Initio Nuclear Thermodynamics

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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.

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Letter

Ab initio study of nuclear clustering in hot dilute nuclear matter

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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.

- 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