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CENTER FOR SCIENCE & THOUGHT

JÜLICH Forschungszentrum

– The Sino-German CRC 110 –

Symmetries and the Emergence of Structure in QCD

– Nuclear Lattice EFT –

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

Deutsche Forschungsgemeinschaft DFG

国家自然科学基金委员会 National Natural Science Foundation of China

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- Fundamentals of NLEFT
- Assorted results and high-lights
  - The minimal interaction
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- Perspectives

NLEFT within the CRC 110

A bit of history

- Basic developments in NLEFT here at Bonn/FZJ in collaboration with Dean Lee (NCSU), later Bochum also joined
- Major funding sources:

  TRR 16 “Subnuclear structure of matter” (Bonn, Bochum, Giessen) 2004-2016

  HGF VH-VI-417 “Nuclear Astrophysics” (GSI, TU Darmstadt, Bonn,...) 2011-2017
- If you have a new method, you must do something the others could not do!

  $\hookrightarrow$ take-home message for the young people!

PRL 106, 192501 (2011) Selected for a Viewpoint in *Physics* PHYSICAL REVIEW LETTERS week ending 13 MAY 2011

Ab Initio Calculation of the Hoyle State

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(Received 24 February 2011; published 9 May 2011)

The Hoyle state plays a crucial role in the helium burning of stars heavier than our Sun and in the production of carbon and other elements necessary for life. This excited state of the carbon-12 nucleus was postulated by Hoyle as a necessary ingredient for the fusion of three alpha particles to produce carbon at stellar temperatures. Although the Hoyle state was seen experimentally more than a half century ago nuclear theorists have not yet uncovered the nature of this state from first principles. In this Letter we report the first *ab initio* calculation of the low-lying states of carbon-12 using supercomputer lattice simulations and a theoretical framework known as effective field theory. In addition to the ground state and excited spin-2 state, we find a resonance at $-85(3)$ MeV with all of the properties of the Hoyle state and in agreement with the experimentally observed energy.

DOI: 10.1103/PhysRevLett.106.192501 PACS numbers: 21.10.Dr, 21.45.−v, 21.60.De, 26.20.Fj

CRC 16

PRL 109, 252501 (2012) PHYSICAL REVIEW LETTERS week ending 21 DECEMBER 2012

Structure and Rotations of the Hoyle State

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(Received 14 August 2012; published 17 December 2012)

The excited state of the ^{12}C nucleus known as the “Hoyle state” constitutes one of the most interesting, difficult, and timely challenges in nuclear physics, as it plays a key role in the production of carbon via fusion of three alpha particles in red giant stars. In this Letter, we present *ab initio* lattice calculations which unravel the structure of the Hoyle state, along with evidence for a low-lying spin-2 rotational excitation. For the ^{12}C ground state and the first excited spin-2 state, we find a compact triangular configuration of alpha clusters. For the Hoyle state and the second excited spin-2 state, we find a “bent-arm” or obtuse triangular configuration of alpha clusters. We also calculate the electromagnetic transition rates between the low-lying states of ^{12}C.

DOI: 10.1103/PhysRevLett.109.252501 PACS numbers: 21.10.Dr, 21.60.De, 23.20.−g, 27.20.+n

CRC 110

NLEFT within the CRC 110

- In FP1, part of **B7** "Chiral Dynamics of Nuclei and Hypernuclei"
  PLs: N. Kaiser, UGM, A. Nogga

  ↪ very succesful, split into two projects in FP2

- In FP2, part of **B9** "Lattice Nuclear Physics"
  PLs: T. Luu, UGM

  ↪ LQCD part develops slowly, move into **A2** in FP3

- In FP3, the whole **B9** "Lattice Nuclear Physics" is NLEFT
  PLs: H. Krebs, UGM

  ↪ seed for the ERC AdG "EXOTIC" (2021-2026)

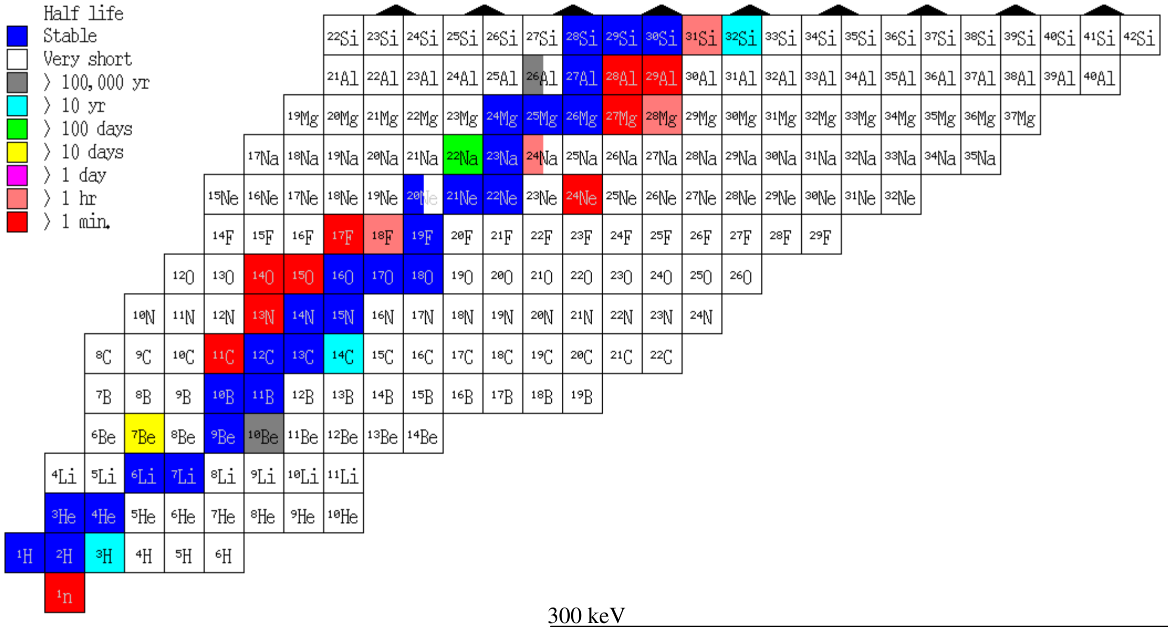
  ↪ seed for a Research Unit in Nuclear Physics (in preparation)

⇒ Impossible to review all results, just discuss selcted hi-lites

Fundamentals of NLEFT

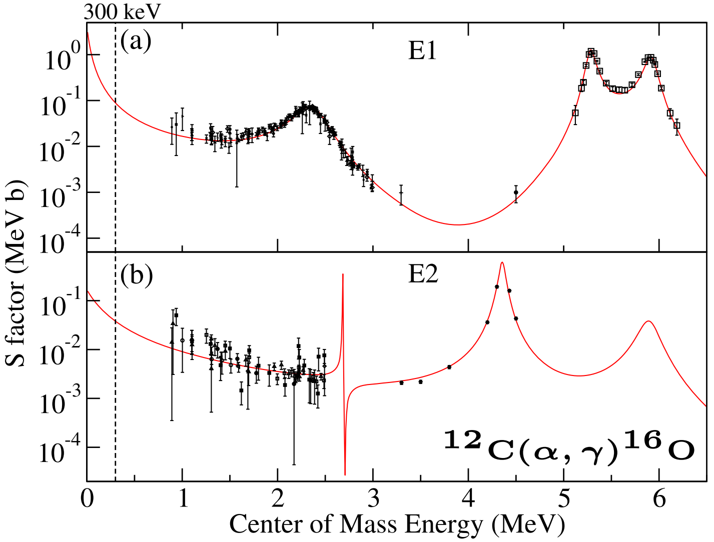
Our goal: Ab initio nuclear structure & reactions

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



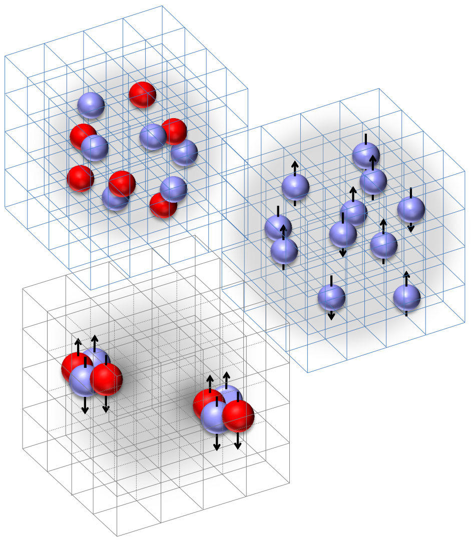
Ⓒ National Nuclear Data Center

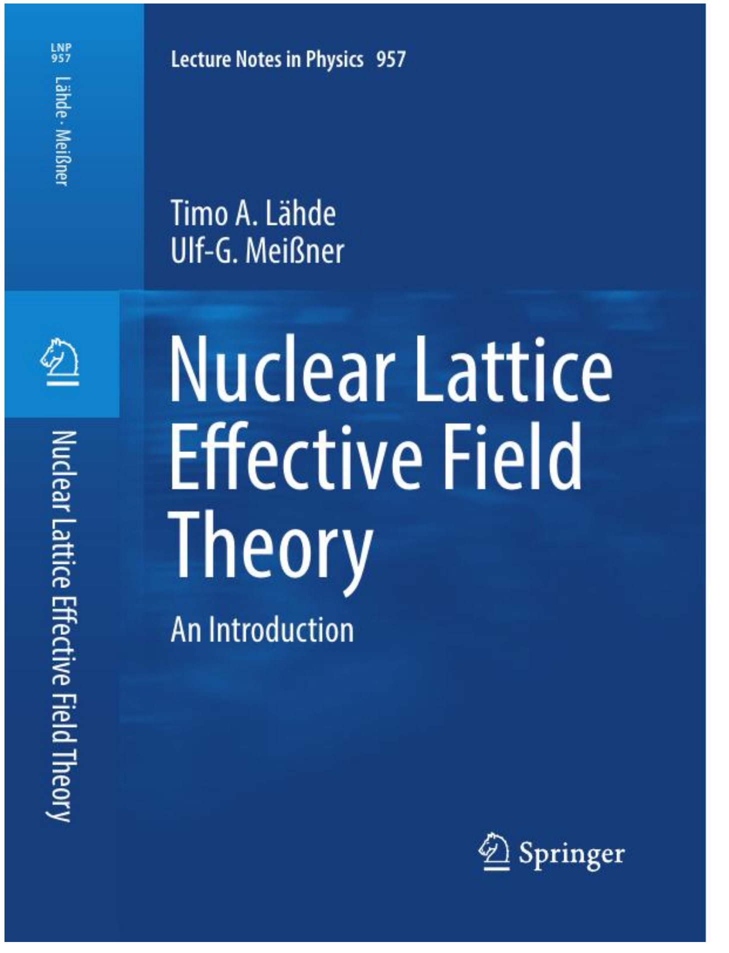
- Nuclear reactions, nuclear astrophysics:
  - ⋆ alpha-particle scattering
  - ⋆ triple-alpha reaction
  - ⋆ alpha-capture on carbon
  - ⋮



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

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

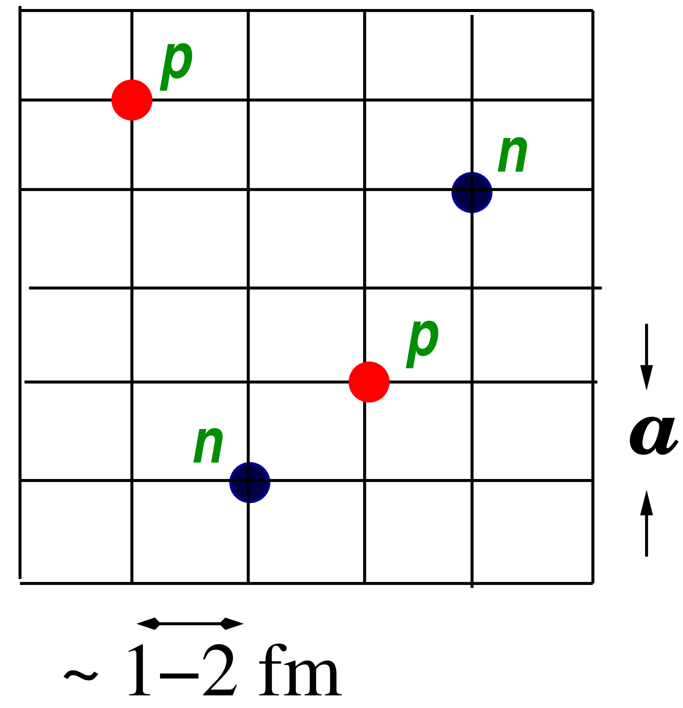
- discretize space-time $V = L_s \times L_s \times L_s \times L_t$:
  nucleons are point-like particles on the sites

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

  $\to$ see Epelbaum, Hammer, UGM, Rev. Mod. Phys. **81** (2009) 1773

- typical lattice parameters

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



- 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

Transfer matrix method

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

  Euclidean time

  with Ψ_A a Slater determinant for A free nucleons

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

- Transient energy

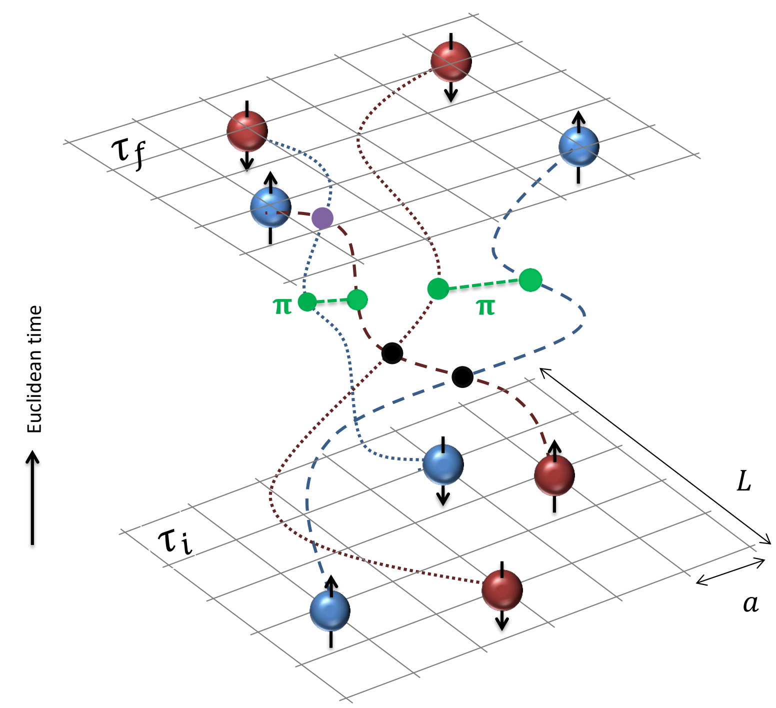
$$E_A(\tau) = -\frac{d}{d\tau} \ln Z_A(\tau)$$

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

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

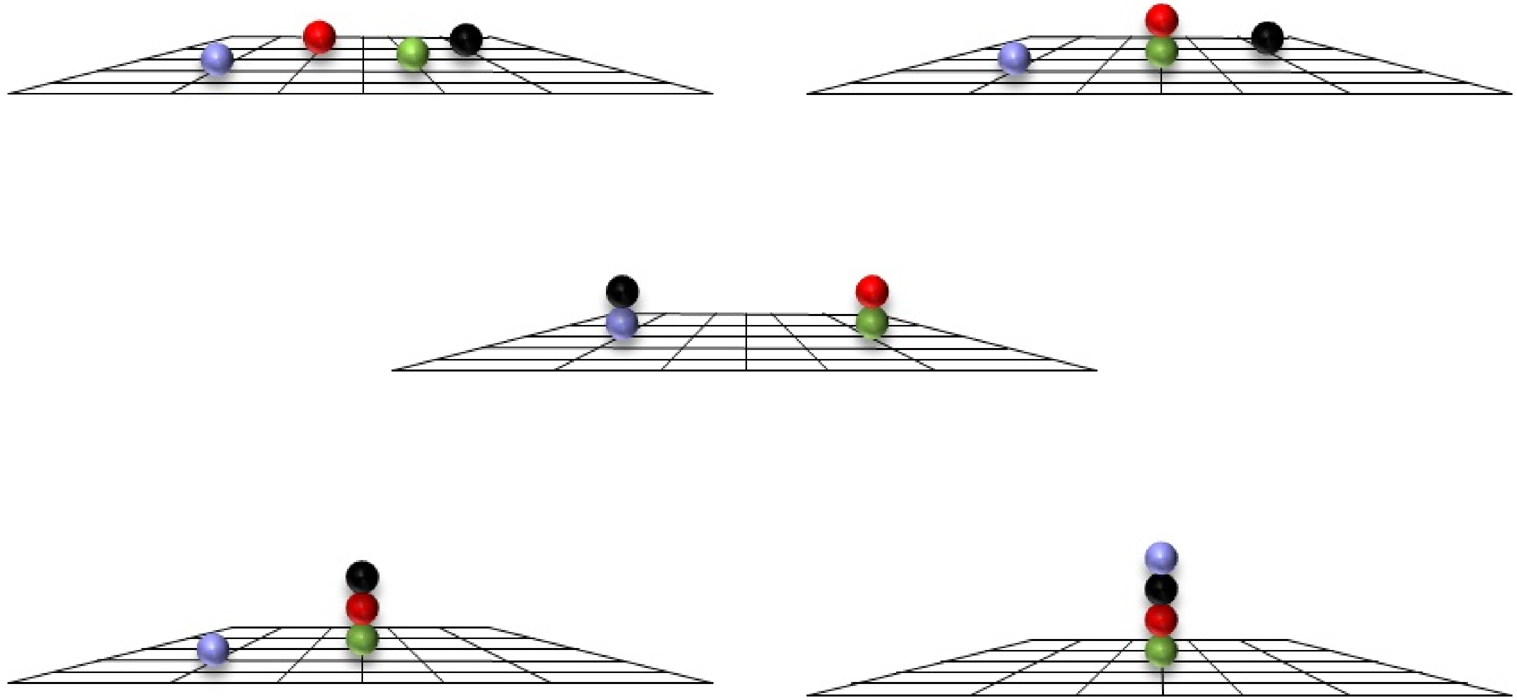
$$Z_A^{\mathcal{O}} = \langle \Psi_A | \exp(-\tau H/2)\, \mathcal{O}\, \exp(-\tau H/2)\, | \Psi_A \rangle$$

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



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

Configurations

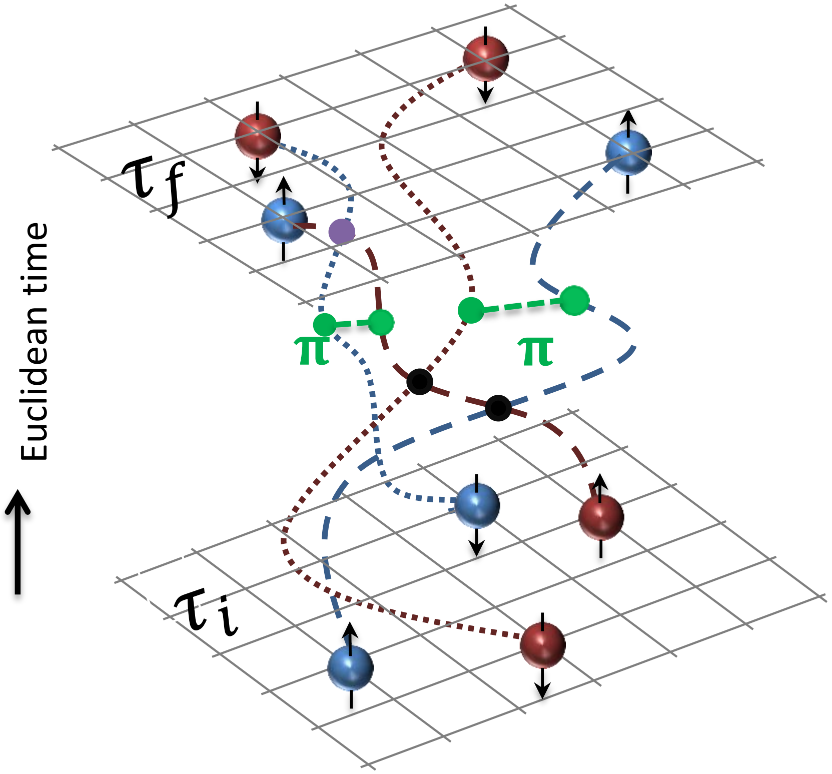


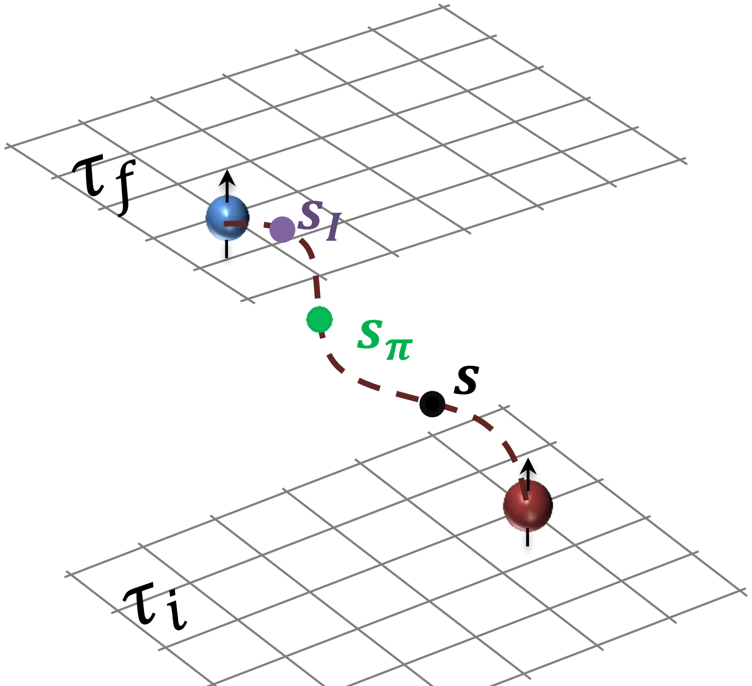
> ⇒ all *possible* configurations are sampled
>
> ⇒ preparation of *all possible* initial/final states
>
> ⇒ *clustering* emerges *naturally*

Auxiliary field method

- Represent interactions by auxiliary fields (Gaussian quadrature):

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

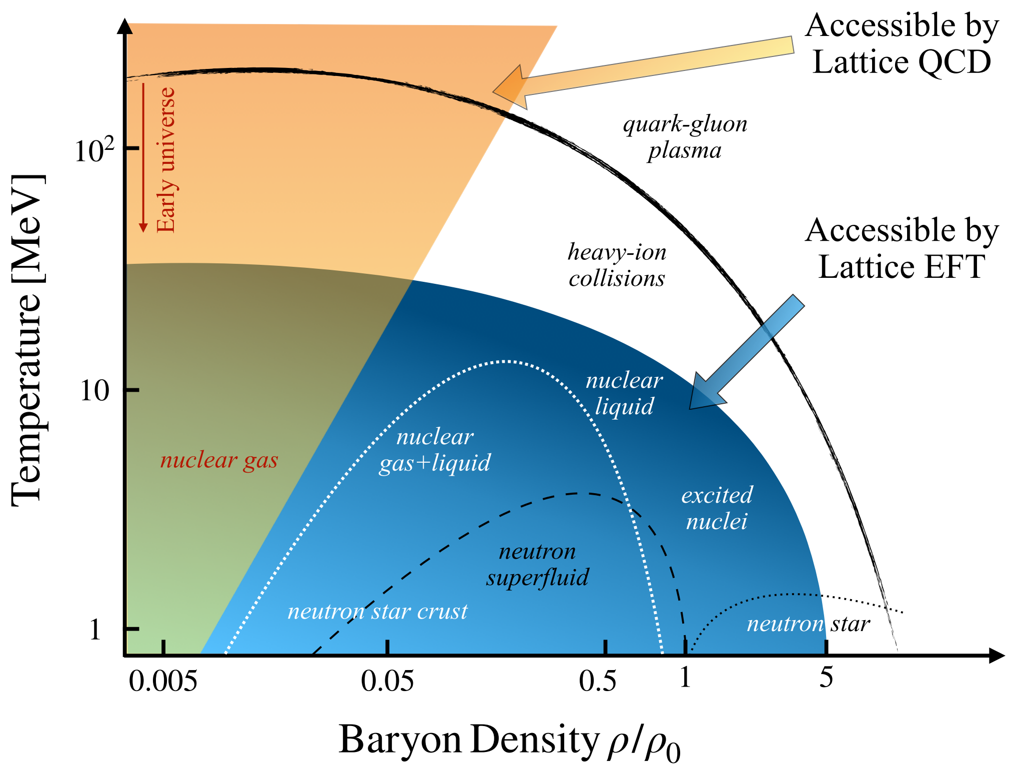




optimally suited for parallel computing!

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

A minimal nuclear interaction

- Basic problem: Straightforward application of chiral EFT forces leads to problems when one goes beyond light nuclei (e.g. the radius problem)

- Main idea: Construct a minimal nuclear interactions that reproduces the ground state properties of light nuclei, medium-mass nuclei, and neutron matter simultaneously with no more than a few percent error in the energies and charge radii

- This can be achieved by making use of Wigner's SU(4) spin-isospin symmetry

Wigner, Phys. Rev. **C 51** (1937) 106

- If the nuclear Hamiltonian does not depend on spin and isospin, then it is obviously invariant under SU(4) transformations [really $U(4) = U(1) \times SU(4)$]:

$$N \to UN\,, \quad U \in SU(4)\,, \quad N = \begin{pmatrix} p \\ n \end{pmatrix}$$

$$N \to N + \delta N\,, \quad \delta N = i\epsilon_{\mu\nu}\sigma^\mu\tau^\nu\, N\,, \quad \sigma^\mu = (1, \sigma_i)\,, \quad \tau^\mu = (1, \tau_i)$$

Remarks on Wigner's SU(4) symmetry

- Wigner SU(4) spin-isospin symmetry in the context of pionless nuclear EFT

  ↪ large scattering lengths — Mehen, Stewart, Wise, Phys. Rev. Lett. **83** (1999) 931

- Wigner SU(4) spin-isospin symmetry is particularly beneficial for NLEFT

  ↪ suppression of sign oscillations — Chen, Lee, Schäfer, Phys. Rev. Lett. **93** (2004) 242302

  ↪ provides a very much improved LO action when smearing is included
  Lu, Li, Elhatisari, Lee, Epelbaum, UGM, Phys. Lett. B **797** (2019) 134863

- Initimately related to α-clustering in nuclei

  ↪ cluster states in ^{12}C like the famous Hoyle state
  Epelbaum, Krebs, Lee, UGM, Phys. Rev. Lett. **106** (2011) 192501

  ↪ nuclear physics is close to a quantum phase transition
  Elhatisari et al., Phys. Rev. Lett. **117** (2016) 132501

Essential elements for nuclear binding

Lu, Li, Elhatisari, Epelbaum, Lee, UGM, Phys. Lett. B **797** (2019) 134863 [arXiv:1812.10928]

- Highly SU(4) symmetric LO action without pions, only **four** parameters

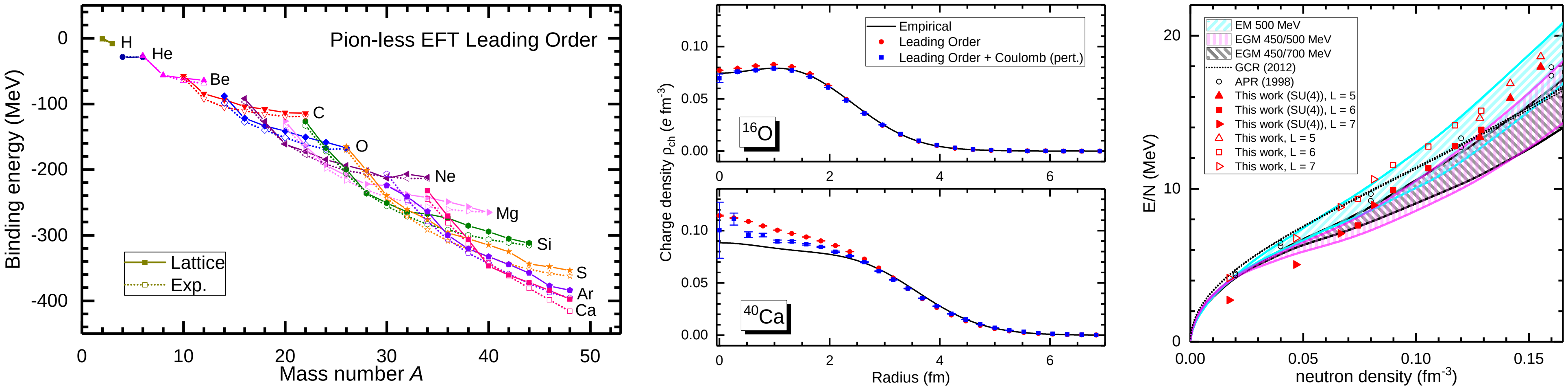
$$H_{\mathrm{SU}(4)} = H_{\mathrm{free}} + \frac{1}{2!} C_2 \sum_n \tilde{\rho}(n)^2 + \frac{1}{3!} C_3 \sum_n \tilde{\rho}(n)^3$$

$$\tilde{\rho}(n) = \sum_i \tilde{a}_i^\dagger(n)\tilde{a}_i(n) + s_L \sum_{|n'-n|=1} \sum_i \tilde{a}_i^\dagger(n')\tilde{a}_i(n')$$

$$\tilde{a}_i(n) = a_i(n) + s_{NL} \sum_{|n'-n|=1} a_i(n')$$

s_L controls the locality of the interactions, s_{NL} the non-locaity of the smearing

→ describes binding energies, radii, charge densities and the EoS of neutron matter



Wigner's SU(4) symmetry and the carbon spectrum

- Study of the spectrum (and other properties) of ^{12}C

  $\hookrightarrow$ spin-orbit splittings are known to be weak

  Hayes, Navratil, Vary, Phys. Rev. Lett. **91** (2003) 012502 Johnson, Phys. Rev. C **91** (2015) 034313

  $\hookrightarrow$ start with cluster and shell-model configurations

- Fit the four parameters:

  C_2, C_3 – ground state energies of ^{4}He and ^{12}C

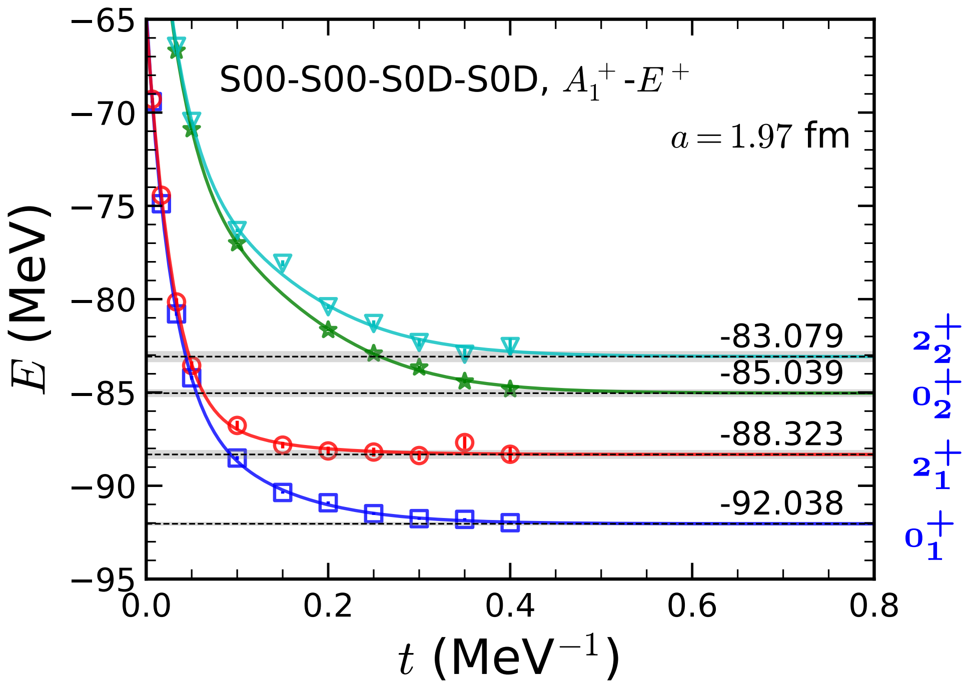
  s_L – radius of ^{12}C around 2.4 fm

  s_{NL} – best overall description of the transition rates

- Calculation of em transitions

  requires coupled-channel approach

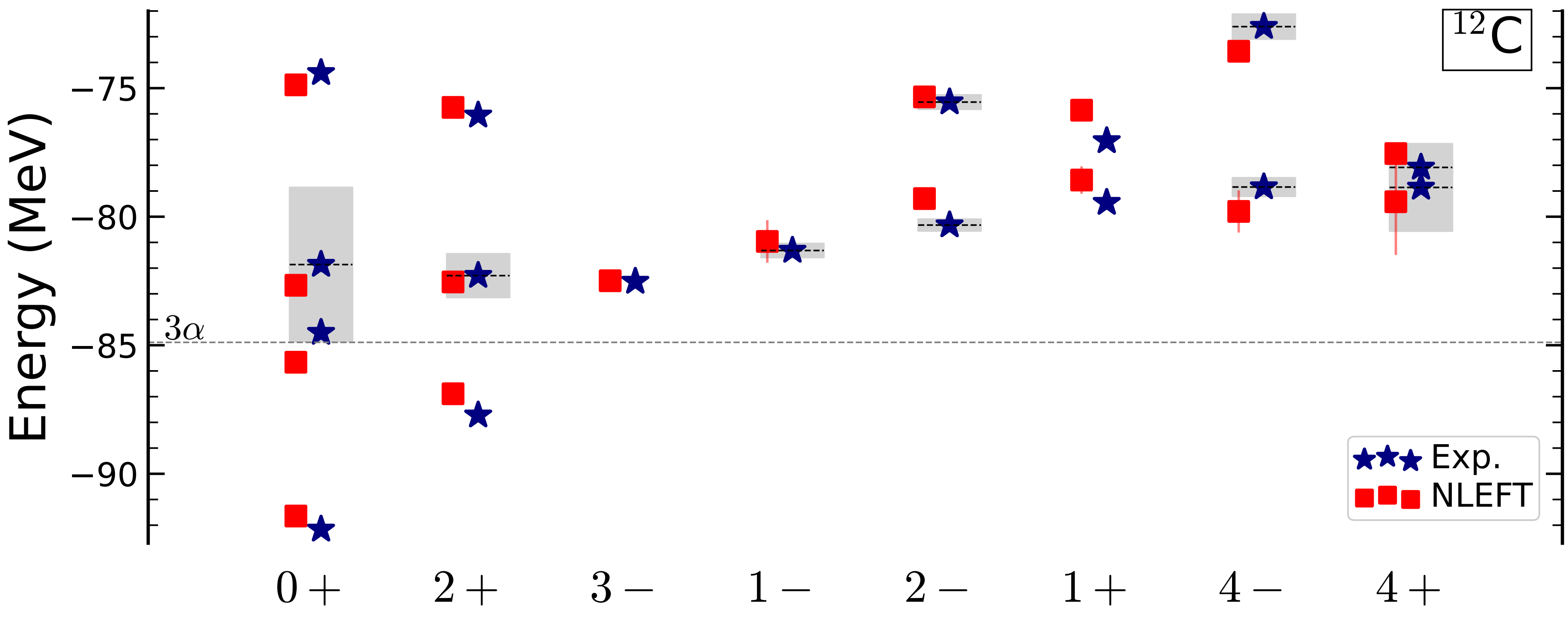
  e.g. 0^+ and 2^+ states



Spectrum of ^{12}C

Shen, Elhatisari, Lähde, Lee, Lu, UGM, Nature Commun. **14** (2023) 2777

- Improved description when 3NFs are included, amazingly good

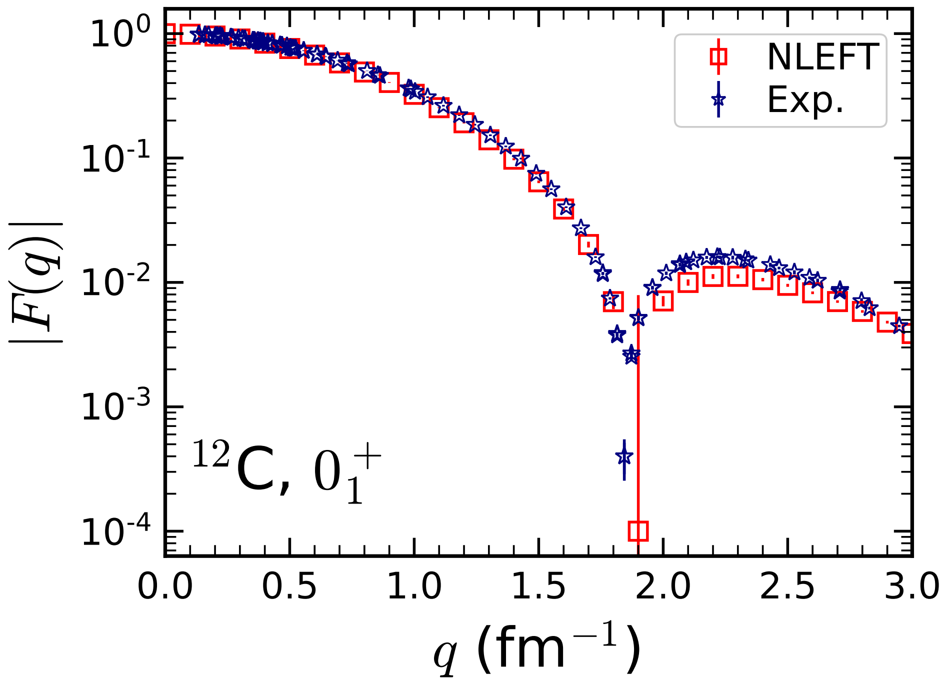


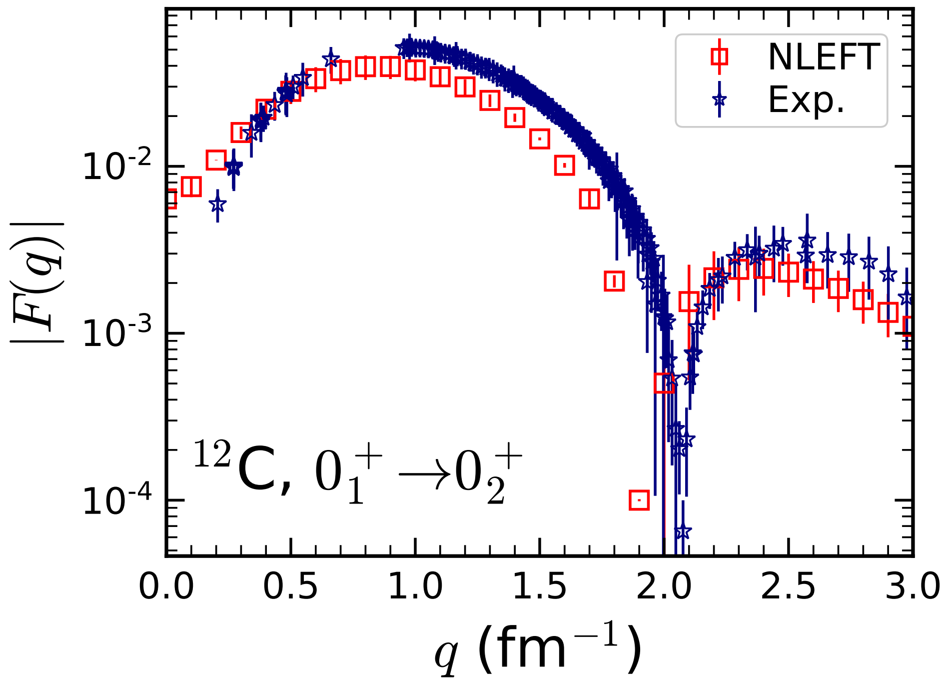
→ solidifies earlier NLEFT statements about the structure of the 0_2^+ and 2_2^+ states

Electromagnetic properties

Shen, Elhatisari, Lähde, Lee, Lu, UGM, Nature Commun. **14** (2023) 2777

- Radii, quadrupole moments & em transition rates agree wih experiment
- Form factors and transition ffs [essentially parameter-free]:



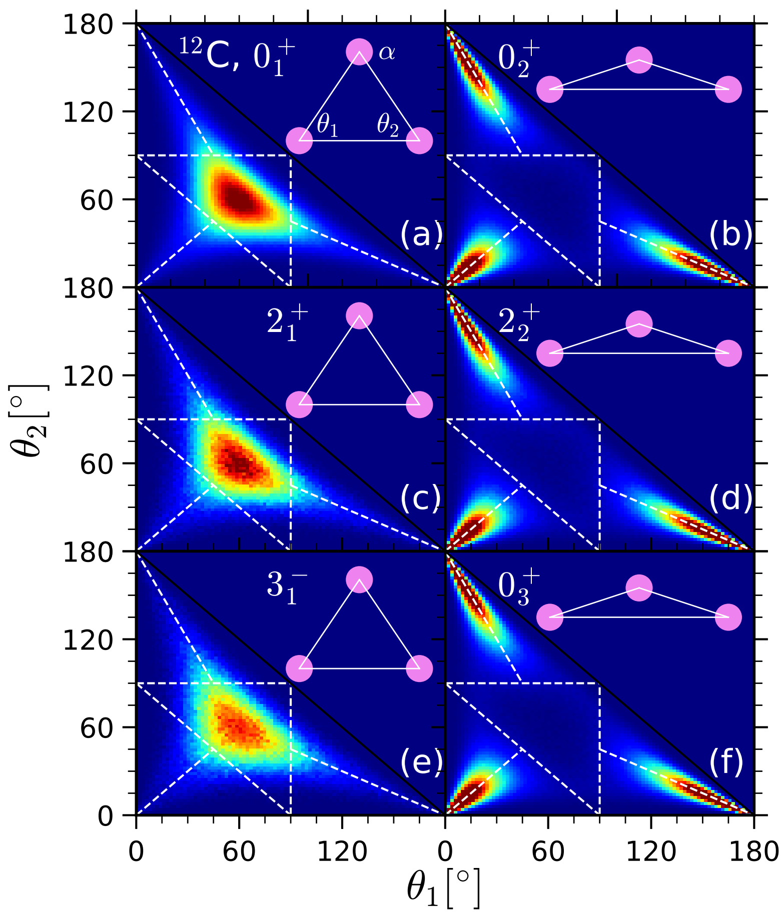


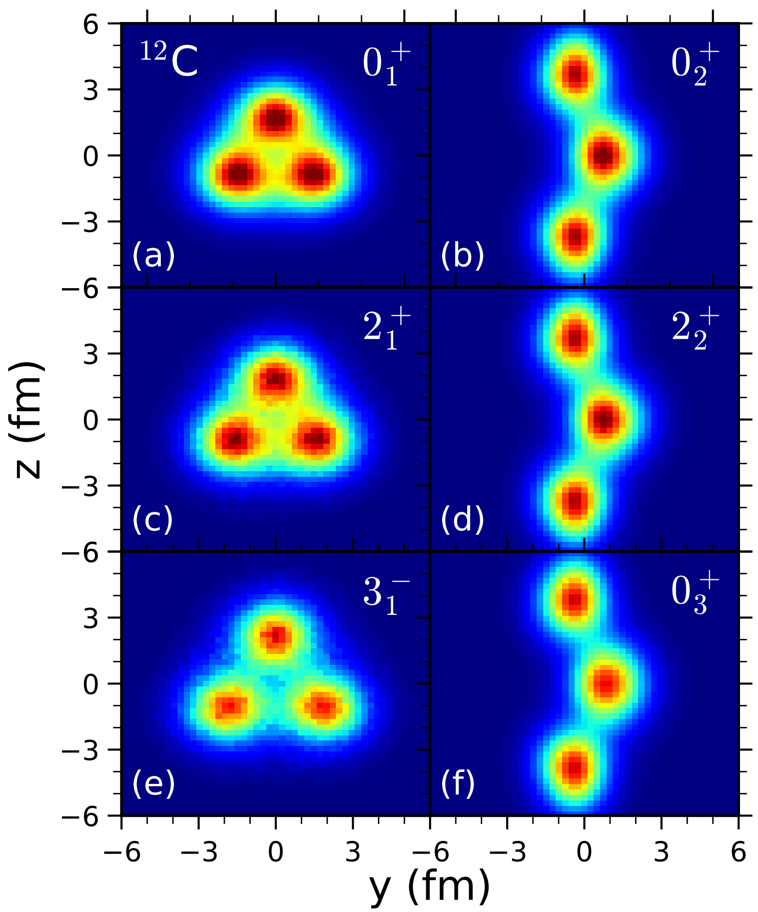
Sick, McCarthy, Nucl. Phys. A **150** (1970) 631
Strehl, Z. Phys. **234** (1970) 416
Crannell et al., Nucl. Phys. A **758** (2005) 399

Chernykh et al., Phys. Rev. Lett. **105** (2010) 022501

Emergence of geometry

- Use the pinhole algorithm to measure the distribution of α-clusters/matter:

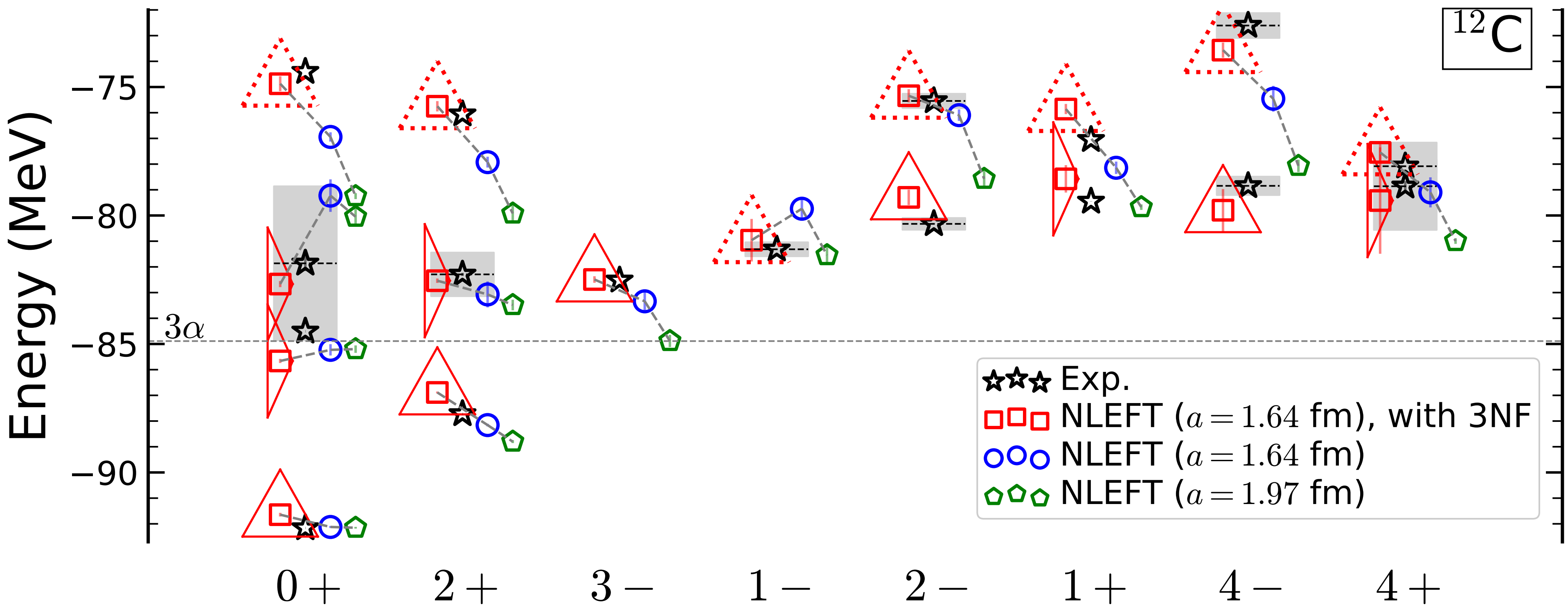




- equilateral & obstuse triangles $\rightarrow$ $\mathbf{2^+}$ states are excitations of the $\mathbf{0^+}$ states

Emergence of duality

- ^{12}C spectrum shows a cluster/shell-model duality

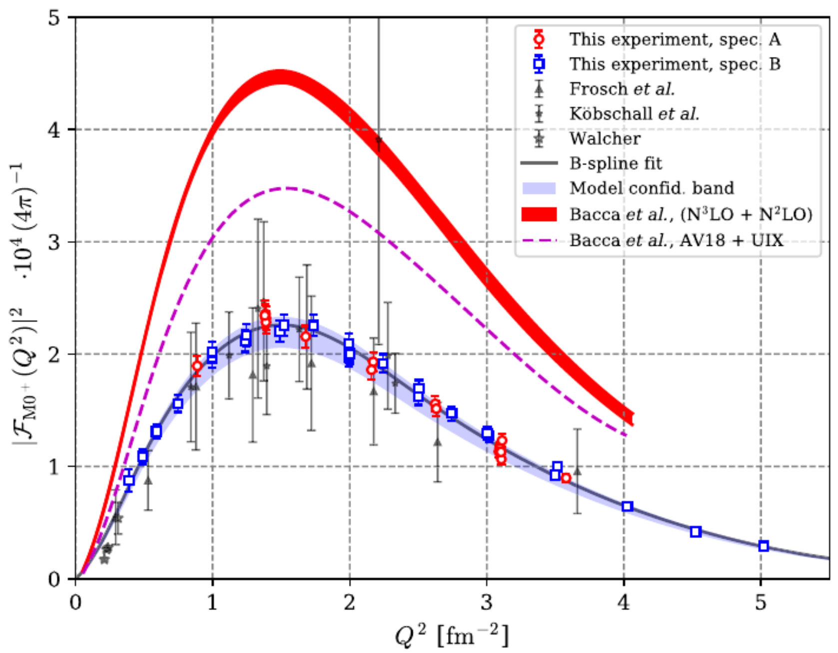


- dashed triangles: strong 1p-1h admixture in the wave function

The ^{4}He form factor puzzle

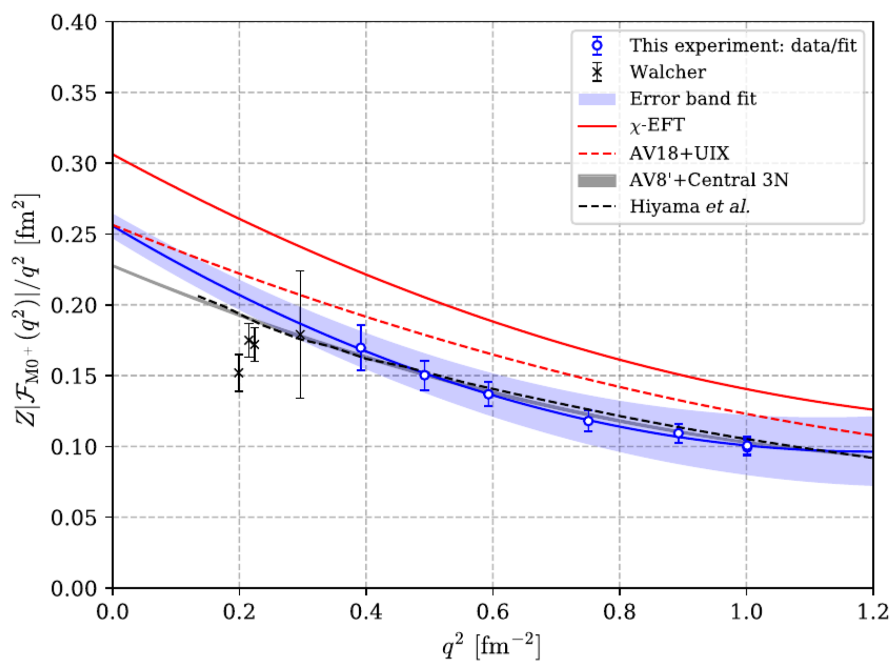
- Recent Mainz measurements of $F_{M0}(0_2^+ \to 0_1^+)$ appear to be in stark disagreement with *ab initio* nuclear theory Kegel et al., Phys. Rev. Lett. **130** (2023) 152502

- Monopole transition ff



[calculations from 2013]

- low-momentum expansion



$\Rightarrow$ **A low-energy puzzle for nuclear forces?**

Ab initio calculation of the ^{4}He transition form factor

UGM, Shen, Elhatisari, Lee, Phys. Rev. Lett. **132** (2024) 062501 [2309.01558 [nucl-th]]

- Use the essential elements action, **all parameters fixed!**

- Calculate the transition ff and its low-energy expansion form the transition density

$$\rho_{\rm tr}(r) = \langle 0_1^+ | \hat\rho(\vec r) | 0_2^+ \rangle$$

$$F(q) = \frac{4\pi}{Z}\int_0^\infty \rho_{\rm tr}(r) j_0(qr) r^2 dr = \frac{1}{Z}\sum_{\lambda=1}^{\infty} \frac{(-1)^\lambda}{(2\lambda+1)!} q^{2\lambda}\langle r^{2\lambda}\rangle_{\rm tr}$$

$$\frac{Z|F(q^2)|}{q^2} = \frac{1}{6}\,\langle r^2\rangle_{\rm tr}\left[1 - \frac{q^2}{20}\mathcal{R}_{\rm tr}^2 + \mathcal{O}(q^4)\right]$$

$$\mathcal{R}_{\rm tr}^2 = \langle r^4\rangle_{\rm tr}/\langle r^2\rangle_{\rm tr}$$

- The first excited state sits in the continuum & close to the ^3H-p threshold

↪ use large volumes $L = 10, 11, 12$ or $L = 13.2$ fm, 14.5 fm, 15.7 fm

↪ the lattice spacing is fixed to $a = 1.32$ fm, corresponding $\Lambda = \pi/a = 465$ MeV

The first excited state

- 3 coupled channels with 0^+ q.n's $\rightarrow$ accelerates convergence as $L_t \rightarrow \infty$
- Shell-model wave functions (4 nucleons in $1s_{1/2}$, twice 3 in $1s_{1/2}$ and 1 in $2s_{1/2}$)

L [fm]	$E(0_1^+)$ [MeV]	$E(0_2^+)$ [MeV]	ΔE [MeV]
13.2	$-28.32(3)$	$-8.37(14)$	$0.28(14)$
14.5	$-28.30(3)$	$-8.02(14)$	$0.42(14)$
15.7	$-28.30(3)$	$-7.96(9)$	$0.40(9)$

$\hookrightarrow$ statistical and large-L_t errors

$\hookrightarrow$ agreement w/ experiment: $E(0_1^+) = 28.3$ MeV, $\Delta E = 0.4$ MeV

$\hookrightarrow$ ΔE consistent w/ no-core Gamov shell model (no 3NFs)

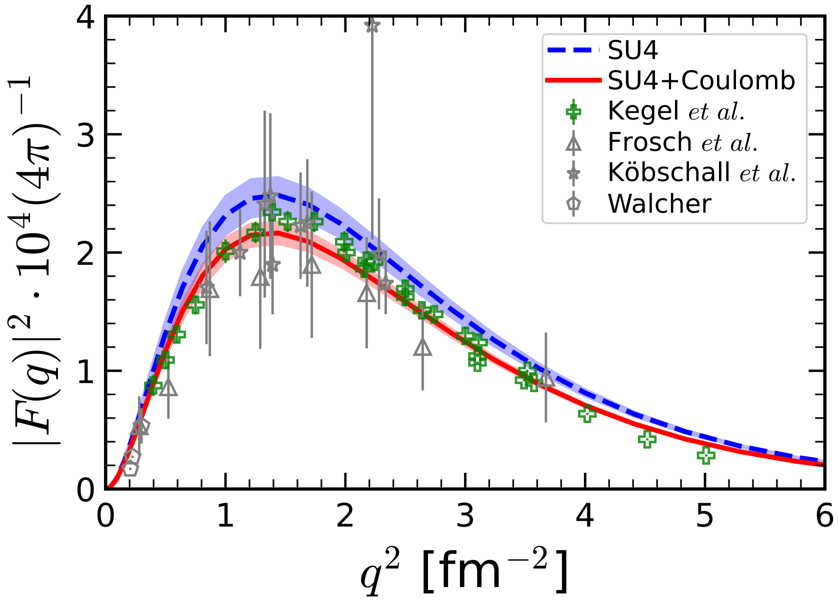
Michel, Nazarewicz, Ploszajczak, Phys. Rev. Lett. **131** (2023) 242502

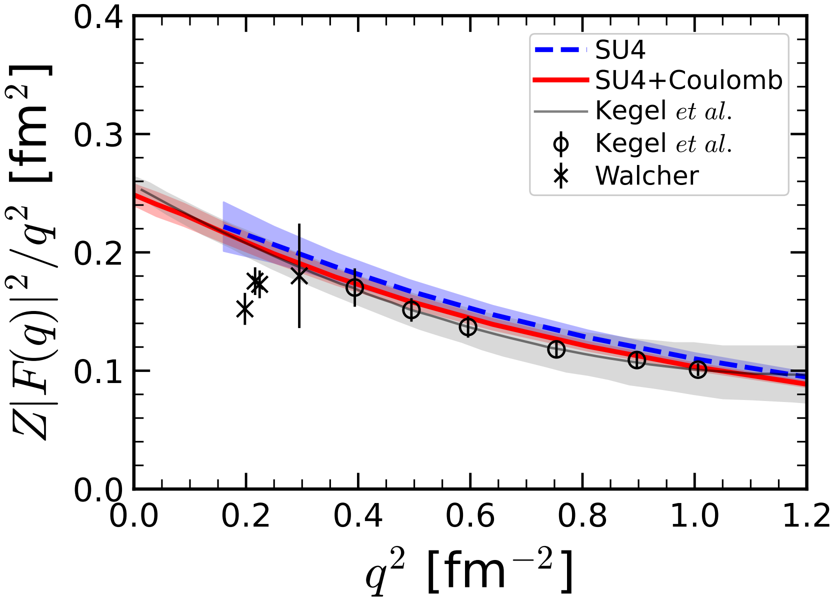
$\hookrightarrow$ consistent w/ the Efimov tetramer analysis $\Delta E = 0.38(2)$ MeV

von Stecher, D'Incao, Greene, Nat. Phys. **5** (2009) 417; Hammer, Platter, EPJA **32** (2007) 113

The transition form factor

- Transition form factor
- Low-momentum expansion





↪ Excellent description of the data

↪ **No puzzle** to the nuclear forces!

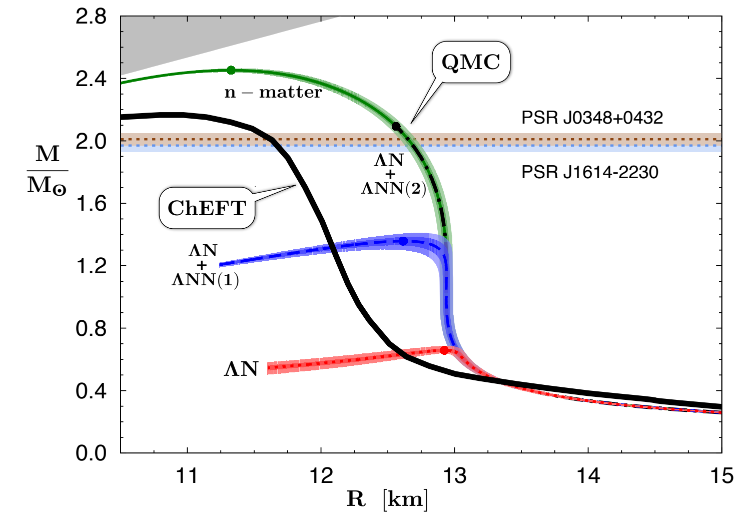
↪ Can be improved using N3LO action + wave function matching

Elhatisari et al., 2210.17488 [nucl-th]

↪ Now consider neutron stars and the “hyperon puzzle”

Towards hyper-neutron matter

Tong, Elhatisari, UGM, 2405.01887 [nucl-th]



@ W. Weise

- Densities in the interior of neutron stars
  up to $5 \cdot \rho_0$ [$\rho_0 = 0.17$ fm^{-3}]
  ↪ possible appearance of hyperons
  → "hyperon puzzle"
  ↪ many possible solutions
  (3-body forces, BSM physics, modifed gravity)
  ↪ Neutron matter EoS plays an important role
  in **multimessenger astronomy** [gravitational waves]

- Can we address this topic w/ NLEFT? If so, how?
  ↪ large densities require a small lattice spacing
  ↪ need to extend the minimal nuclear interaction to such densities
  ↪ need to extend the minimal nuclear interaction to the strangeness sector

The minimal interaction with strangeness I

Tong, Elhatisari, UGM, 2405.01887 [nucl-th]

- 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

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

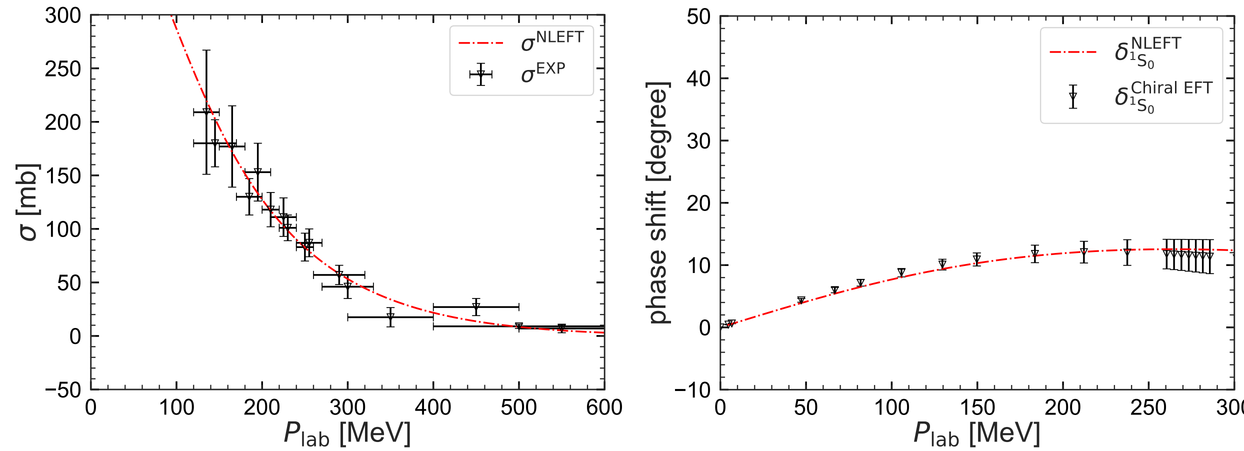
$\hookrightarrow$ must determine 4 LECs! [smearing parameters from the nucleon sector]

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

The minimal interaction with strangeness II

Tong, Elhatisari, UGM, 2405.01887 [nucl-th]

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



- 3BF LECs from the separation energies of Λ and $\Lambda\Lambda$ hyper-nuclei [* prediction]:

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

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

Nucleus	NLEFT [MeV]	Exp. [MeV]
${}^5_\Lambda$He	$3.40(1)(1)$	$3.10(3)$
${}^9_\Lambda$Be	$5.72(5)(4)$	$6.61(7)$
${}^{13}_\Lambda$C	$10.54(17)(29)^*$	$11.80(16)$
${}^6_{\Lambda\Lambda}$He	$7.36(1)(4)$	$6.91(16)$
${}^{10}_{\Lambda\Lambda}$Be	$13.30(7)(12)$	$14.70(40)$
${}^{12}_{\Lambda\Lambda}$Be	$21.22(56)(21)^*$	$21.48(121)$

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

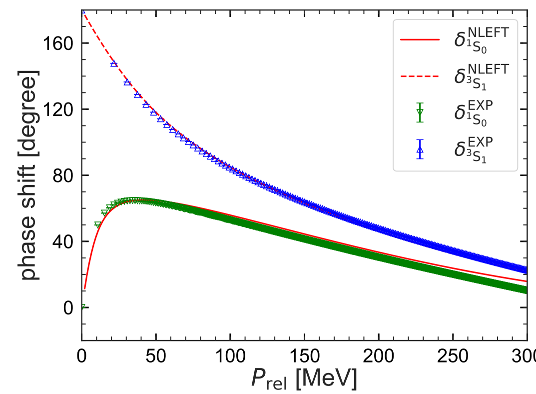
Pure neutron matter

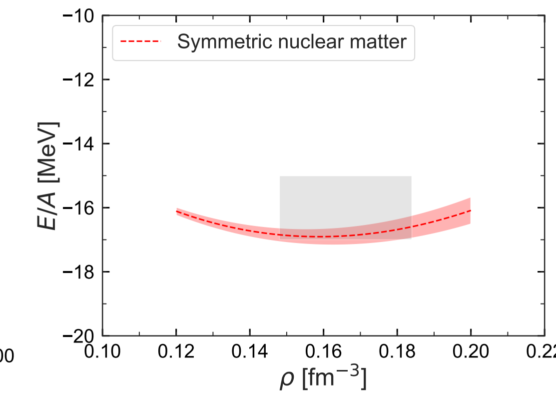
Tong, Elhatisari, UGM, 2405.01887 [nucl-th]

- Input: S-wave phase shifts (2N)

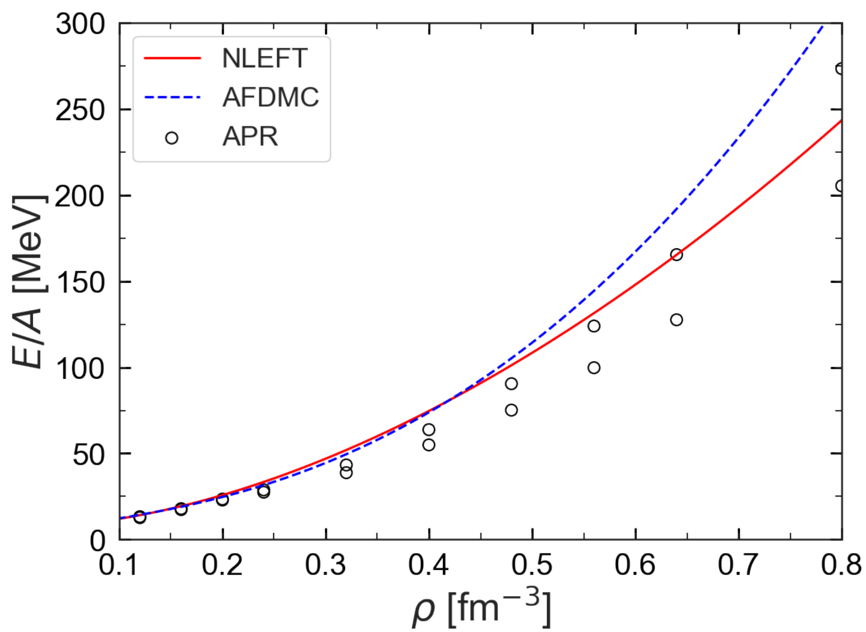
  & symmetric nuclear matter (3N)
- Note: extension of the minimal

  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

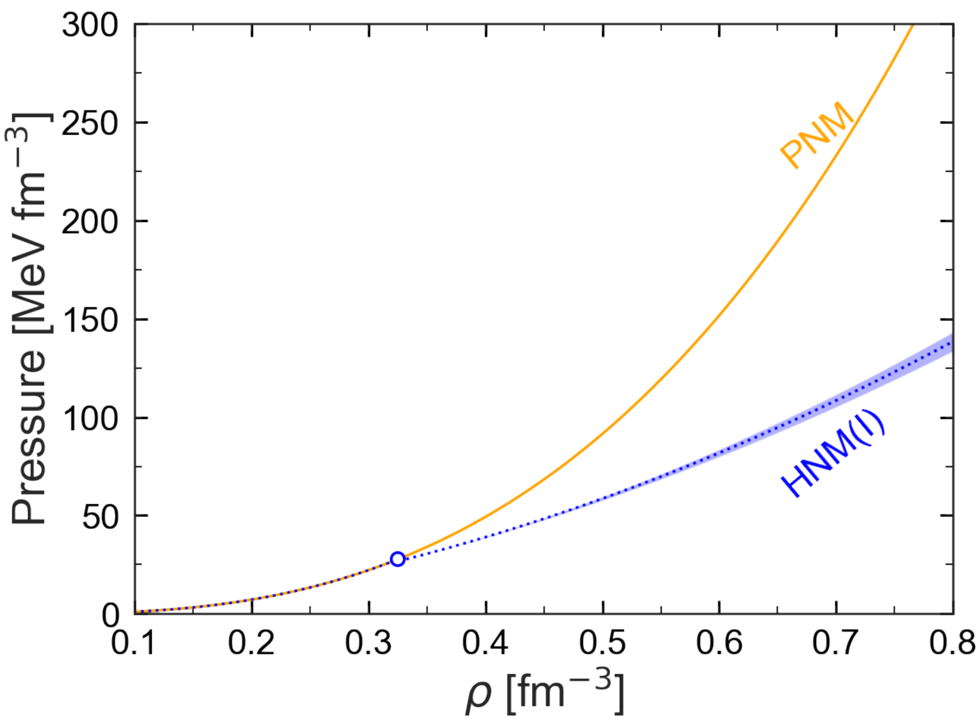
neutron stars based on this PNM EoS

Neutron star properties

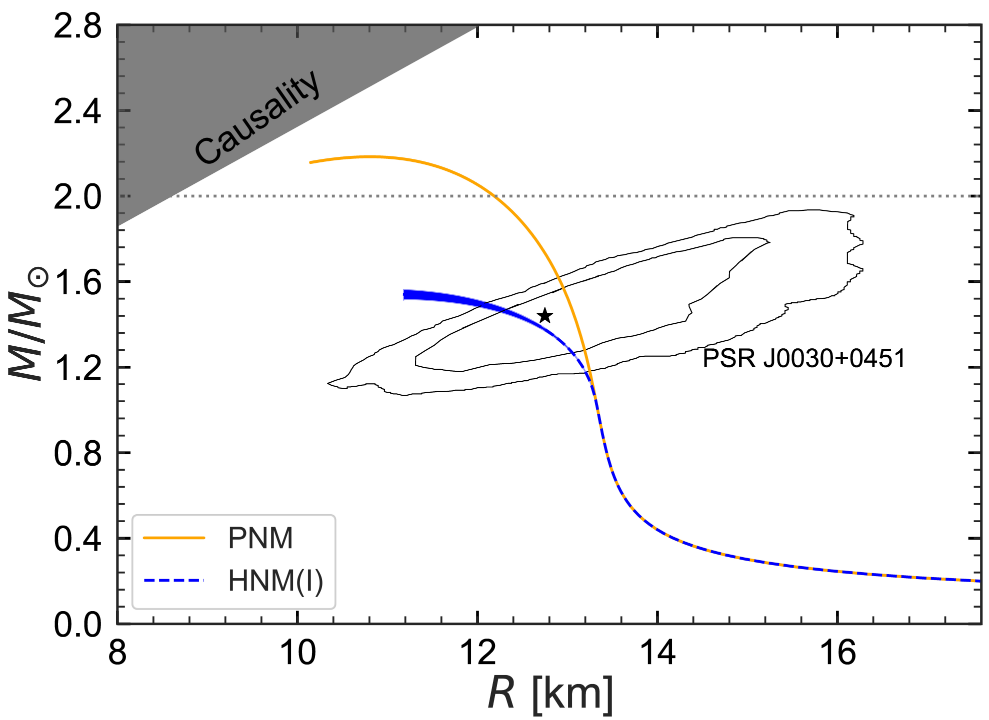
Tong, Elhatisari, UGM, 2405.01887 [nucl-th]

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

  - EoS (PNM and HMN(I))



  - Mass-radius relation



- Max. neutron star mass: $M_{\rm max} = 2.19(1)(2)\, M_\odot$ for PNM

  $M_{\rm max} = 1.52(1)(1)\, M_\odot$ for HNM(I) $\rightarrow$ need repulsion

EoS of hyper-neutron matter

Tong, Elhatisari, UGM, 2405.01887 [nucl-th]

- 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

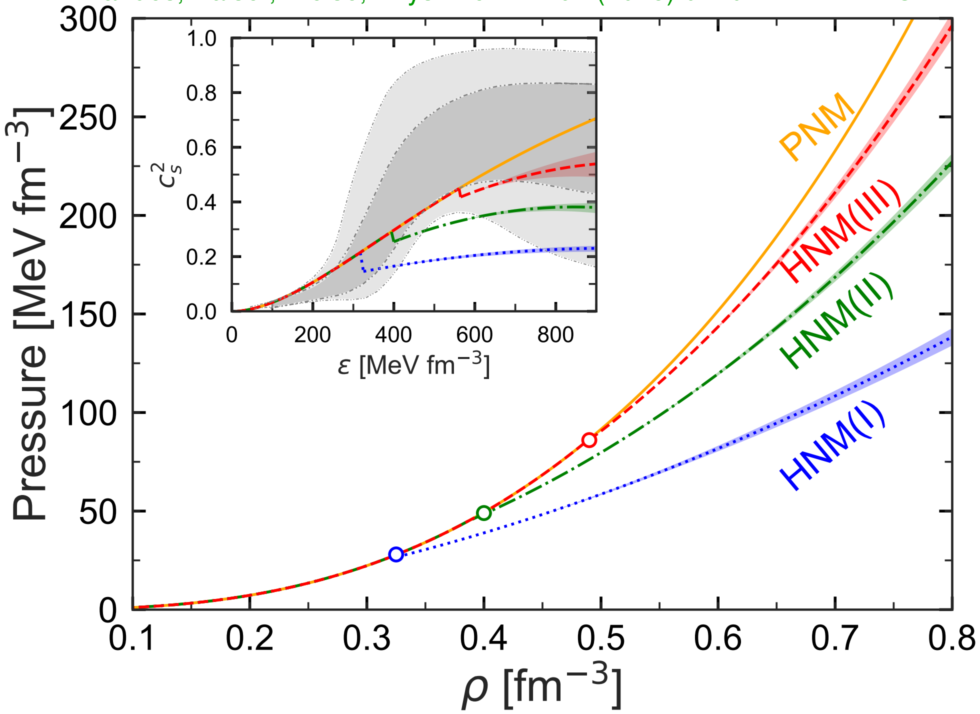
  $\hookrightarrow$ take $M_{\rm max}$ as data point: $M_{\rm max} = 1.93 M_\odot$ for HNM(II)

  $M_{\rm max} = 2.12 M_\odot$ for HNM(III)

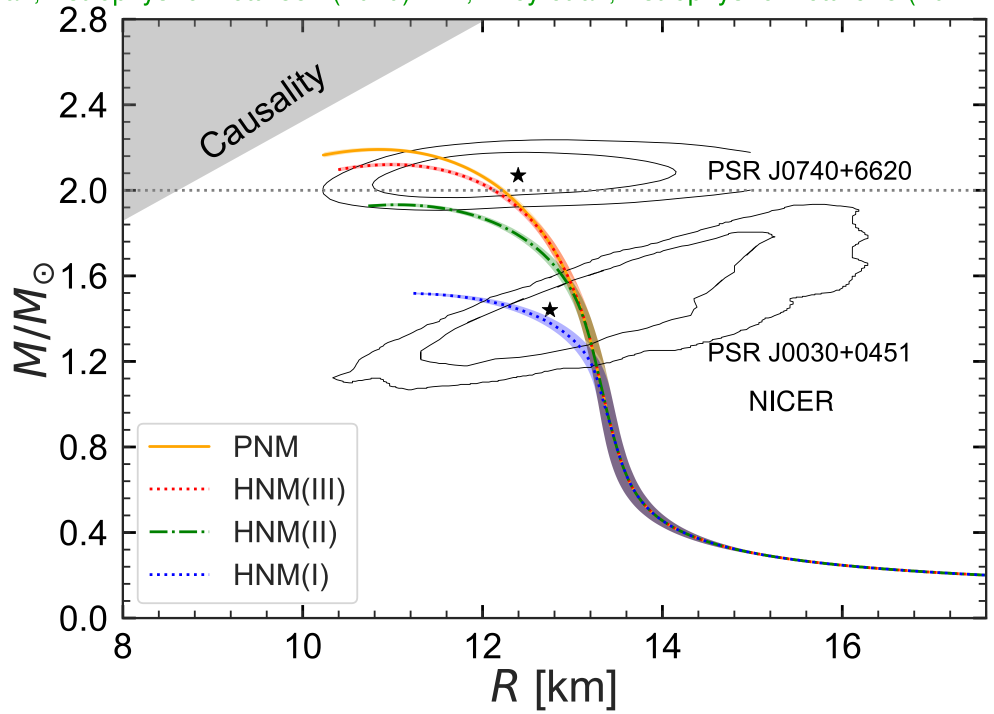
- EoS & speed of sound

- Mass-radius relation

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



NICER: Miller et al., Astrophys. J. Lett. **887** (2019) L24; Riley et al., Astrophys. J. Lett. **918** (2021 L27



Finite temperature physics

- Just two teasers for finite T calculations

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

***Ab Initio* Nuclear Thermodynamics**

Bing-Nan Lu,[1] Ning Li,[1] Serdar Elhatisari,[2] Dean Lee,[1] Joaquín E. Drut,[3] Timo A. Lähde,[4] Evgeny Epelbaum,[5] and Ulf-G. Meißner[6,4,7]

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[7]*Tbilisi State University, 0186 Tbilisi, Georgia*

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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.

Phys. Lett. B 850 (2024) 138463

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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

$\hookrightarrow$ liquid-vapor phase transition

$\hookrightarrow$ location of the critical point

- new light cluster distillation method

$\hookrightarrow$ abundances of dimers, trimers, tetramers

$\hookrightarrow$ benchmark for virial calculations

Chiral Interactions at N3LO

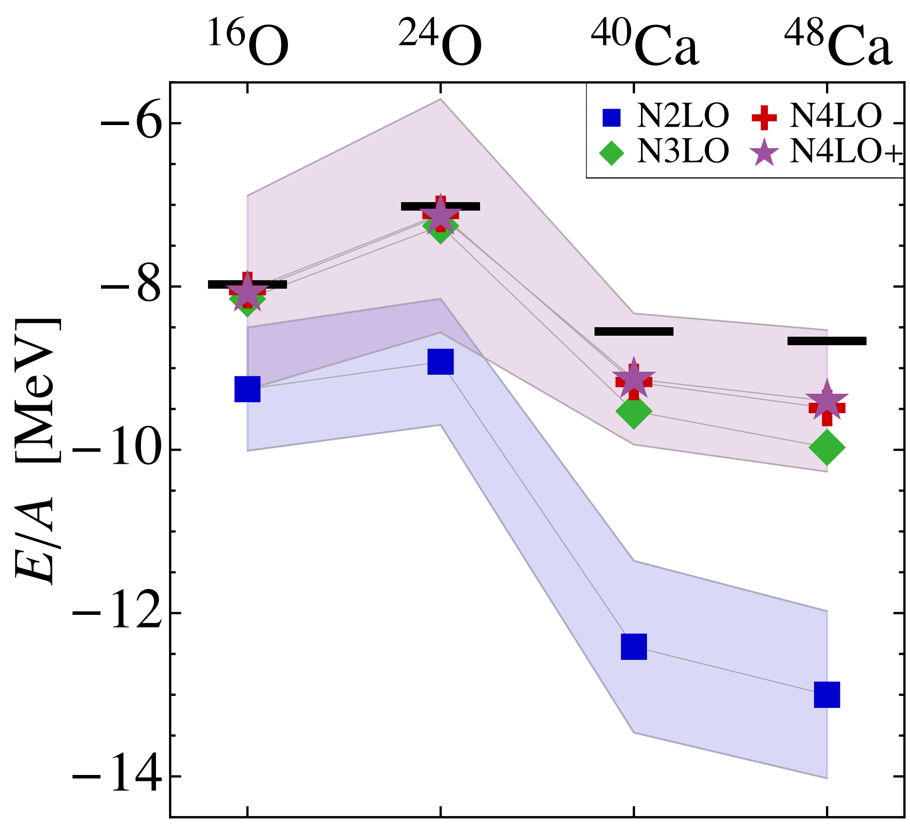
One motivation: The puzzle of the nuclear radii

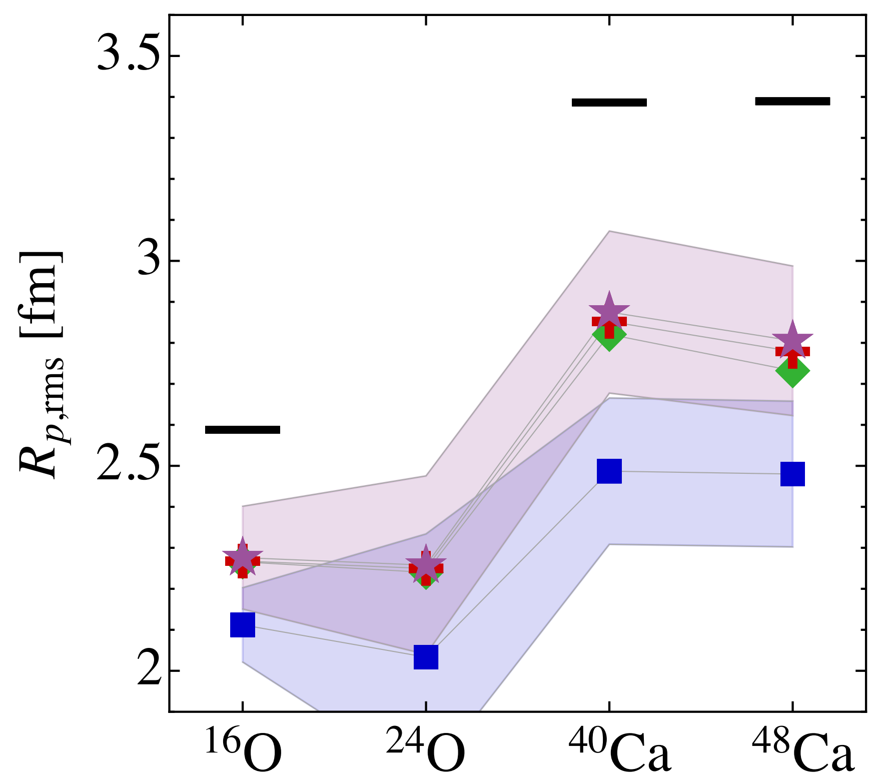
- Modern *ab initio* methods get correct energies, but incorrect radii

Cipollone et al., Phys. Rev. C **92** (2015) 014306, ...

- E.g. shell model with SRG evolved chiral NN and NNN interactions

LENPIC, Phys. Rev. C **106** (2022) 064002





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

  $\hookrightarrow$ essentially done $\surd$ $\rightarrow$ as just discussed

  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) $\surd$

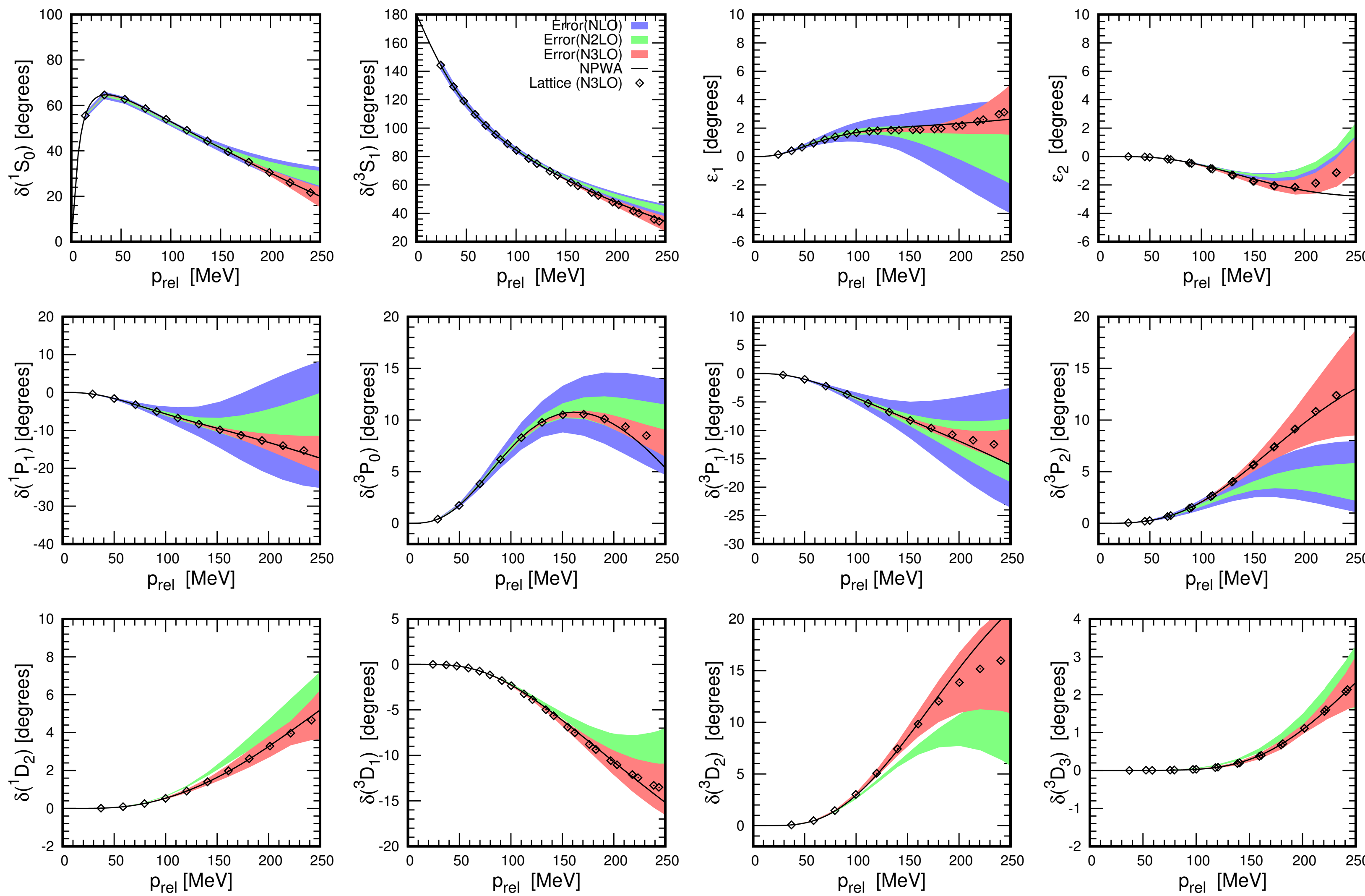
  $\hookrightarrow$ third for nuclear reactions/astrophysics (first results) $\surd$

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 $a = 1.32$ fm (cf. Nijmegen PWA)

NLO
N2LO
N3LO

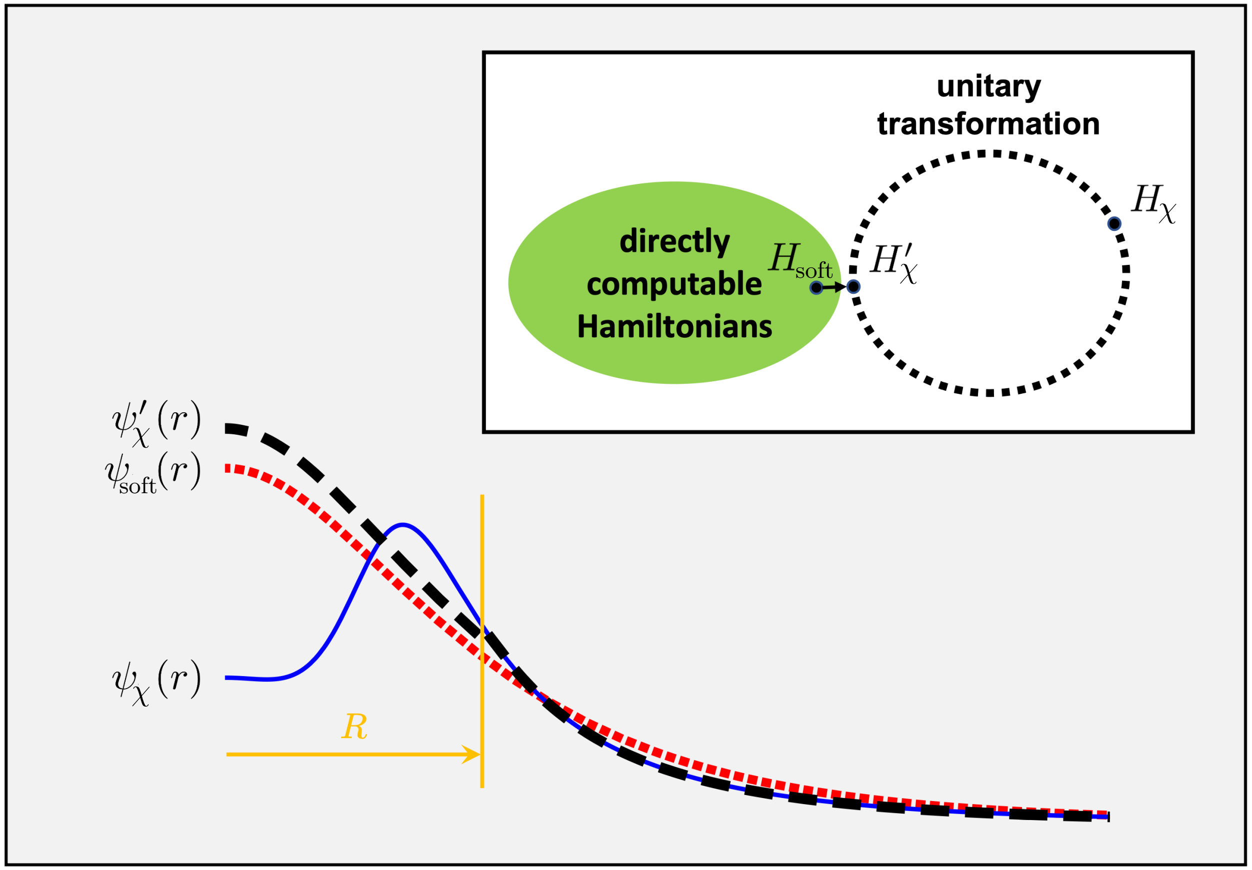


uncertainty estimates á la Epelbaum, Krebs, UGM,
Eur. Phys. J. A **51** (2015) 53

Wave function matching

Elhatisari et al., acc. for publication in *Nature* [arXiv:2210.17488 [nucl-th]]

- Graphical representation of w.f. matching



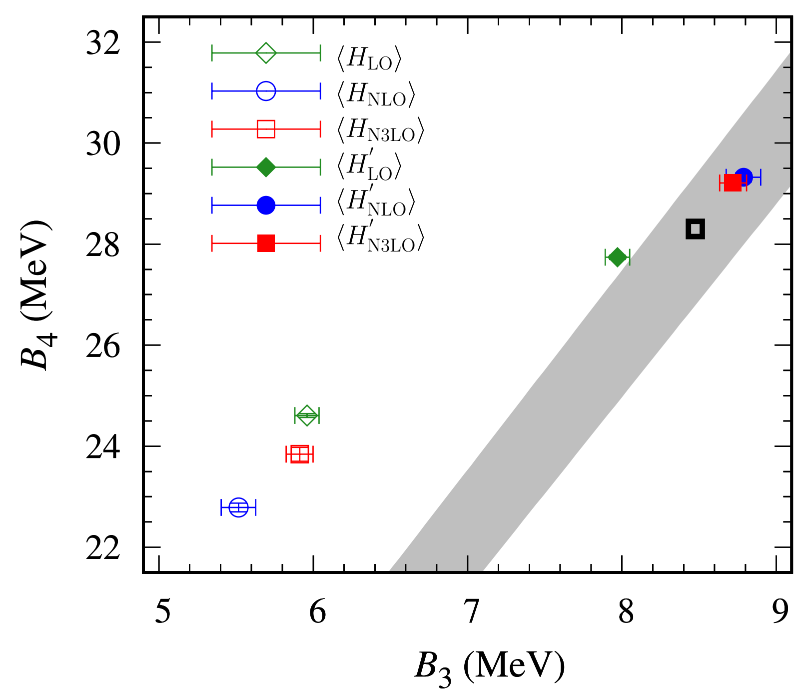
- W.F. matching is a "Hamiltonian translator":
  eigenenergies from $\boldsymbol{H_1}$ but w.f. from $\boldsymbol{H_2 = U^\dagger H_1 U}$

Wave function matching for light nuclei

Elhatisari et al., acc. for publication in *Nature* [arXiv:2210.17488 [nucl-th]], L. Bovermann, PhD thesis

- W.F. matching for the light nuclei

Nucleus	$B_{\rm LO}$ [MeV]	$B_{\rm N3LO}$ [MeV]	Exp. [MeV]
$E_{\chi,{\rm d}}$	1.79	2.21	2.22
$\langle\psi^0_{\rm soft}\|\,H_{\chi,{\rm d}}\,\|\psi^0_{\rm soft}\rangle$	0.45	0.62	
$\langle\psi^0_{\rm soft}\|\,H'_{\chi,{\rm d}}\,\|\psi^0_{\rm soft}\rangle$	1.65	2.01	
$\langle\psi^0_{\rm soft}\|\,H_{\chi,{\rm t}}\,\|\psi^0_{\rm soft}\rangle$	5.96(8)	5.91(9)	8.48
$\langle\psi^0_{\rm soft}\|\,H'_{\chi,{\rm t}}\,\|\psi^0_{\rm soft}\rangle$	7.97(8)	8.72(9)	
$\langle\psi^0_{\rm soft}\|\,H_{\chi,\alpha}\,\|\psi^0_{\rm soft}\rangle$	24.61(4)	23.84(14)	28.30
$\langle\psi^0_{\rm soft}\|\,H'_{\chi,\alpha}\,\|\psi^0_{\rm soft}\rangle$	27.74(4)	29.21(14)	



- reasonable accuracy for the light nuclei

- Tjon-band recovered with H'_χ

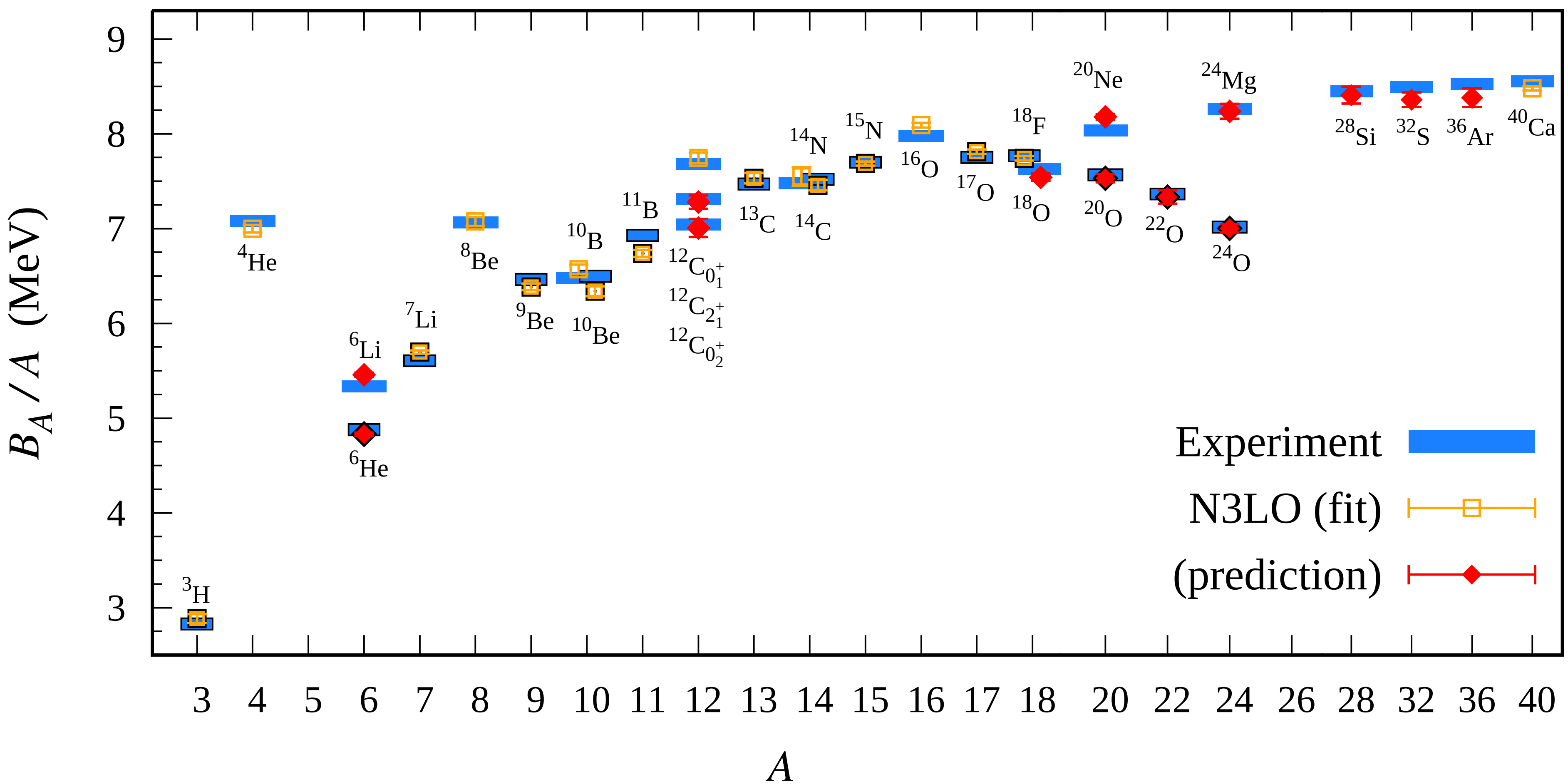
  Platter, Hammer, UGM, Phys. Lett. B **607** (2005) 254

$\hookrightarrow$ now let us go to larger nuclei....

Nuclei at N3LO

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

Elhatisari et al., acc. for publication in *Nature* [arXiv:2210.17488 [nucl-th]]

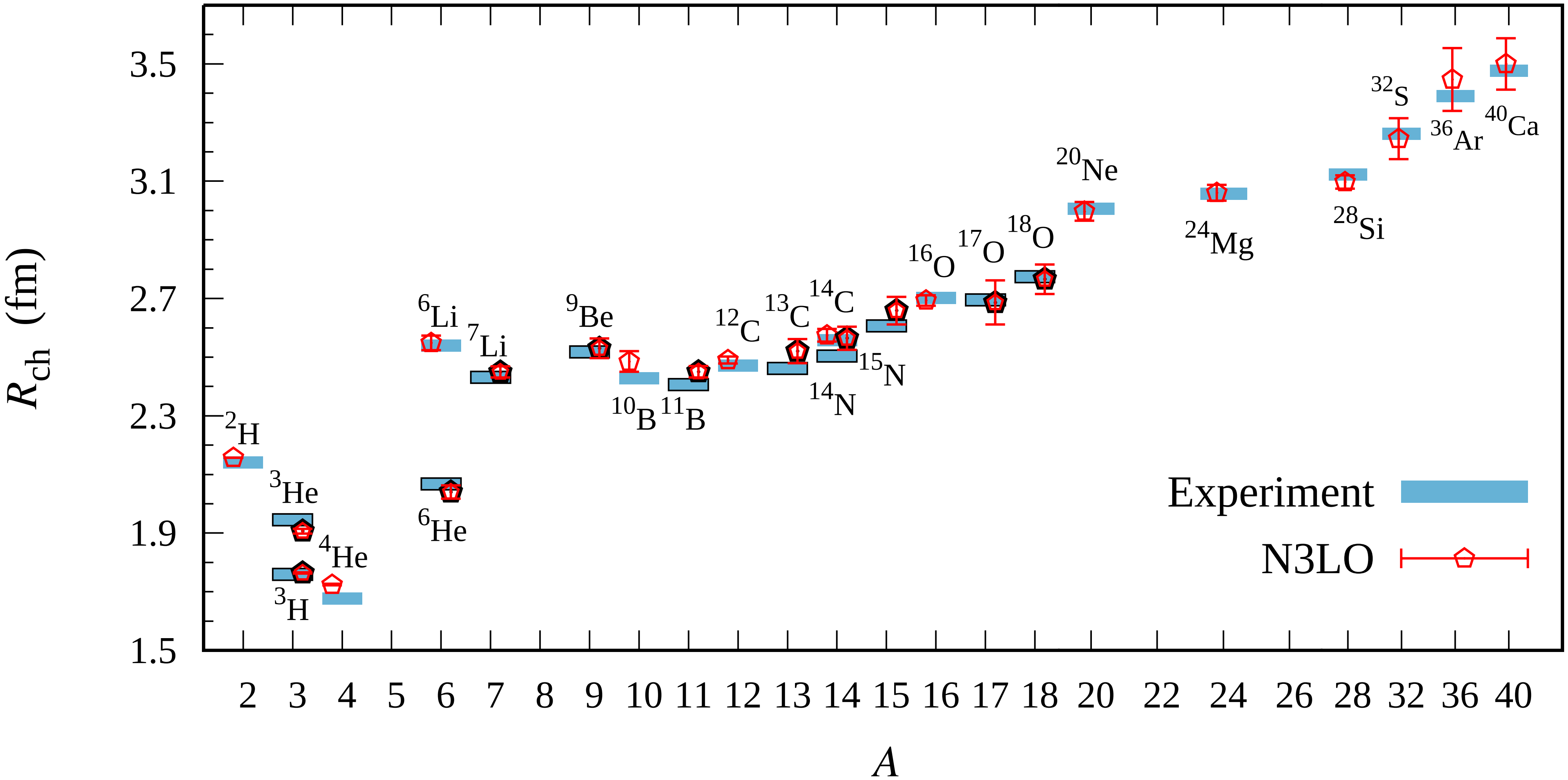


→ excellent starting point for precision studies

Prediction: Charge radii at N3LO

Elhatisari et al., acc. for publication in *Nature* [arXiv:2210.17488 [nucl-th]]

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

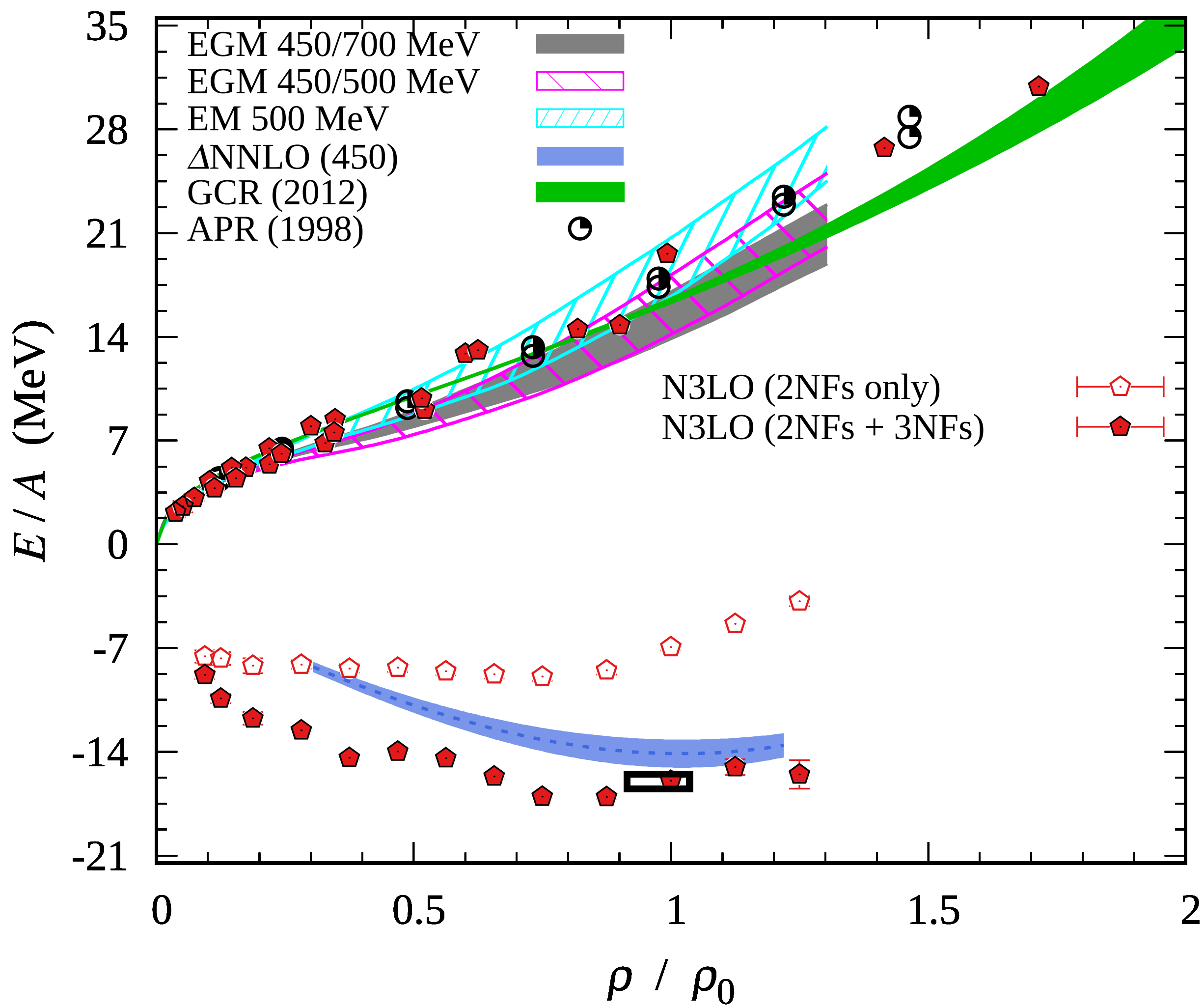


$\hookrightarrow$ no radius problem!

Prediction: Neutron & nuclear matter at N3LO

Elhatisari et al., acc. for publication in *Nature* [arXiv:2210.17488 [nucl-th]]

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

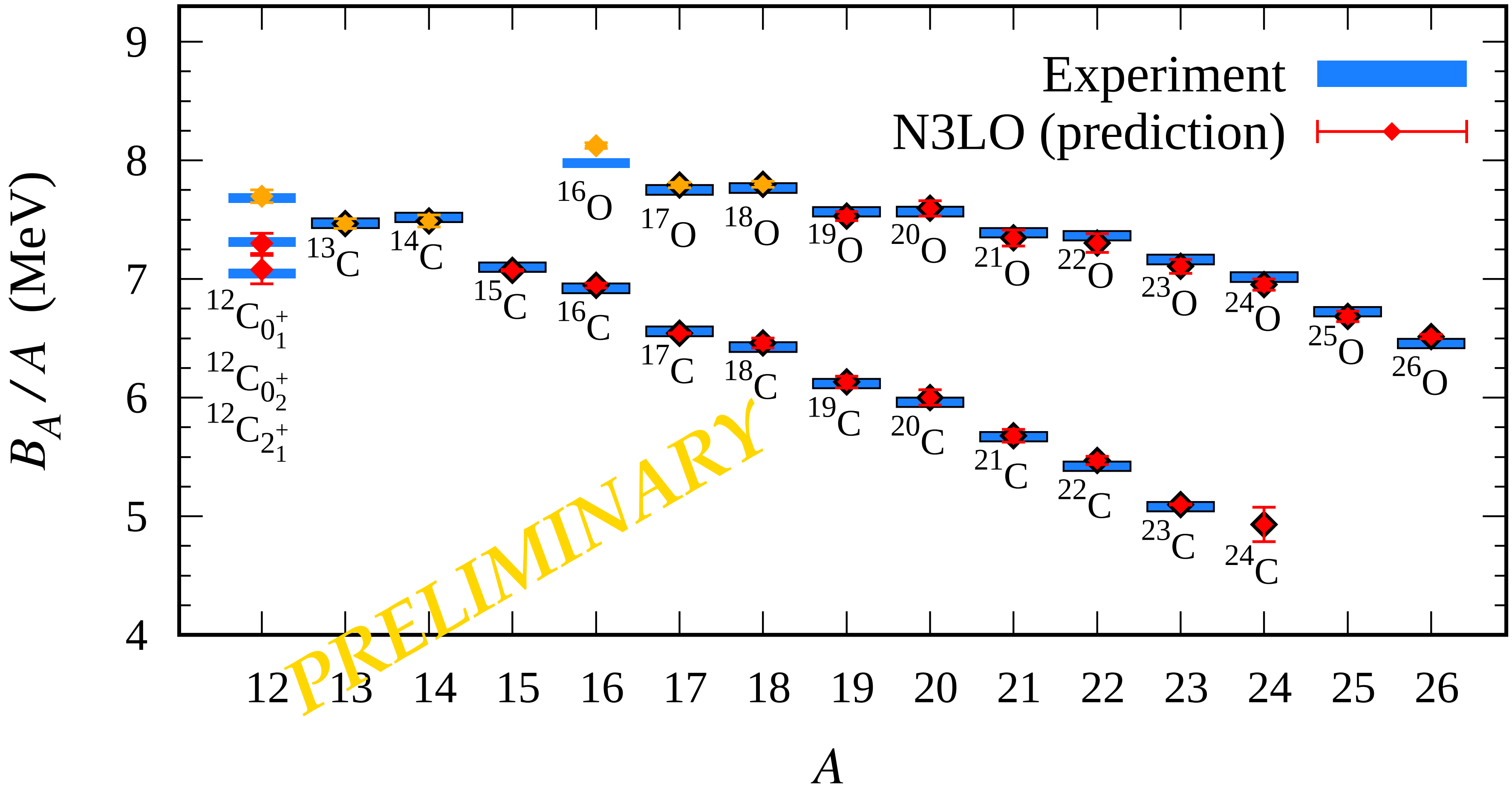


$\hookrightarrow$ can be improved using average twisted b.c.'s (Lu et al. (2020)

Prediction: Isotope chains of carbon & oxyen

NLEFT collaboration, in progress

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



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

Chiral Interactions (at N3LO): Applications to scattering

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

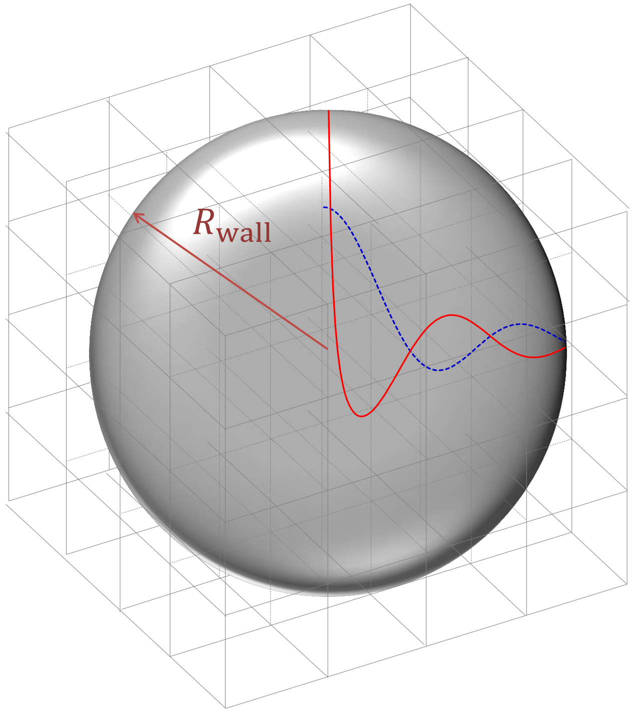
↪ works in many cases, problems w/ partial-wave mixing and cluster-cluster scattering

- 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 $R_{\rm wall}$

  ↪ 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 w/ chiral H

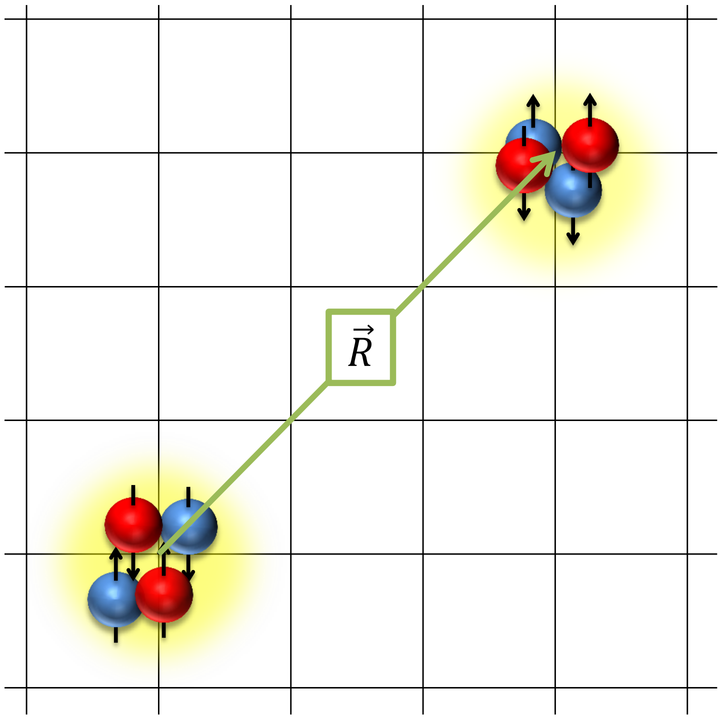
$$|\vec{R}\rangle_\tau = \exp(-H\tau)|\vec{R}\rangle$$

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

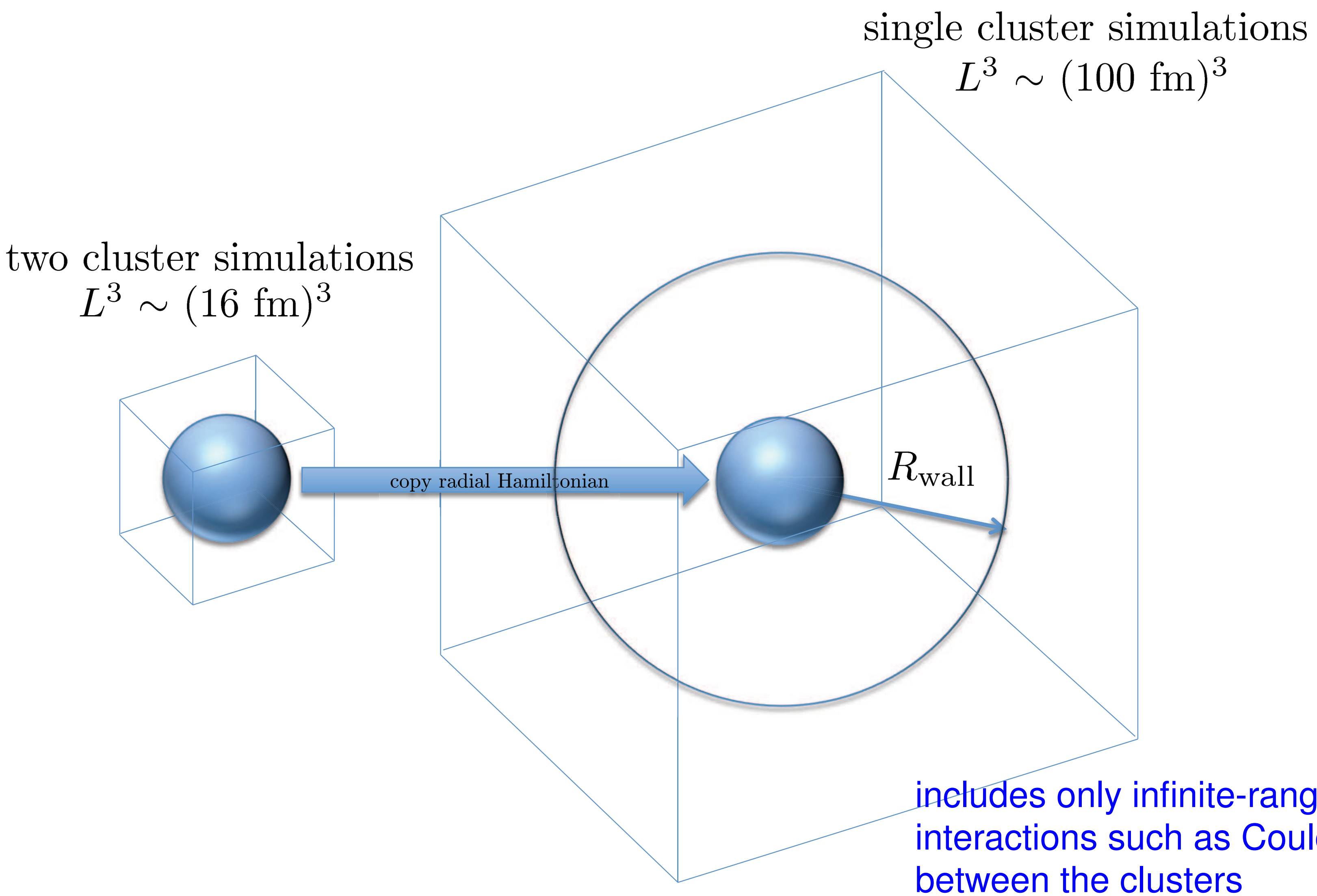
- Adiabatic Hamiltonian (requires norm matrices)

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

- favorable scaling: $t_{\mathrm{CPU}} \sim (A_1 + A_2)^2$



Adiabatic Hamiltonian with Coulomb



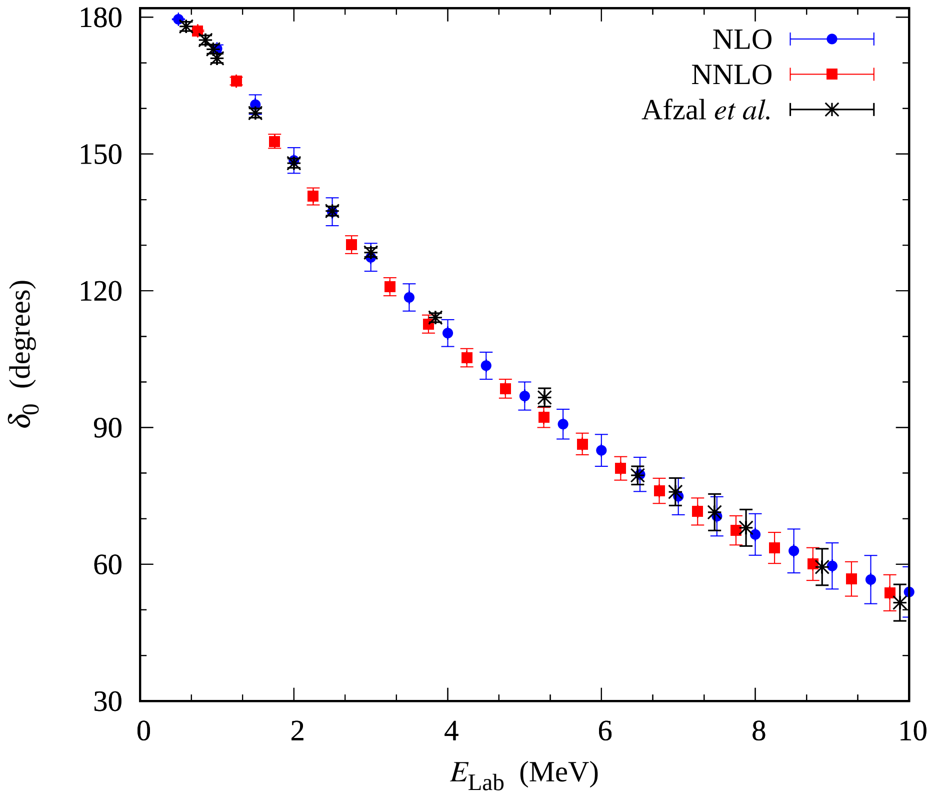
includes only infinite-range interactions such as Coulomb between the clusters

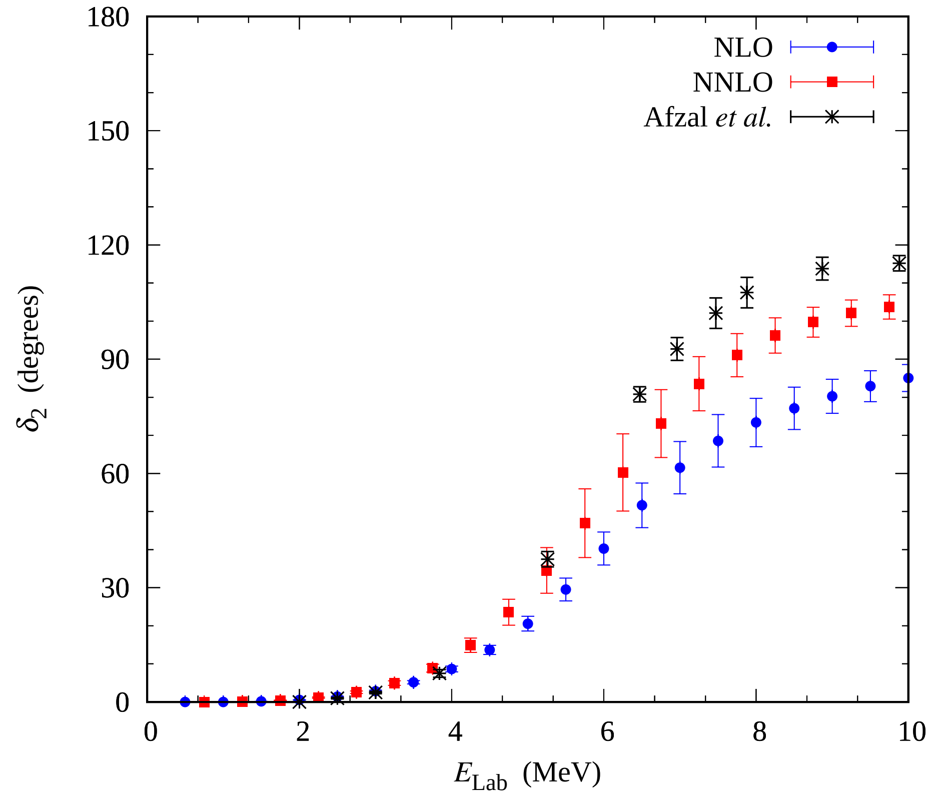
25

Breakthrough: *Ab initio* α-α scattering

Elhatisari, Lee, Rupak, Epelbaum, Krebs, Lähde, Luu, UGM, Nature **528** (2015) 111
Elhatisari, Lähde, Lee, UGM, Vonk, JHEP **02** (2022) 001

- **Parameter-free** S-wave and D-wave phase shifts at NNLO, updated in 2022





$E_R^{\rm NNLO} = -0.11(1)$ MeV [$+0.09$ MeV]

$E_R^{\rm NNLO} = 2.93(5)$ MeV [$2.92(18)$ MeV]

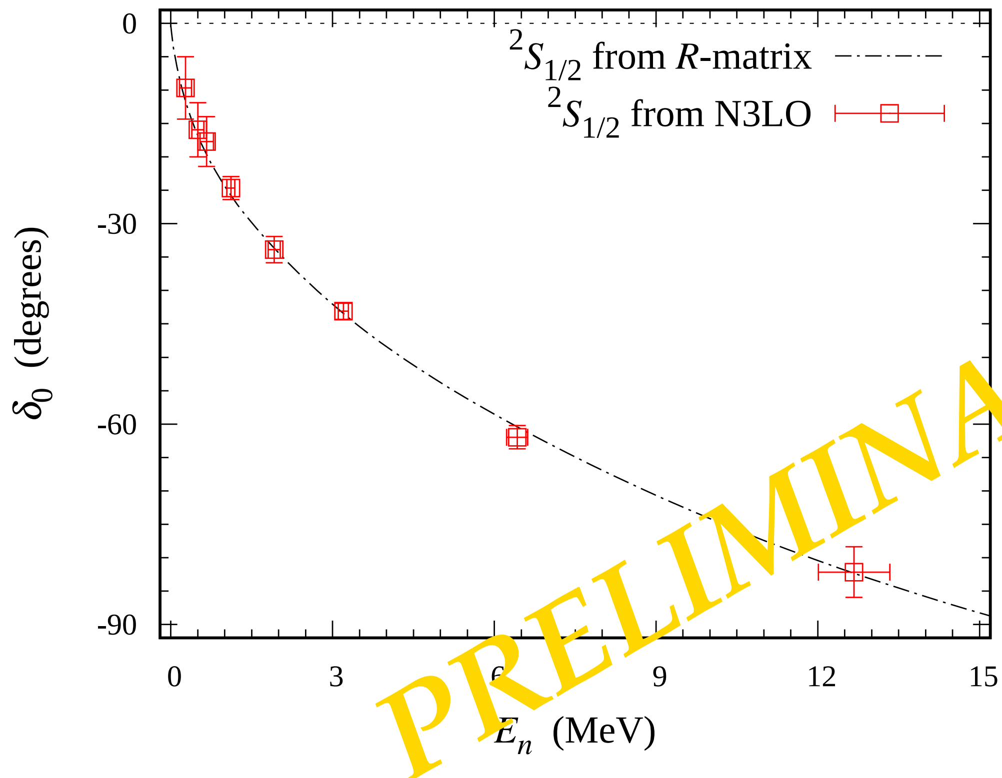
$\Gamma_R^{\rm NNLO} = 2.00(16)$ MeV [$1.35(50)$ MeV]

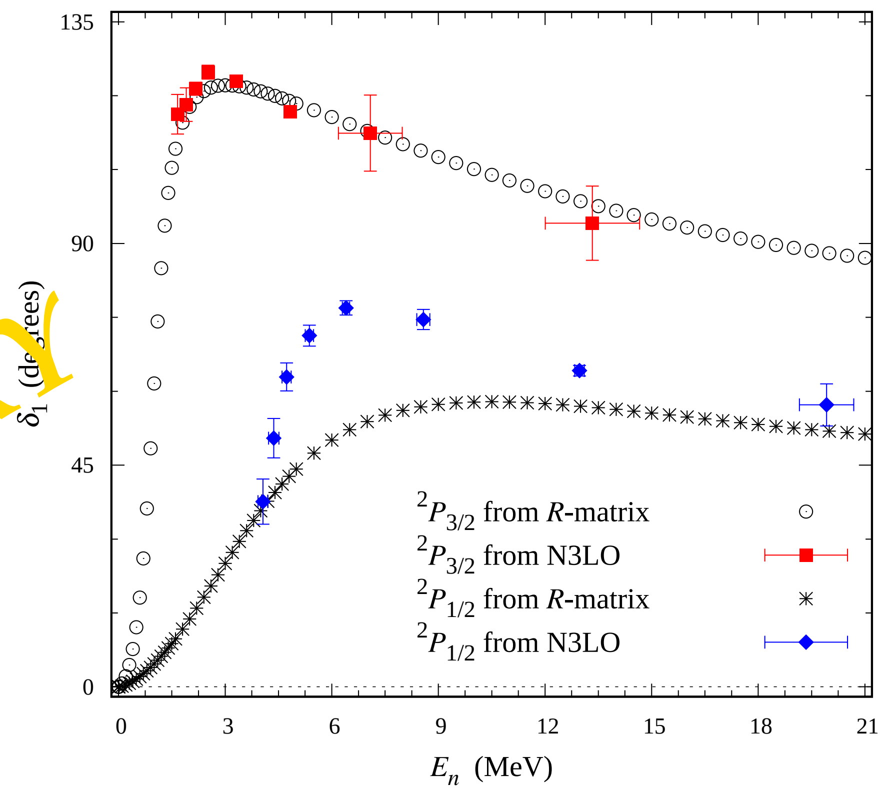
Afzal et al., Rev. Mod. Phys. **41** (1969) 247 [data]

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

On-going projects

Further directions

- Just discuss two important directions

1) β and double-β decays:

$\hookrightarrow$ probing the weak interactions in nuclei

$\hookrightarrow$ providing precise nuclear M.E.s for $0\nu 2\beta$ decays (^{48}Ca, ^{76}Ge, ...)

$\rightarrow$ show first result

2) The "holy grail" of nuclear astrophysics: $\alpha + ^{12}\text{C} \rightarrow ^{16}\text{O} + \gamma$ at E_{Gamov}

$\hookrightarrow$ consider first $\alpha + ^{12}\text{C}$ elastic scattering

$\hookrightarrow$ add the second channel to account for the photon in the final state

$\rightarrow$ show first result

Prediction: Triton β-decay at N3LO

Elhatisari, Hildenbrand, UGM, in preparation

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

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

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

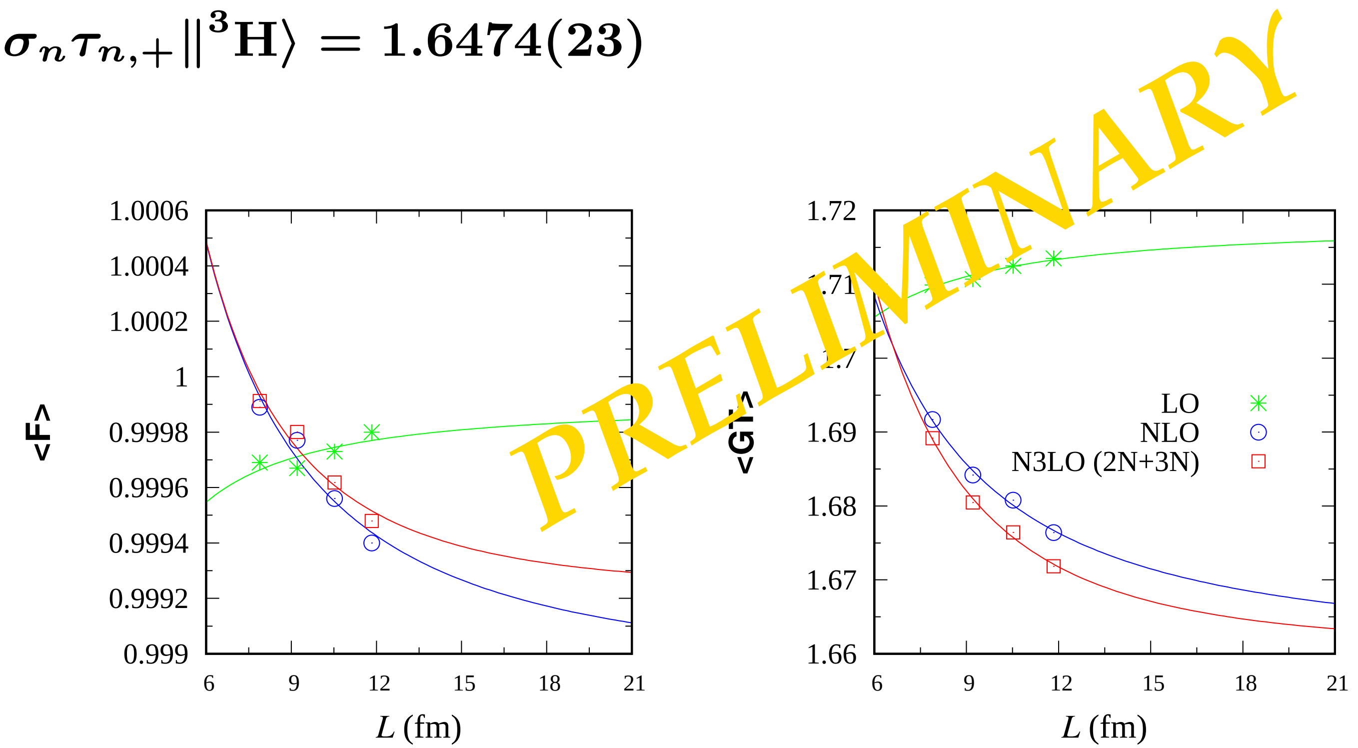
- NLEFT:

$$\boxed{\langle \mathsf{F}\rangle_{\mathrm{N3LO}} = 0.9992(16)}$$

$$\boxed{\langle \mathsf{GT}\rangle_{\mathrm{N3LO}} = 1.661(35)}$$

- No Coulomb at LO

- Larger L underway...

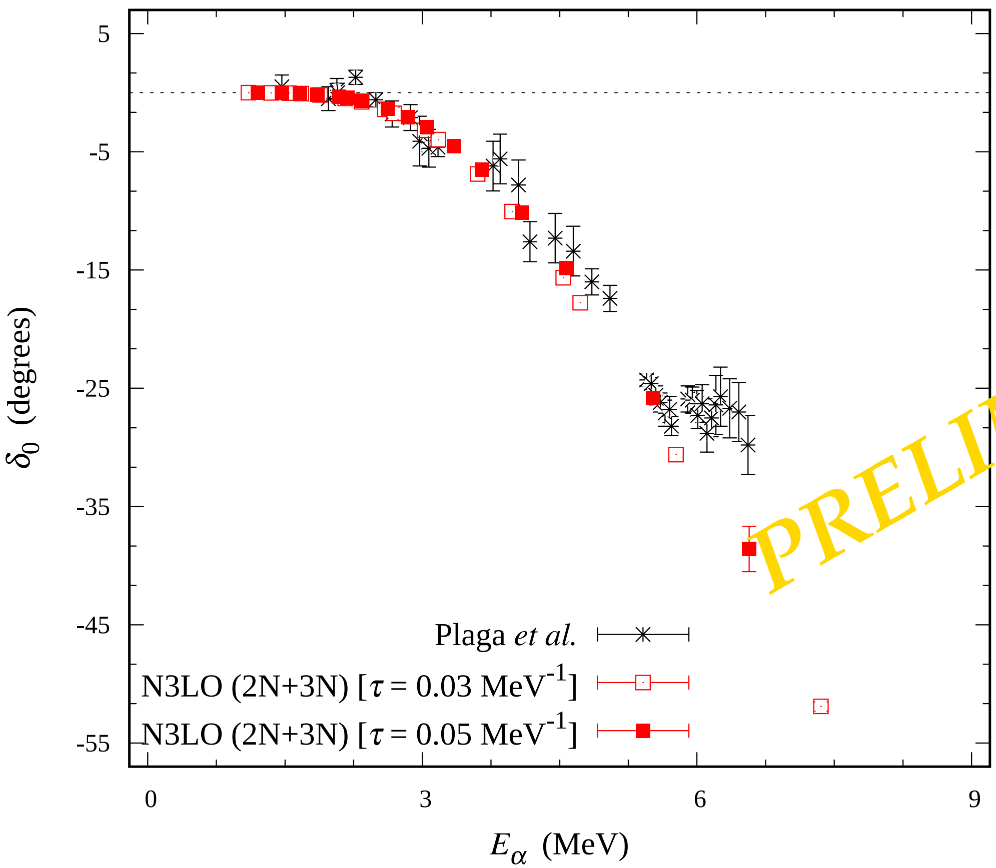


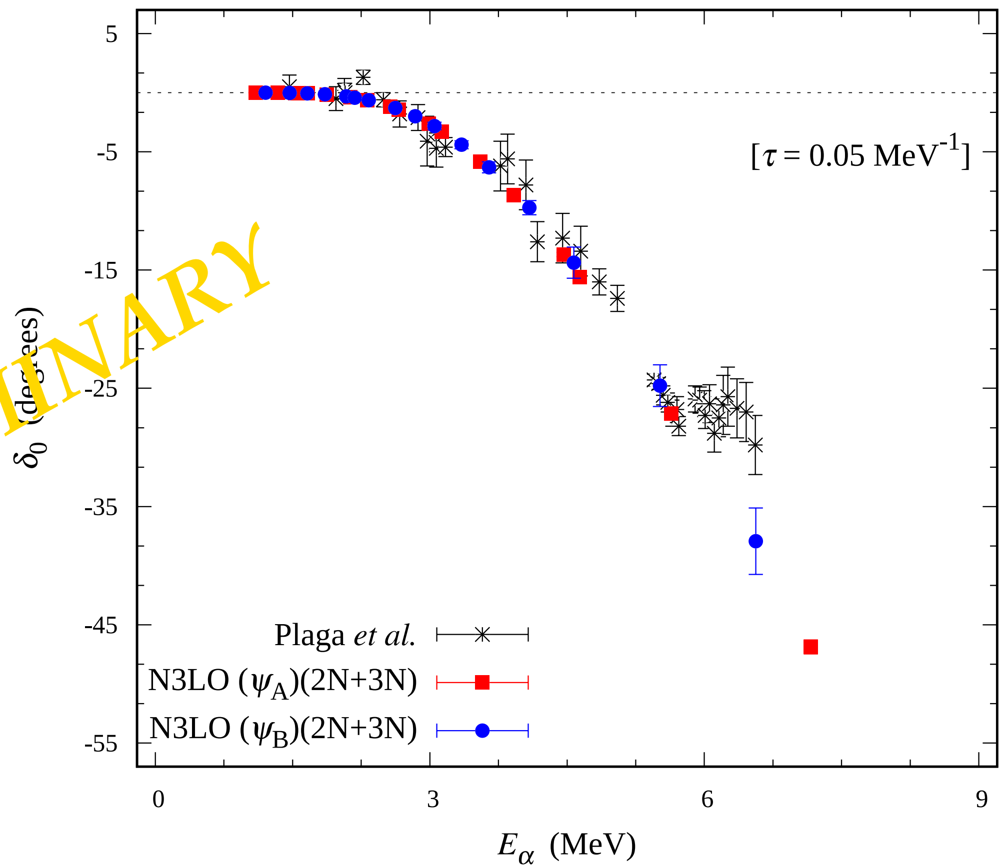
Scattering: Alpha-carbon scattering at N3LO

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

- Use the APM, first step for the holy grail of nuclear astrophysics

  ↪ different Euclidean times & different initial states





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

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

Perspectives

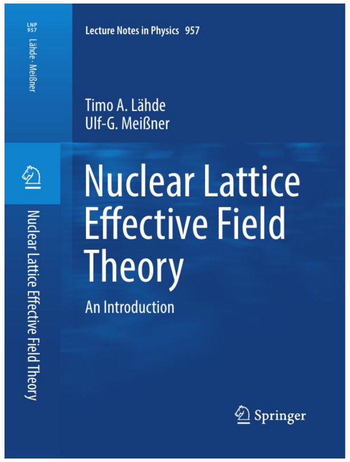
Perspectives

- Established NLEFT as a precision quantum many-body approach $\surd$
  $\hookrightarrow$ CRC 110 instrumental in achieving this! $\hookrightarrow$ ERC AdG

- Very successful within the CRC 110:
  2 Nature, 1 Nat. Comm., 14 Phys. Rev. Lett., 1 Rev. Mod. Phys., ... $\surd$
  plus 1 textbook!

- Also successful in terms of personal: 3 post-doc $\to$ professors
  Bing-Nan Lu (GSCAEP), Ning Li (SCNU), Shihang Shen (Beihang U.)

- On-going and future research:
  - proton and neutron drip lines towards heavy nuclei
  - precision low-energy scattering for BBN and stellar reactions
  - hypernuclear landscape
  - anthropics (fine-tunings in element generation)

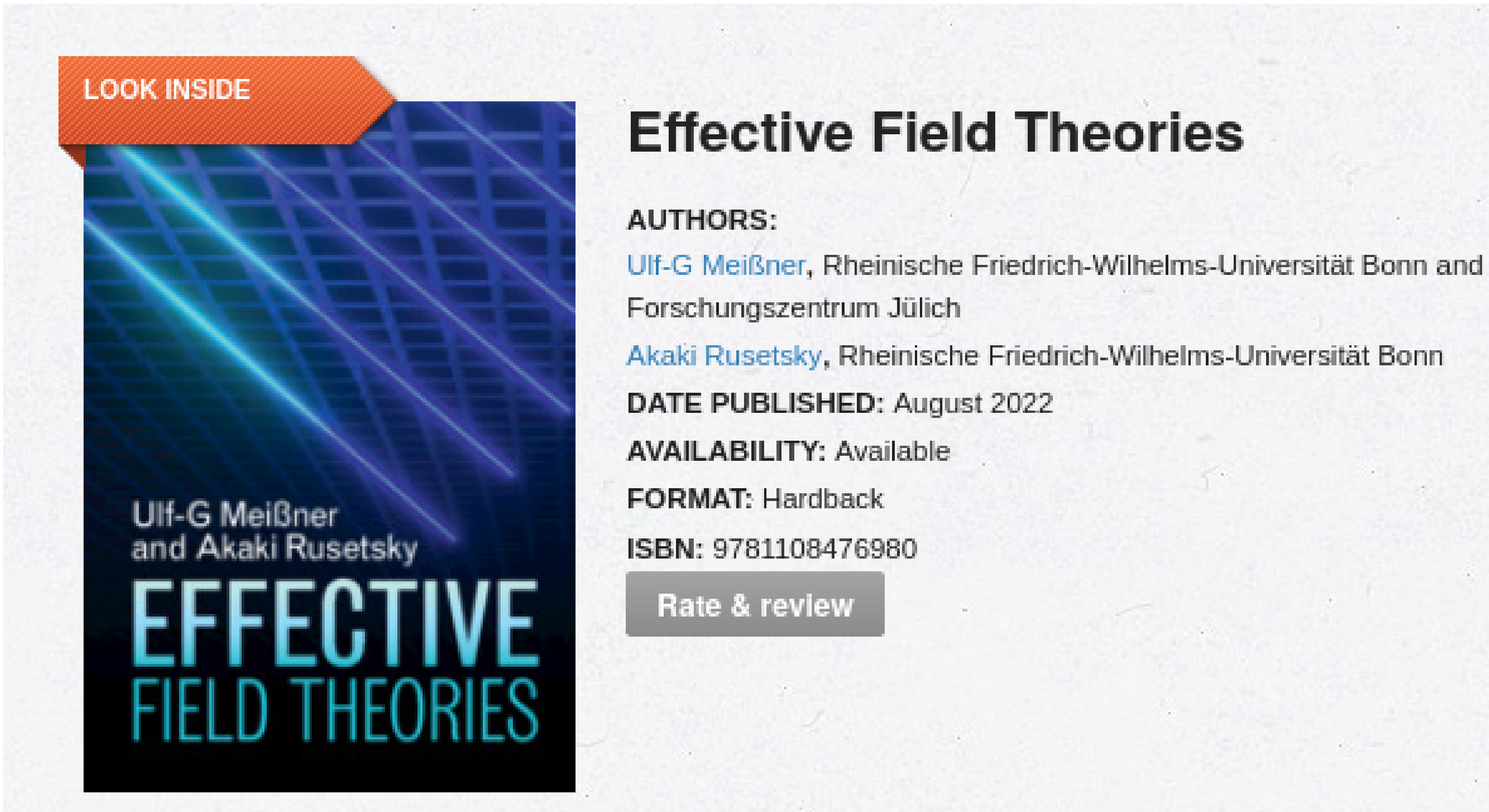


Thank you for your attention !

SPARES

More on EFTs

- Much more details on EFTs in light quark physics:

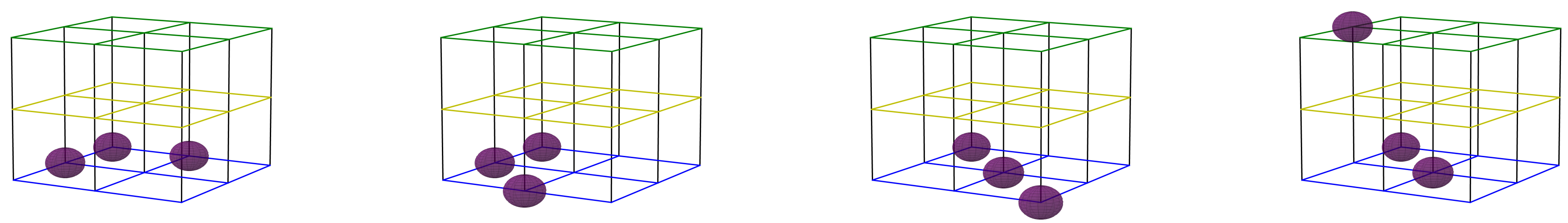


https://www.cambridge.org/de/academic/subjects/physics/theoretical-physics-and-mathematical-physics/effective-field-theories

Configurations

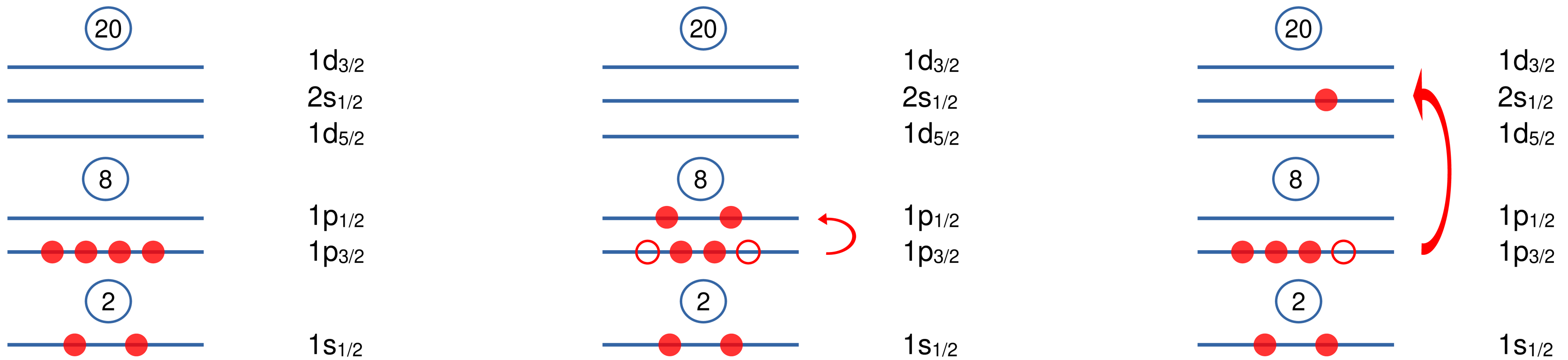
- Cluster and shell model configurations

S1 S2 S3 S4



— isoscele right triangle — "bent-arm" shape — linear diagonal chain — acute isoscele triangle

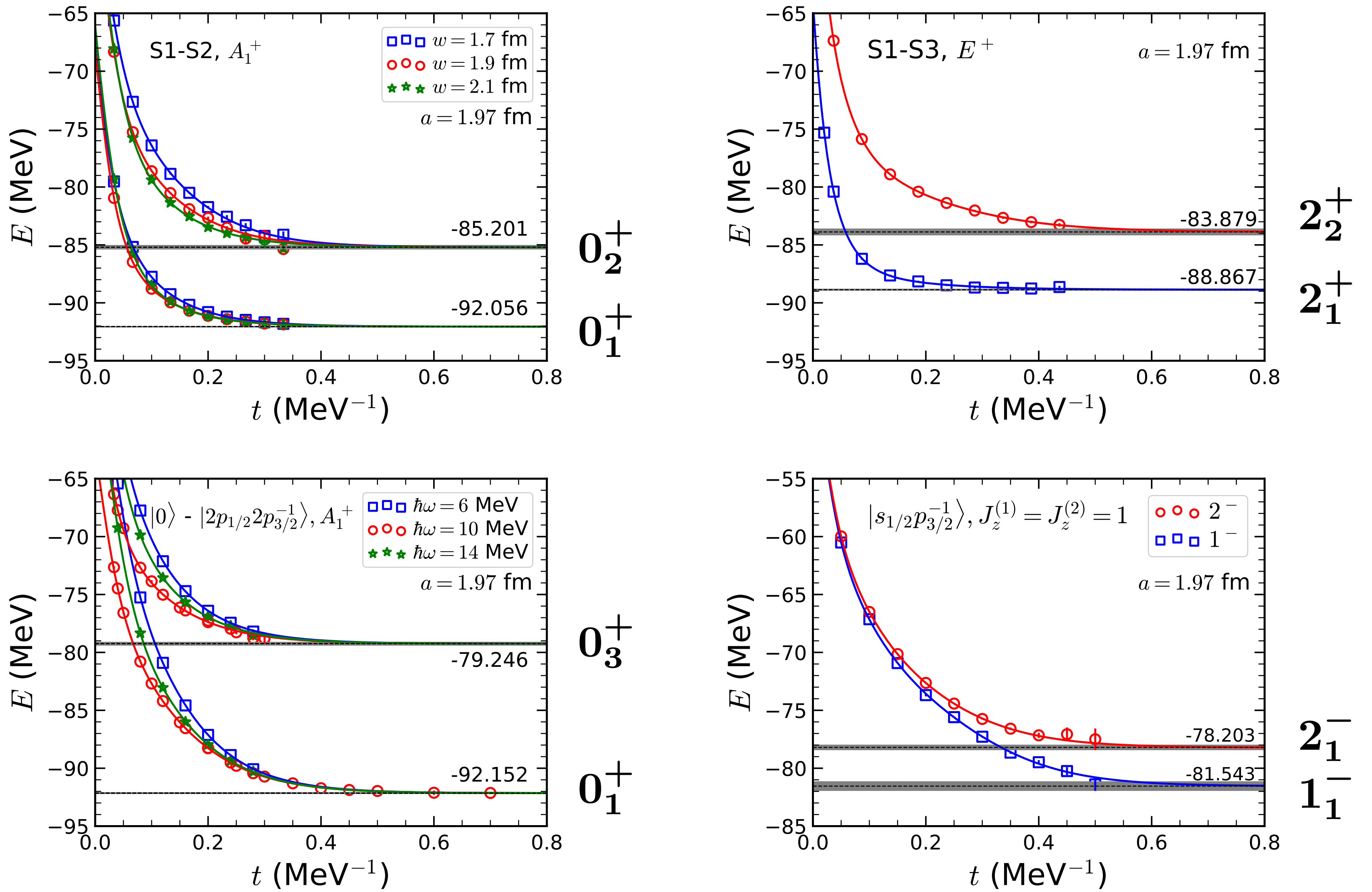
Gaussian wave packets
$w = 1.7 - 2.1$ fm



— ground state $|0\rangle$ — $2p$-$2h$ state, $J_z = 0$ — $1p$-$1h$ state, $J_z^{(1)} = J_z^{(2)} = 1$

Transient energies

- Transient energies from cluster and shell-model configurations



Electromagnetic properties

Shen, Elhatisari, Lähde, Lee, Lu, UGM, Nature Commun. **14** (2023) 2777

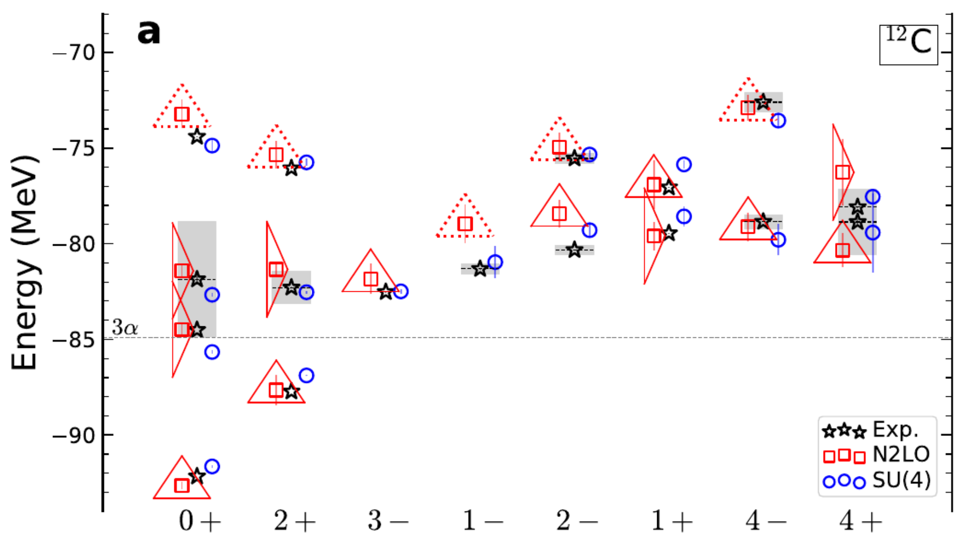
- Radii (be aware of excited states), quadrupole moments & transition rates

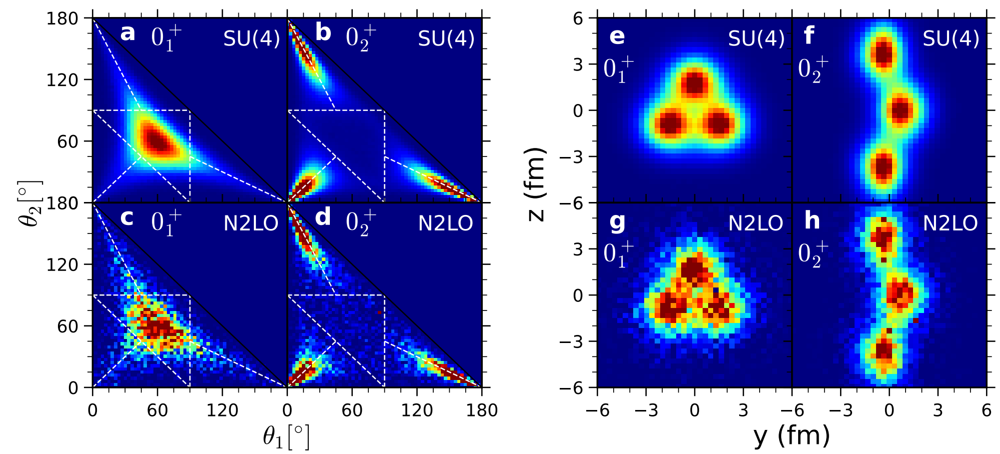
	NLEFT	FMD	α cluster	BEC	RXMC	Exp.
$r_c(0_1^+)$ [fm]	$\mathbf{2.53(1)}$	2.53	2.54	2.53	2.65	$\mathbf{2.47(2)}$
$r(0_2^+)$ [fm]	$\mathbf{3.45(2)}$	3.38	3.71	3.83	4.00	–
$r(0_3^+)$ [fm]	$\mathbf{3.47(1)}$	4.62	4.75	–	4.80	–
$r(2_1^+)$ [fm]	$\mathbf{2.42(1)}$	2.50	2.37	2.38	–	–
$r(2_2^+)$ [fm]	$\mathbf{3.30(1)}$	4.43	4.43	–	–	–

	NLEFT	FMD	α cluster	NCSM	Exp.
$Q(2_1^+)$ [e fm^2]	$\mathbf{6.8(3)}$	–	–	6.3(3)	$\mathbf{8.1(2.3)}$
$Q(2_2^+)$ [e fm^2]	$\mathbf{-35(1)}$	–	–	–	–
$M(E0, 0_1^+ \to 0_2^+)$ [e fm^2]	$\mathbf{4.8(3)}$	6.5	6.5	–	$\mathbf{5.4(2)}$
$M(E0, 0_1^+ \to 0_3^+)$ [e fm^2]	$\mathbf{0.4(3)}$	–	–	–	–
$M(E0, 0_2^+ \to 0_3^+)$ [e fm^2]	$\mathbf{7.4(4)}$	–	–	–	–
$B(E2, 2_1^+ \to 0_1^+)$ [e^2 fm^4]	$\mathbf{11.4(1)}$	8.7	9.2	8.7(9)	$\mathbf{7.9(4)}$
$B(E2, 2_1^+ \to 0_2^+)$ [e^2 fm^4]	$\mathbf{2.5(2)}$	3.8	0.8	–	$\mathbf{2.6(4)}$

Sanity check

- Repeat the calculations w/ the time-honored N2LO chiral interaction
  $\hookrightarrow$ better NN phase shifts than the SU(4) interaction
  $\hookrightarrow$ but calculations are much more difficult (sign problem)





- spectrum as before (good agreement w/ data)
- density distributions as before (more noisy, stronger sign problem)

Wave function matching II

Elhatisari et al., acc. for publication in ... [arXiv:2210.17488 [nucl-th]]

- $\boldsymbol{H}_{\rm soft}$ has tolerable sign oscillations, good for many-body observables
- $\boldsymbol{H}_\chi$ has severe sign oscillations, derived from the underlying theory

$\hookrightarrow$ can we find a unitary trafo, that creates a chiral $\boldsymbol{H}_\chi$ that is pert. th'y friendly?

$$\boldsymbol{H}'_\chi = \boldsymbol{U}^\dagger\, \boldsymbol{H}_\chi\, \boldsymbol{U}$$

☐ Let $|\psi^0_{\rm soft}\rangle$ be the lowest eigenstate of $\boldsymbol{H}_{\rm soft}$

☐ Let $|\psi^0_\chi\rangle$ be the lowest eigenstate of $\boldsymbol{H}_\chi$

☐ Let $|\phi_{\rm soft}\rangle$ be the projected and normalized lowest eigenstate of $\boldsymbol{H}_{\rm soft}$

$$|\phi_{\rm soft}\rangle = \mathcal{P}\,|\psi^0_{\rm soft}\rangle / || |\psi^0_{\rm soft}\rangle ||$$

☐ Let $|\phi_\chi\rangle$ be the projected and normalized lowest eigenstate of $\boldsymbol{H}_\chi$

$$|\phi_\chi\rangle = \mathcal{P}\,|\psi^0_\chi\rangle / || |\psi^0_\chi\rangle ||$$

$$\hookrightarrow \boldsymbol{U}_{R',R} = \theta(r-R)\delta_{R',R} + \theta(R'-r)\theta(R-r)|\phi^\perp_\chi\rangle\langle\phi^\perp_{\rm soft}|$$