Nuclear Lattice Effective Field Theory

– Introduction and Perspectives –

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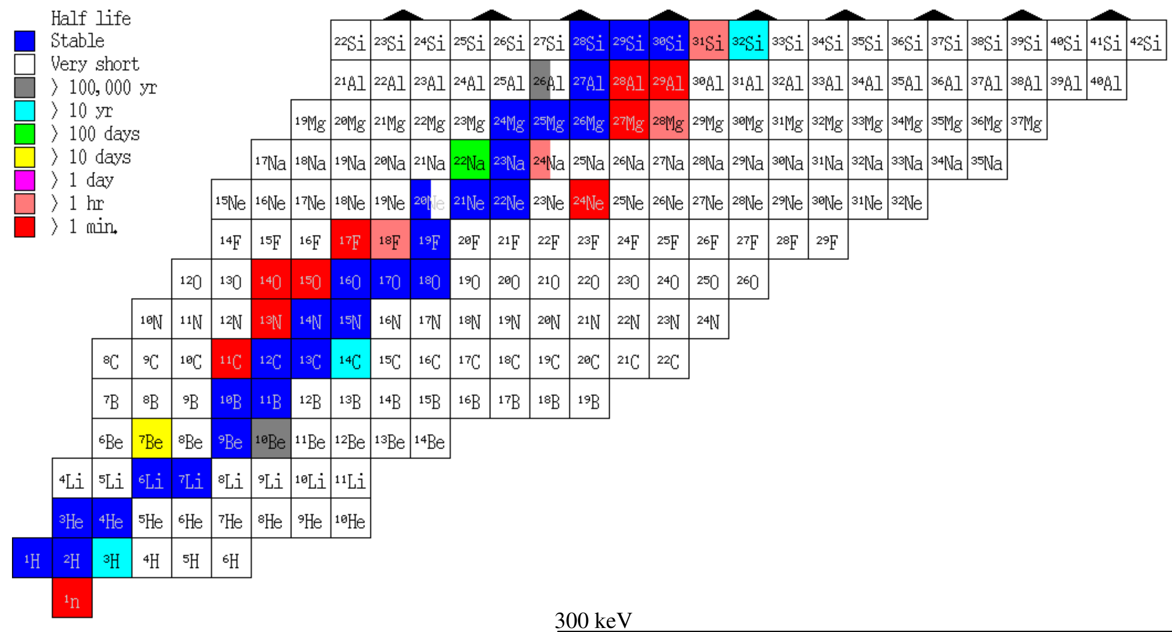
Contents

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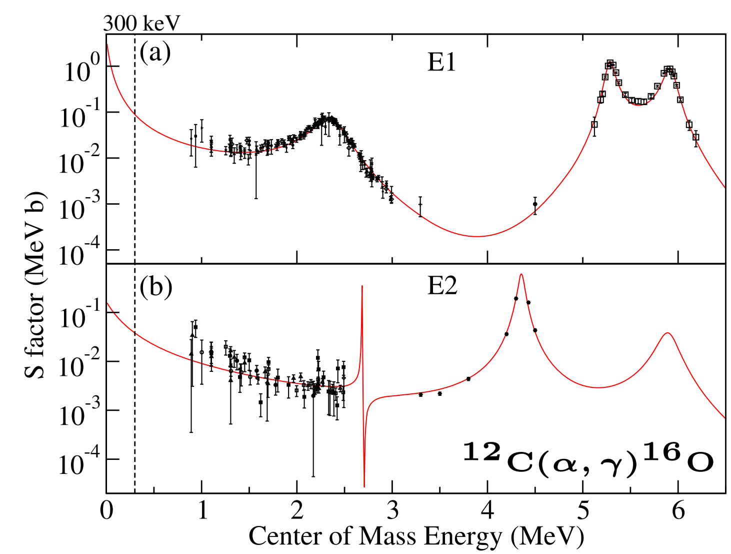
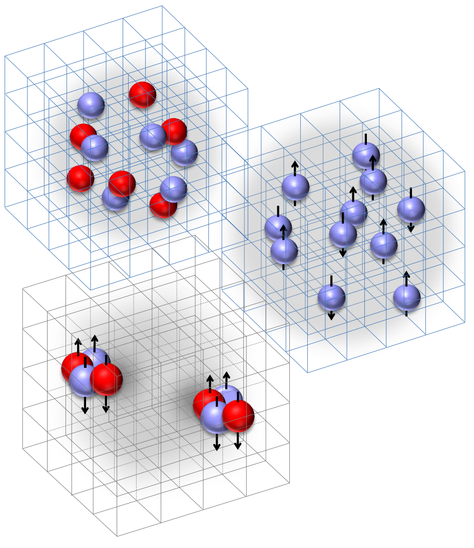
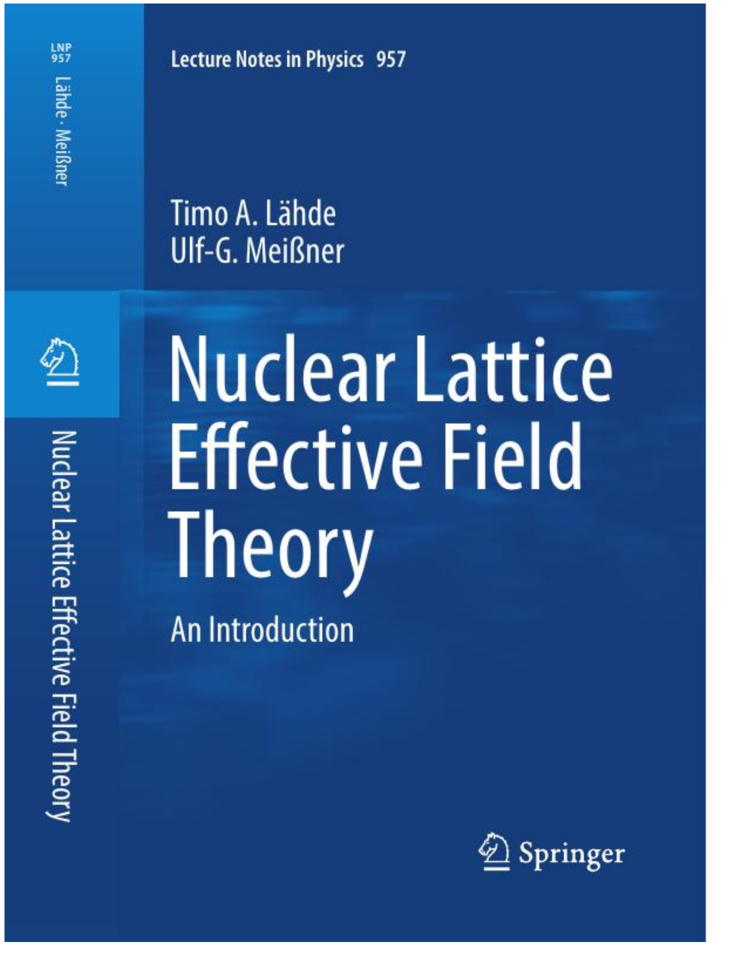
- Nuclear reactions, nuclear astrophysics:
  - ⋆ alpha-particle scattering
  - ⋆ triple-alpha reaction
  - ⋆ alpha-capture on carbon
  - ⋮



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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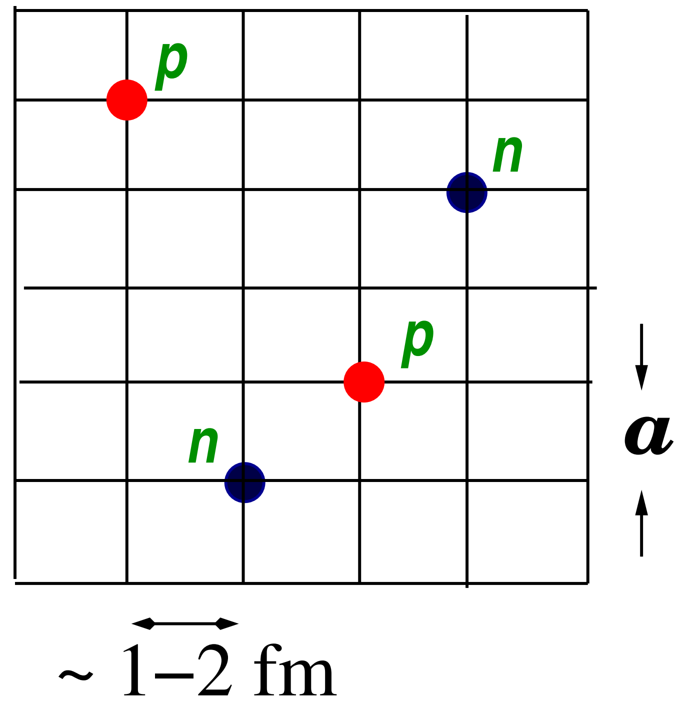
Nuclear lattice effective field theory (NLEFT)

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

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



- 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: $Z_A(\tau) = \langle \Psi_A | \exp(-\tau H) | \Psi_A \rangle$

  with Ψ_A a Slater determinant for A free nucleons

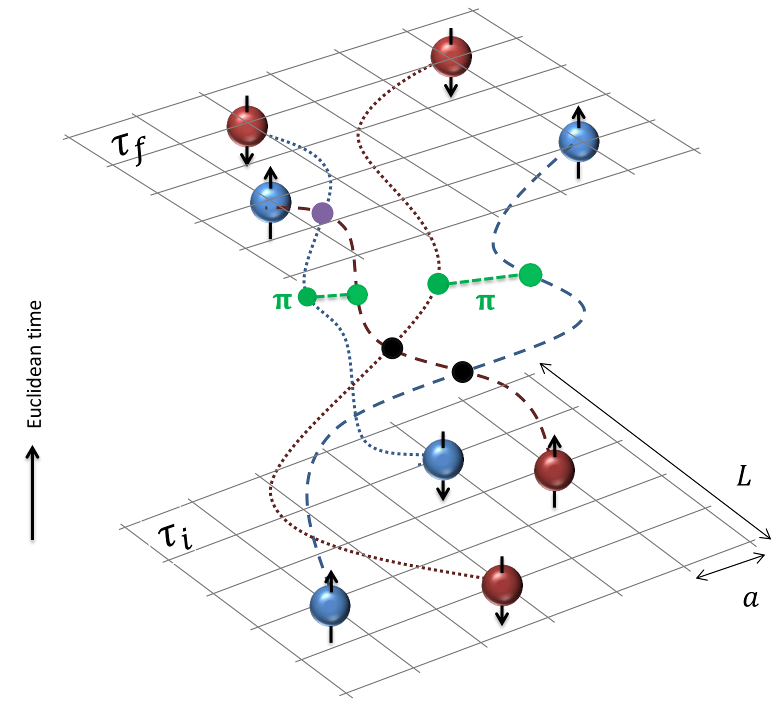
  [or a more sophisticated (correlated) initial/final state]

Euclidean time

- Transient energy

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

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



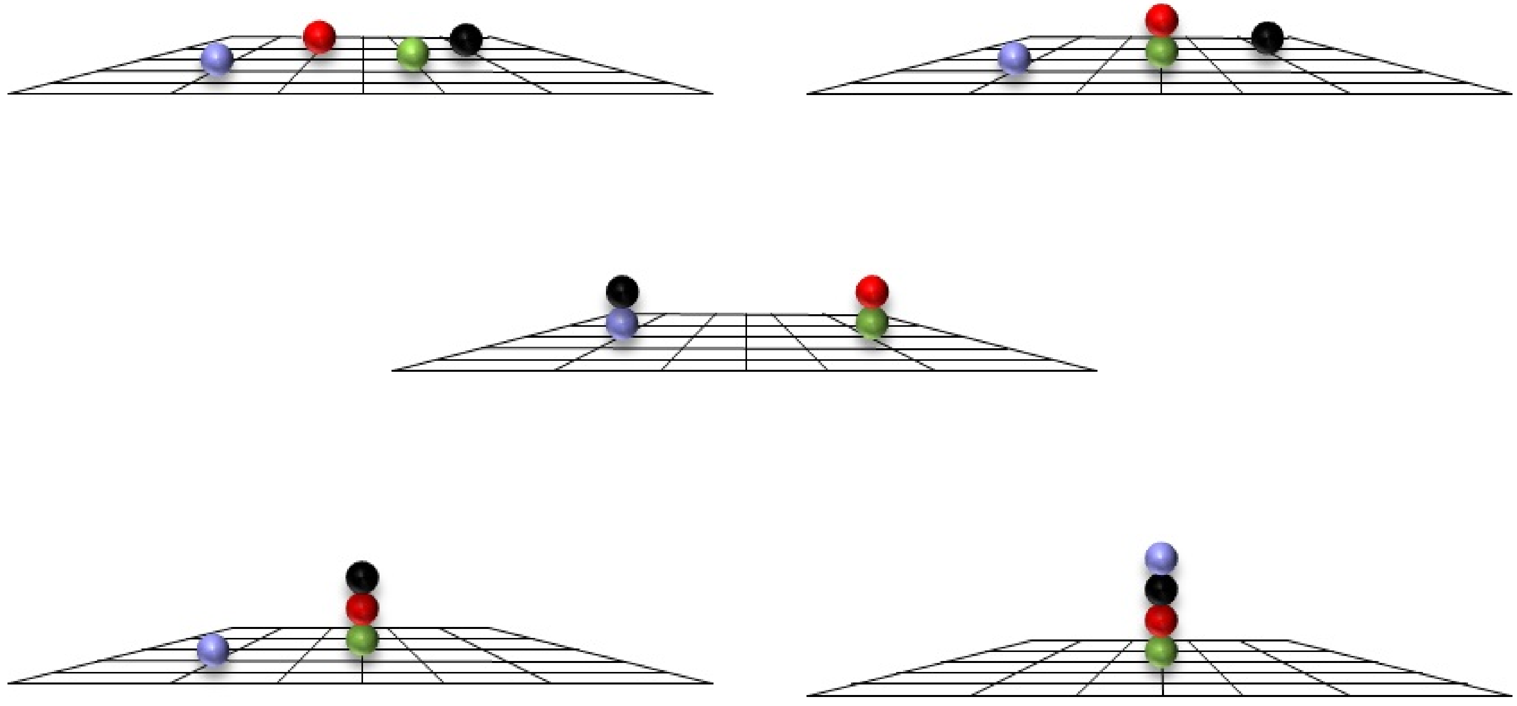
- Exp. value of any normal–ordered operator $\mathcal{O}$

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

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

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

Configurations



⇒ all *possible* configurations are sampled

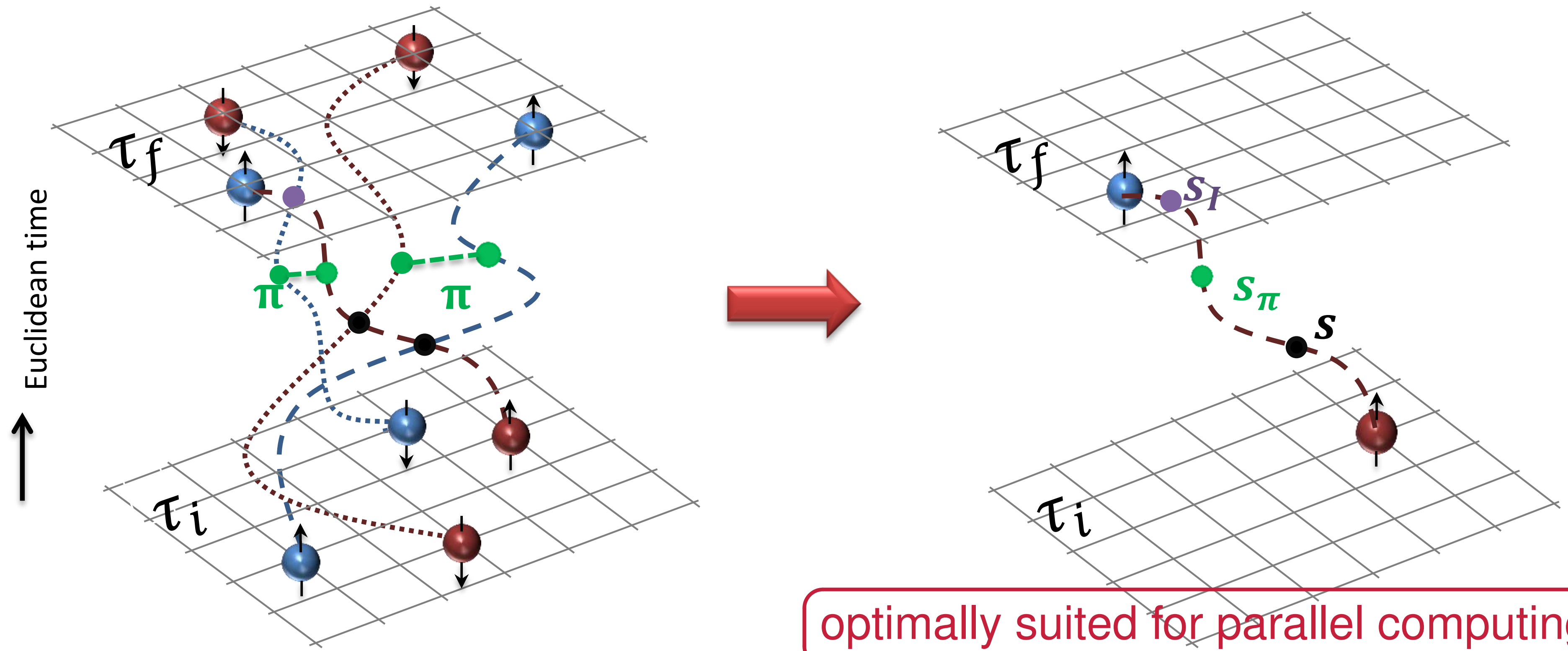
⇒ preparation of *all possible* initial/final states

⇒ *clustering* emerges *naturally*

Auxiliary field method

- Represent interactions by auxiliary fields (Gaussian quadrature):

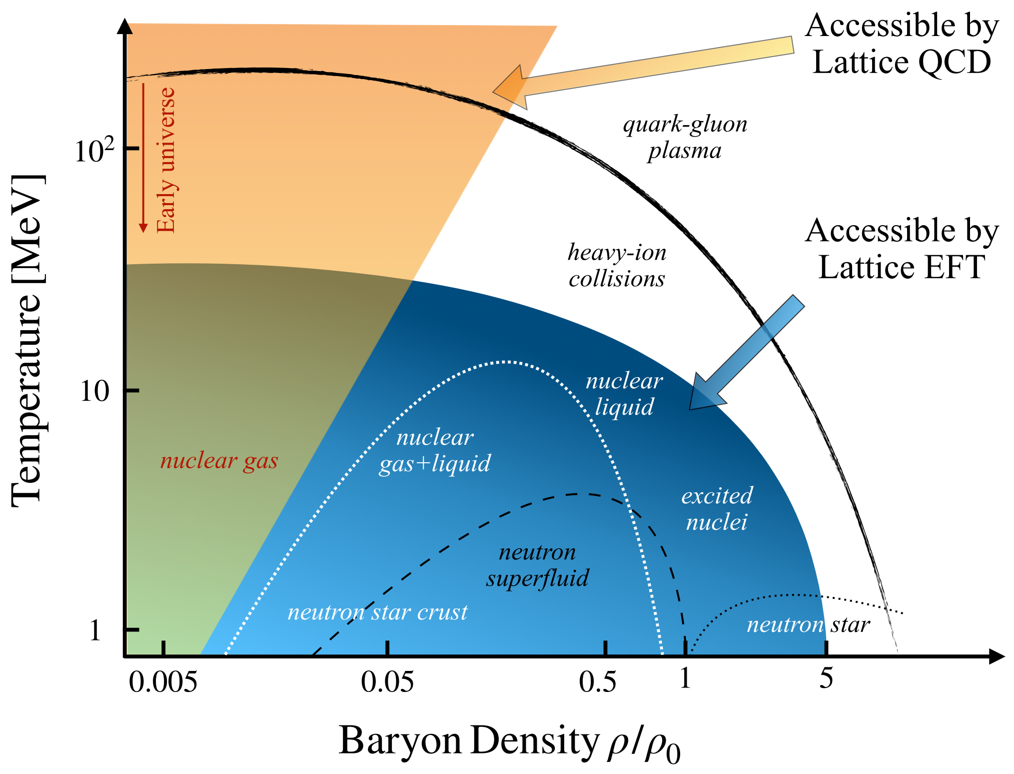
$$\exp\left[-\frac{C}{2}\left(N^\dagger N\right)^2\right] = \sqrt{\frac{1}{2\pi}}\int ds\,\exp\left[-\frac{s^2}{2} + \sqrt{C}\,s\left(N^\dagger N\right)\right]$$



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) + JUPITER + ...

87 Pflops → Exascale

The minimal nuclear interaction: Foundations

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

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

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

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

  $\hookrightarrow$ 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

  $\hookrightarrow$ cluster states in ^{12}C like the famous Hoyle state

  Epelbaum, Krebs, Lee, UGM, Phys. Rev. Lett. **106** (2011) 192501

  $\hookrightarrow$ 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

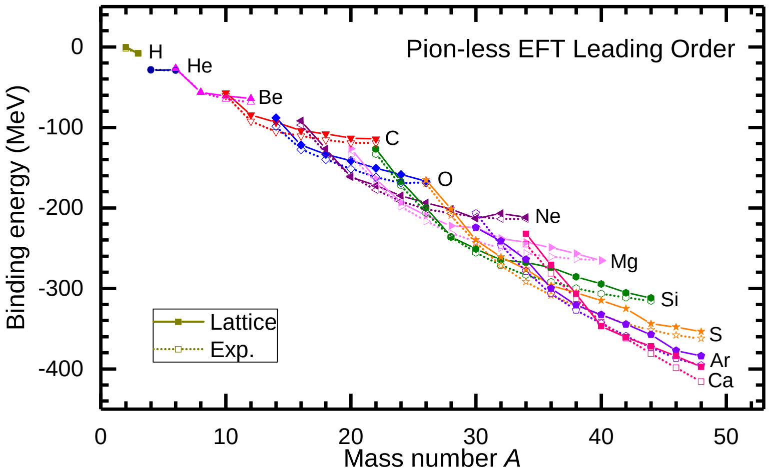
$$H_{\mathrm{SU(4)}} = H_{\mathrm{free}} + \frac{1}{2!} C_2 \sum_n \tilde{\rho}(n)^2 + \frac{1}{3!} C_3 \sum_n \tilde{\rho}(n)^3$$

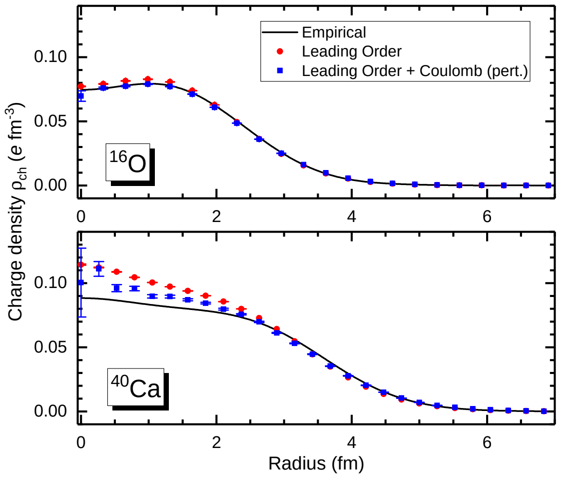
$$\tilde{\rho}(n) = \sum_i \tilde{a}_i^\dagger(n)\tilde{a}_i(n) + s_L \sum_{|n'-n|=1} \sum_i \tilde{a}_i^\dagger(n')\tilde{a}_i(n')$$

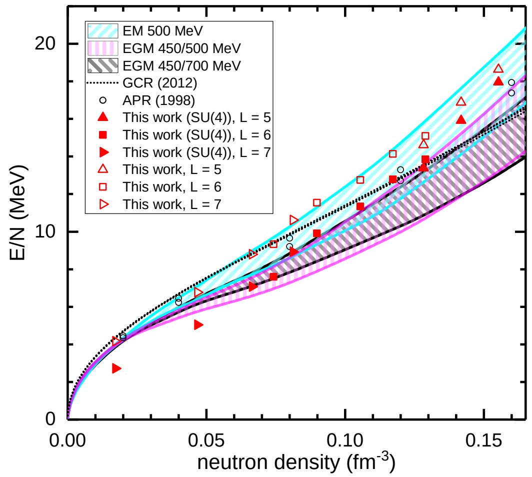
$$\tilde{a}_i(n) = a_i(n) + s_{NL} \sum_{|n'-n|=1} a_i(n')$$

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

$\rightarrow$ describes binding energies, radii, charge densities and the EoS of neutron matter







The minimal nuclear interaction: Applications

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 $\longrightarrow$ next slide

- Fit the four parameters:

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

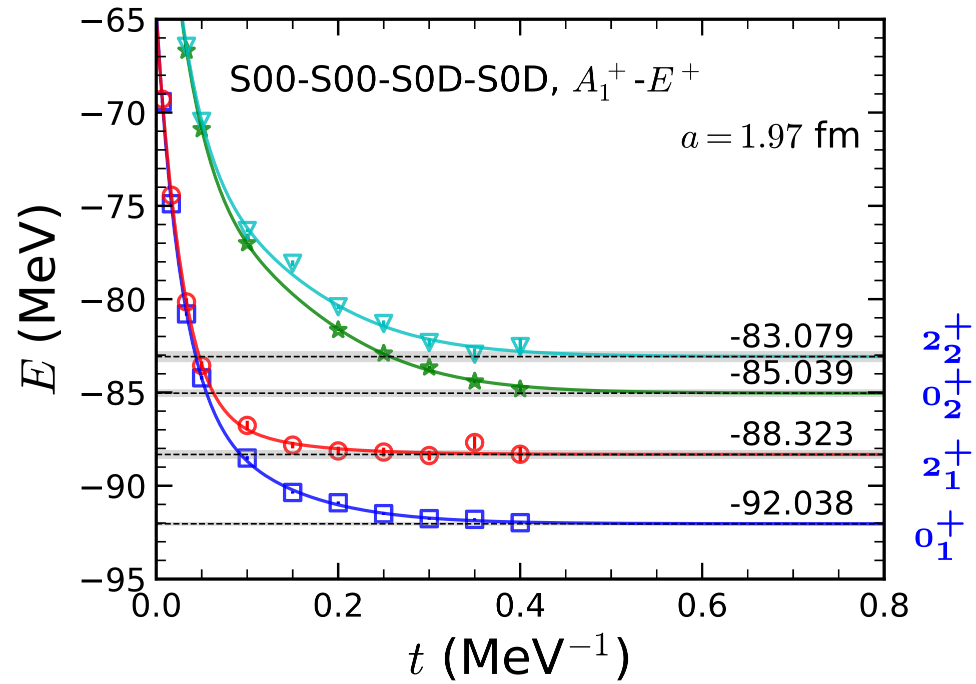
  $s_{\rm L}$ – radius of ^{12}C around 2.4 fm

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

- Calculation of em transitions

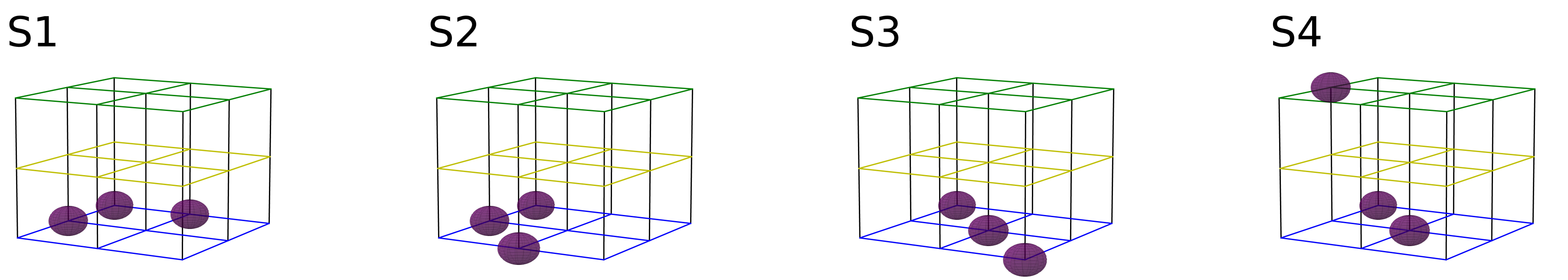
  requires coupled-channel approach

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



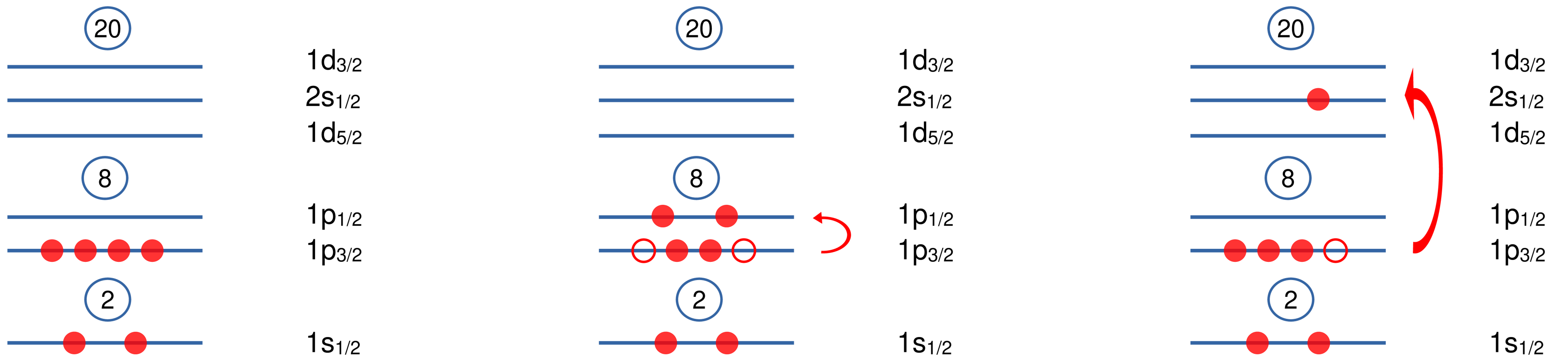
Configurations

- Cluster and shell model configurations



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

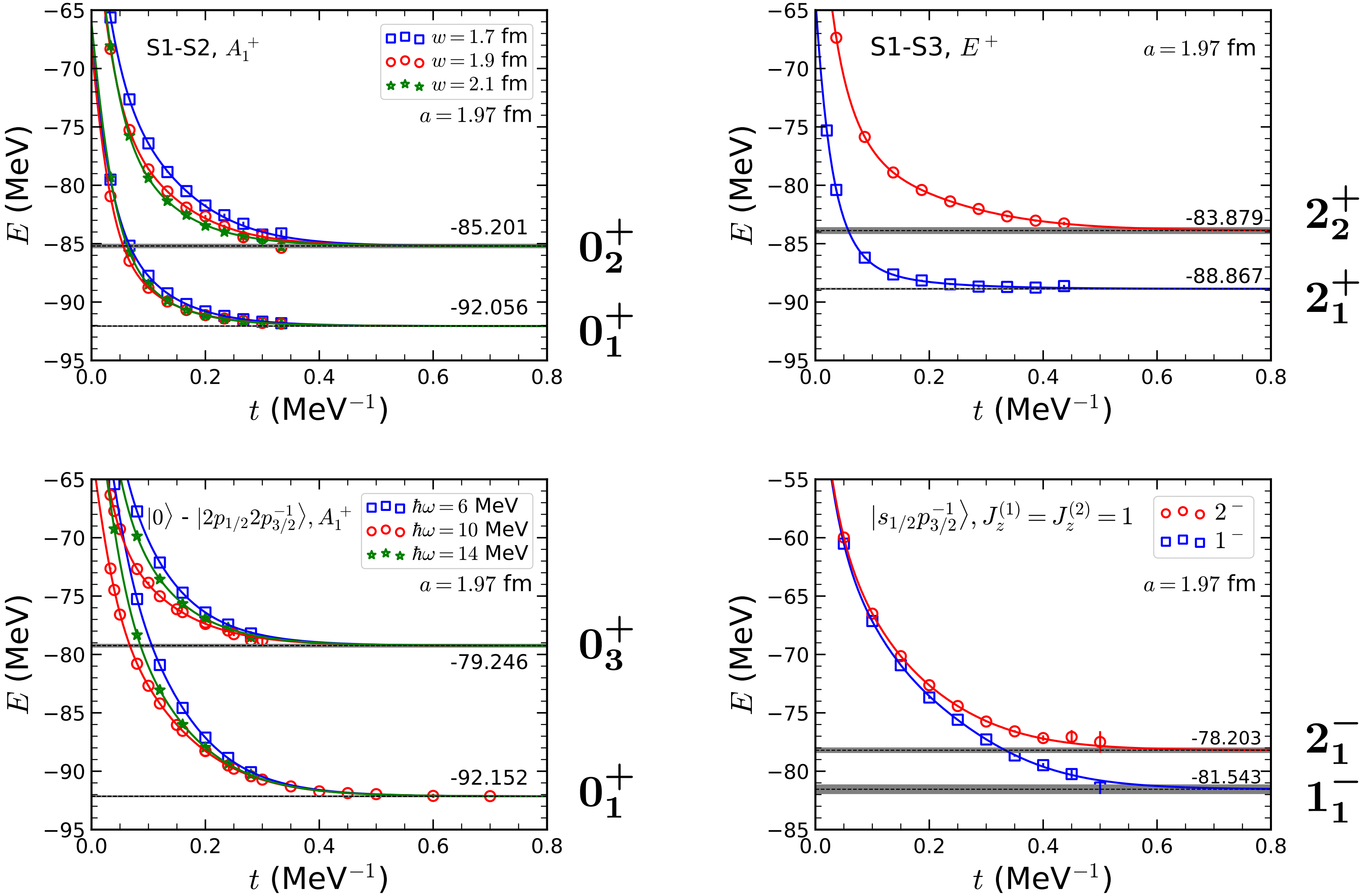
Gaussian wave packets $w = 1.7 - 2.1$ fm



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

Transient energies

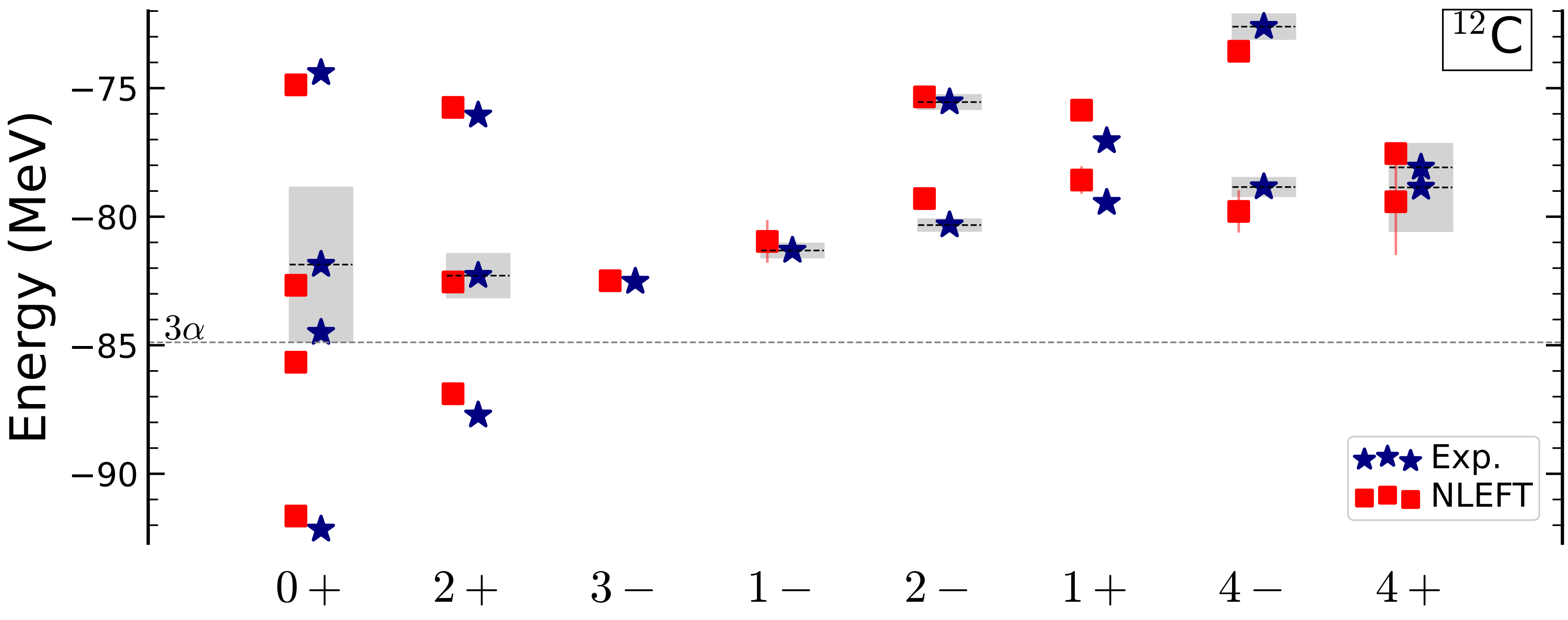
- Transient energies from cluster and shell-model configurations



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 $\mathbf{0_2^+}$ and $\mathbf{2_2^+}$ states

Electromagnetic properties

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

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

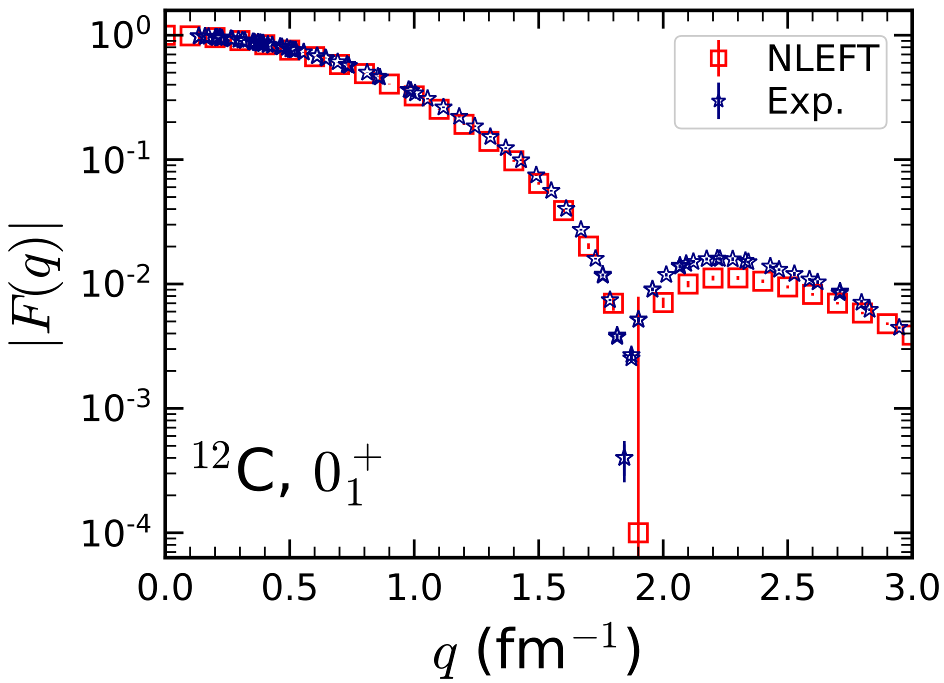
	NLEFT	FMD	α cluster	BEC	RXMC	Exp.
$r_c(0_1^+)$ [fm]	$\mathbf{2.53(1)}$	2.53	2.54	2.53	2.65	$\mathbf{2.47(2)}$
$r(0_2^+)$ [fm]	$\mathbf{3.45(2)}$	3.38	3.71	3.83	4.00	–
$r(0_3^+)$ [fm]	$\mathbf{3.47(1)}$	4.62	4.75	–	4.80	–
$r(2_1^+)$ [fm]	$\mathbf{2.42(1)}$	2.50	2.37	2.38	–	–
$r(2_2^+)$ [fm]	$\mathbf{3.30(1)}$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

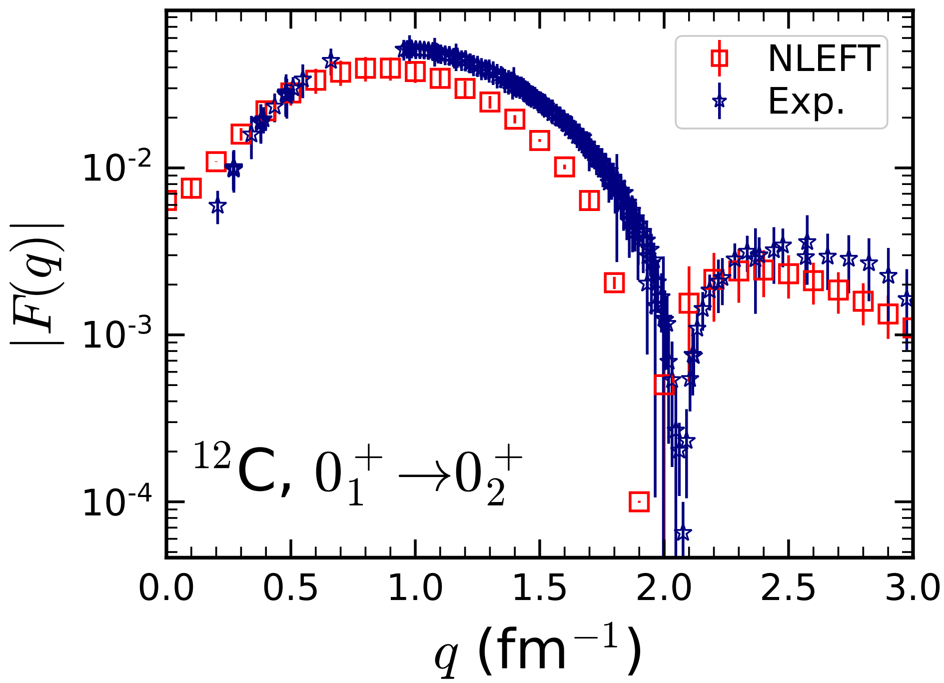
	NLEFT	FMD	α cluster	NCSM	Exp.
$Q(2_1^+)$ [e fm^2]	$\mathbf{6.8(3)}$	–	–	6.3(3)	$\mathbf{8.1(2.3)}$
$Q(2_2^+)$ [e fm^2]	$\mathbf{-35(1)}$	–	–	–	–
$M(E0, 0_1^+ \to 0_2^+)$ [e fm^2]	$\mathbf{4.8(3)}$	6.5	6.5	–	$\mathbf{5.4(2)}$
$M(E0, 0_1^+ \to 0_3^+)$ [e fm^2]	$\mathbf{0.4(3)}$	–	–	–	–
$M(E0, 0_2^+ \to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

Electromagnetic properties cont'd

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

- Form factors and transition ffs [essentially parameter-free]:



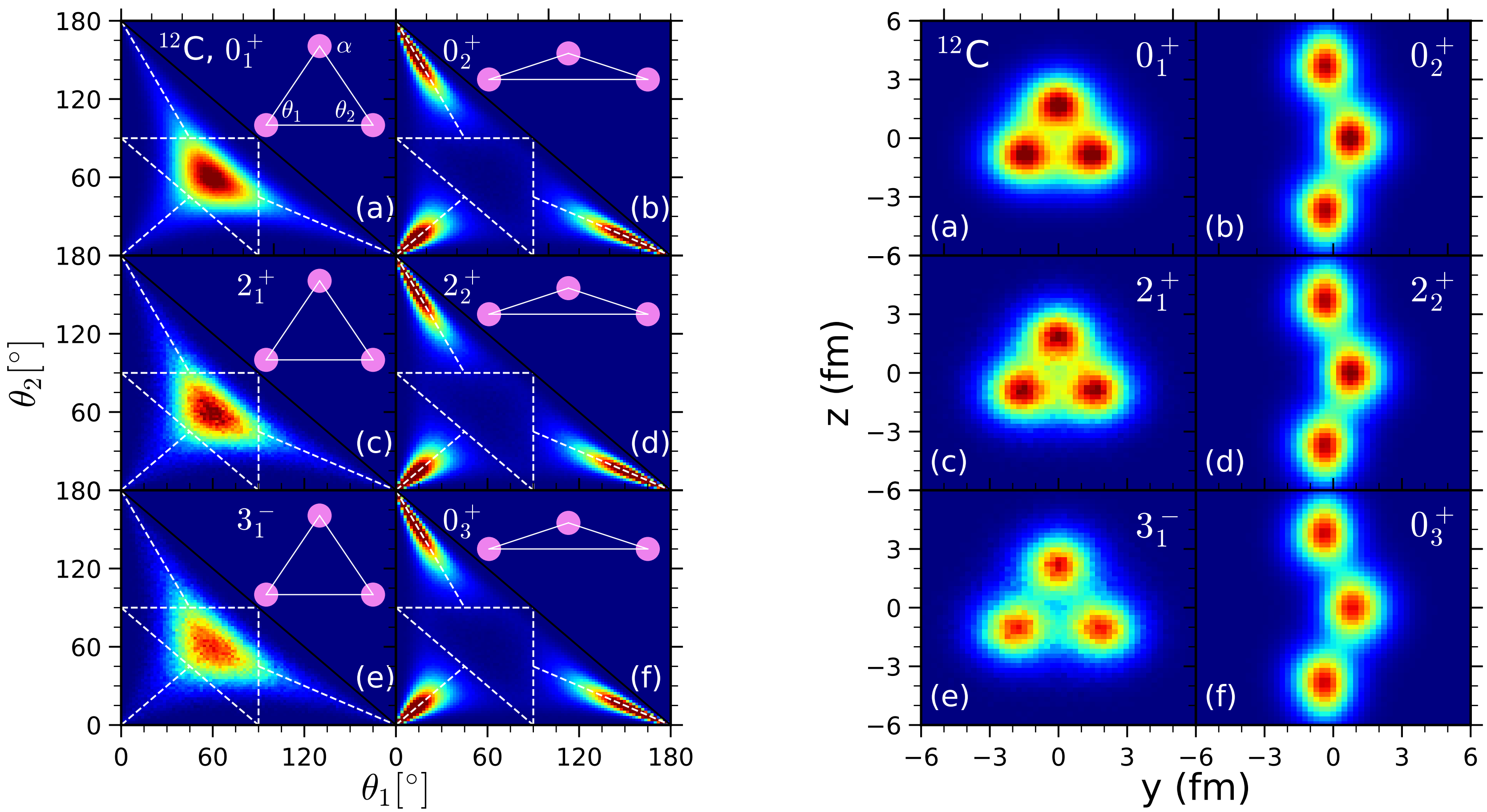


Sick, McCarthy, Nucl. Phys. A 150 (1970) 631
Strehl, Z. Phys. 234 (1970) 416
Crannell et al., Nucl. Phys. A 758 (2005) 399

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

Emergence of geometry

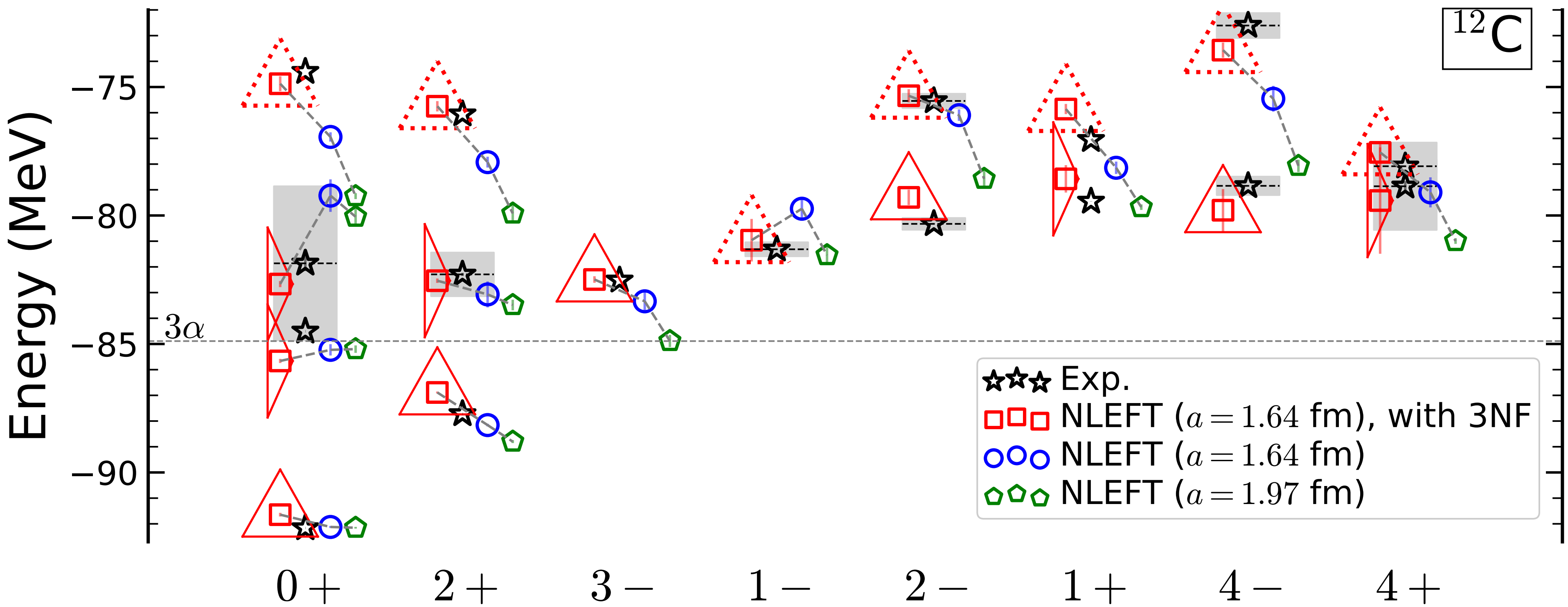
- Use the pinhole algorithm to measure the distribution of α-clusters/matter:



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

Emergence of duality

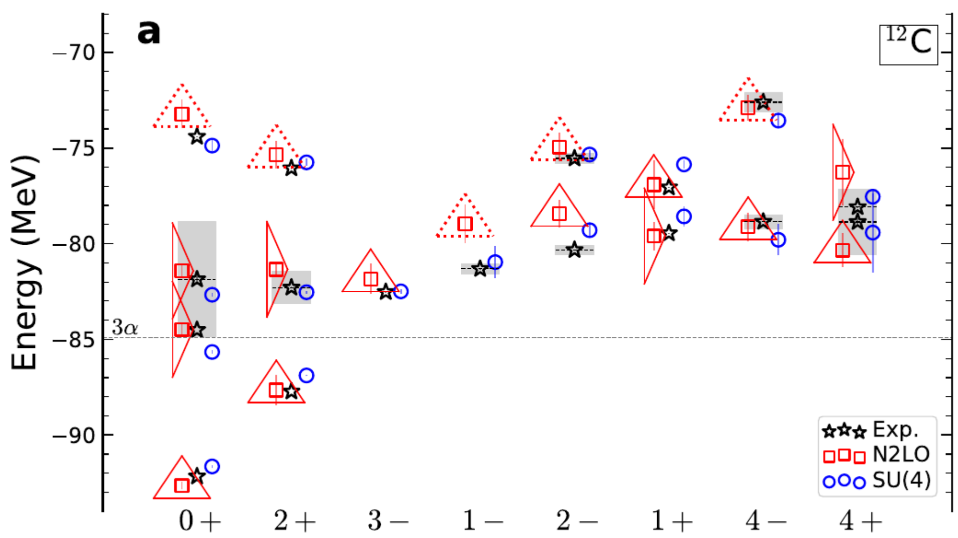
- ^{12}C spectrum shows a cluster/shell-model duality

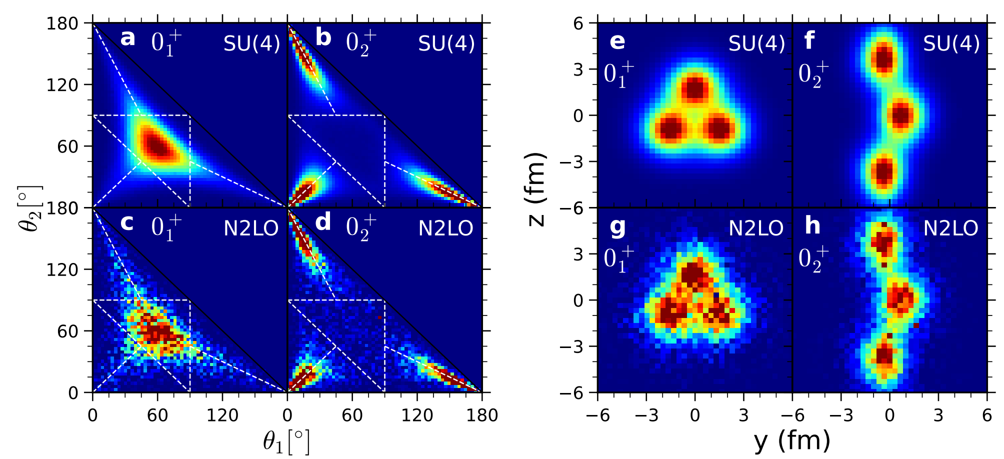


- dashed triangles: strong 1p-1h admixture in the wave function

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)



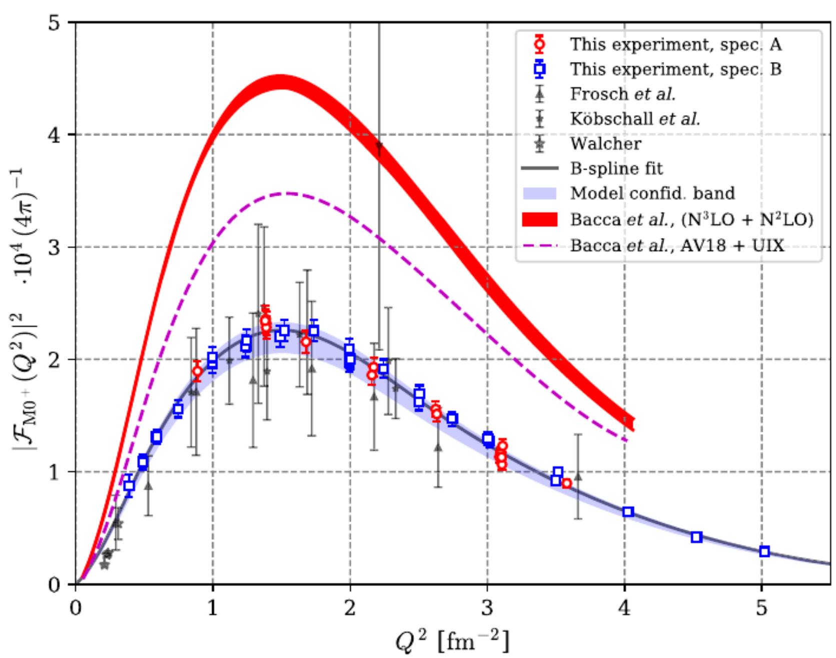


- spectrum as before (good agreement w/ data)
- density distributions as before (more noisy, stronger sign problem)

The ^{4}He form factor puzzle

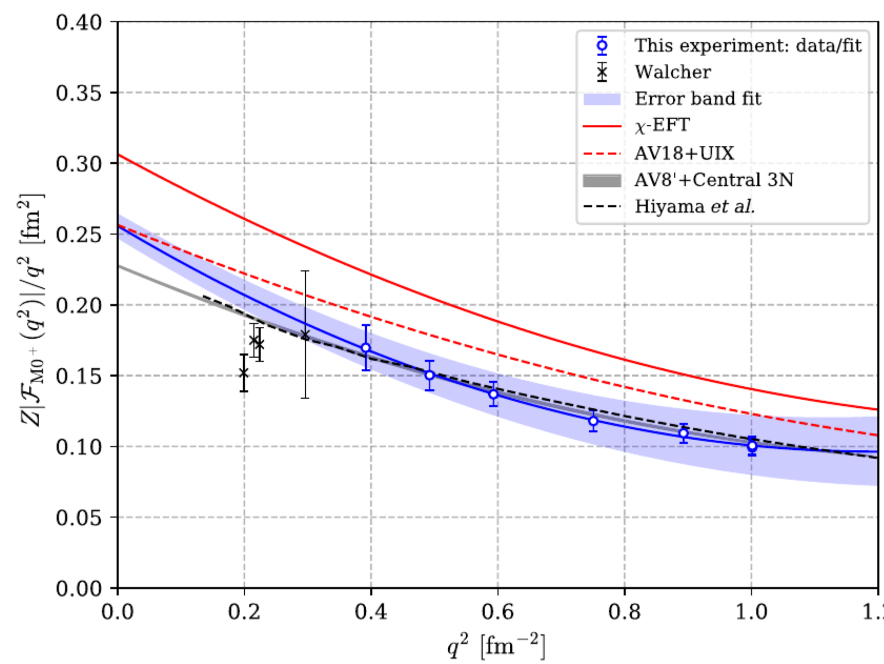
- Recent Mainz measurements of $F_{M0}(0_2^+ \to 0_1^+)$ appear to be in stark disagreement with *ab initio* nuclear theory Kegel et al., Phys. Rev. Lett. **130** (2023) 152502

- 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 $\mathbf{0^+}$ q.n's $\to$ accelerates convergence as $L_t \to \infty$

- Shell-model wave functions (4 nucleons in $\mathbf{1s_{1/2}}$, twice 3 in $\mathbf{1s_{1/2}}$ and 1 in $\mathbf{2s_{1/2}}$)

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

$\hookrightarrow$ statistical and large-L_t errors

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

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

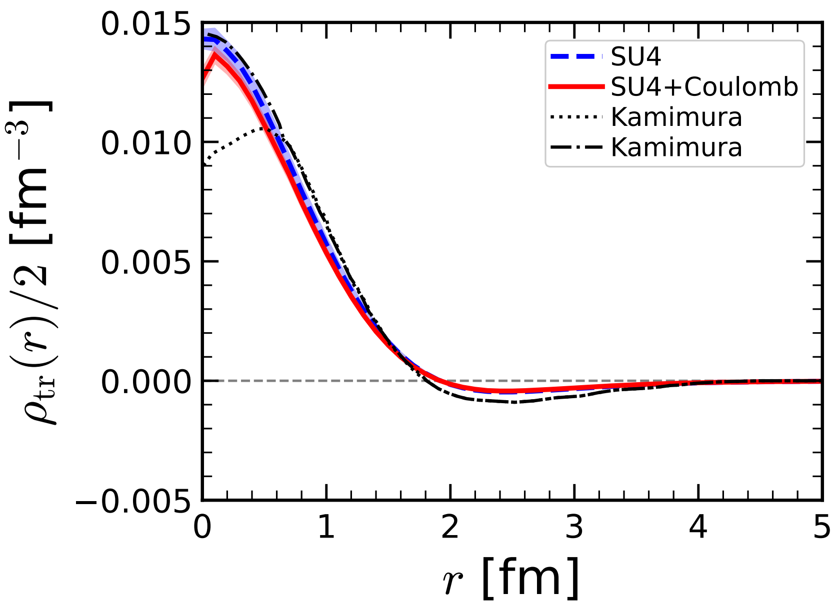
Michel, Nazarewicz, Ploszajczak, Phys. Rev. Lett. **131** (2023) 242502

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

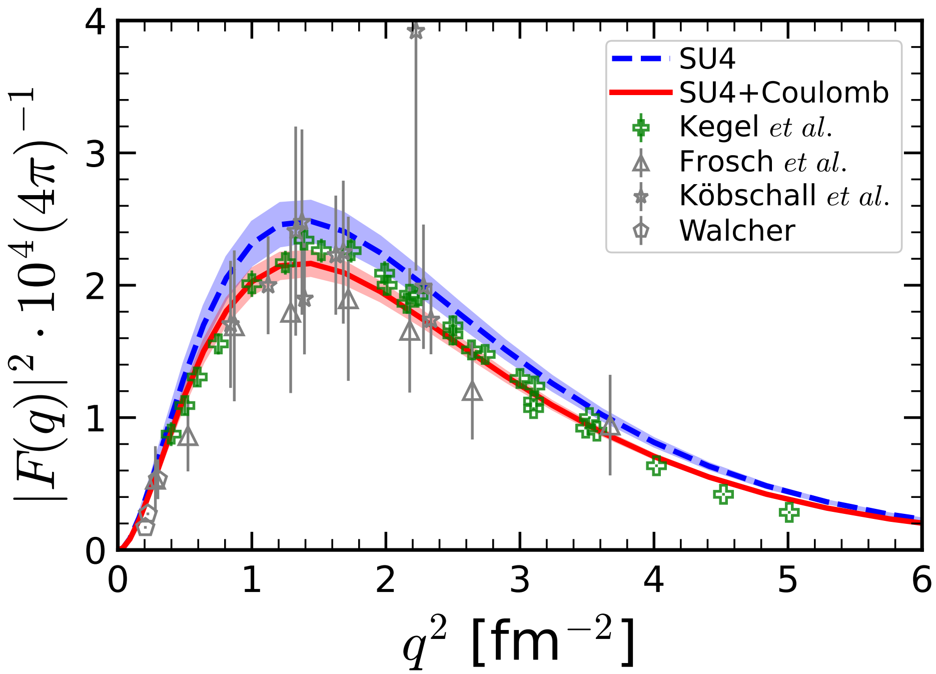
von Stecher, D'Incao, Greene, Nat. Phys. **5** (2009) 417; Hammer, Platter, EPJA **32** (2007) 113

The transition form factor

- Transition charge density



- Transition form factor



$\hookrightarrow$ agrees with the reconstructed one from Kamimura PTEP **2023** (2023) 071D01

$\hookrightarrow$ very small central depletion (no zero)

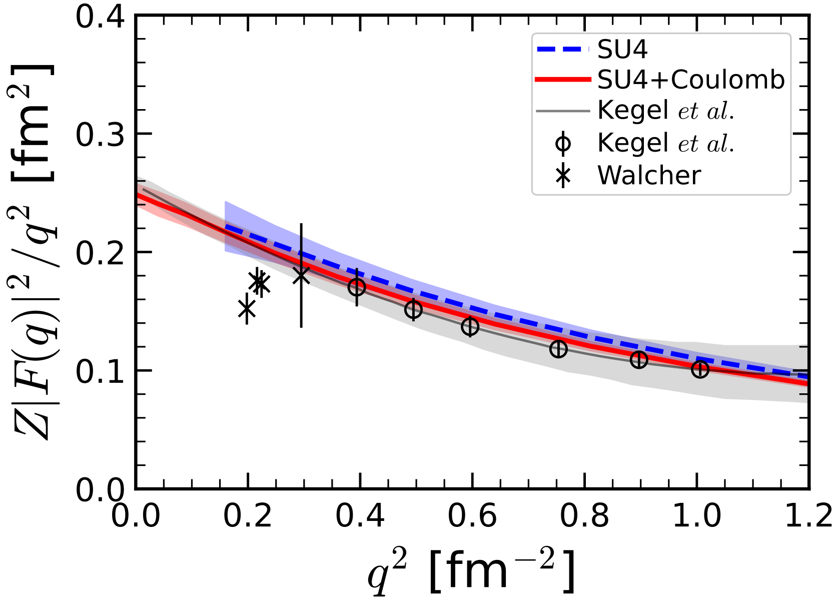
$\hookrightarrow$ excellent description of the data

$\hookrightarrow$ Coulomb required plus smaller uncertainty (improved signal)

$\hookrightarrow$ 3NFs important!

The transition form factor II

- Small momentum expansion



	$\langle r^2\rangle_{\rm tr}$ [fm^2]	$\mathcal{R}_{\rm tr}$ [fm]
Experiment	1.53 ± 0.05	4.56 ± 0.15
Th (AV8'+ centr. 3N)*	1.36 ± 0.01	4.01 ± 0.05
Th (AV18 + UIX)	1.54 ± 0.01	3.77 ± 0.08
Th (NLEFT)	1.49 ± 0.01	4.00 ± 0.04

*Hiyama, Gibson, Kamimura, PRC **70** (2004) 031001

$\hookrightarrow$ Also consistent description of the low-energy data

$\hookrightarrow$ **No puzzle** to the nuclear forces!

$\hookrightarrow$ Can be improved using N3LO action + wave function matching

Elhatisari et al., 2210.17488 [nucl-th]

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

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

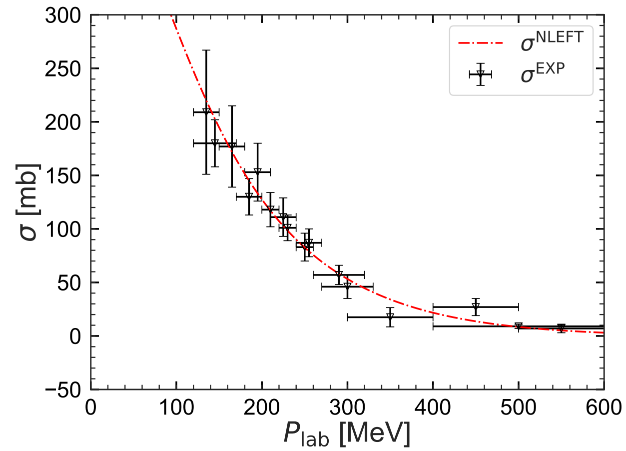
$\hookrightarrow$ must determine 4 LECs! [smearing parameters from the nucleon sector]

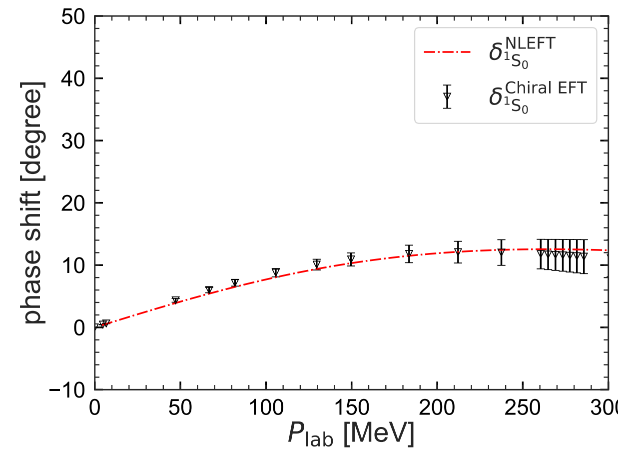
$\hookrightarrow$ first time that the $\Lambda\Lambda N$ three-body force is included

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

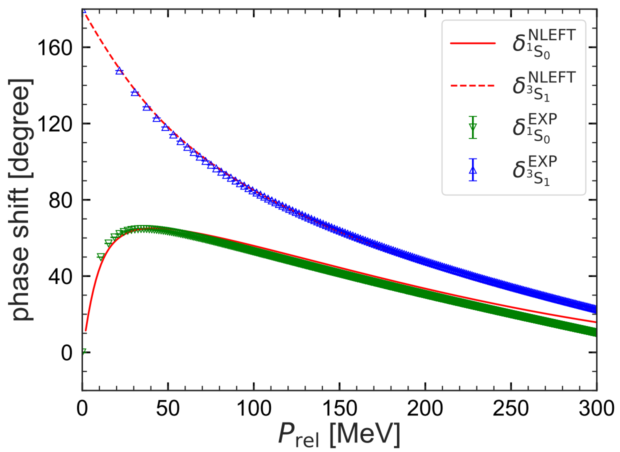
$\hookrightarrow$ this defines our EoS of hyper-nuclear matter called **HMN(I)**

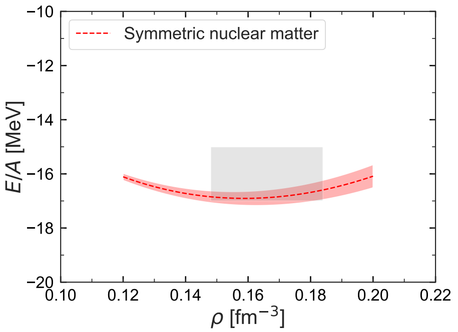
The minimal nuclear interaction: EoS & neutron star properties

Pure neutron matter

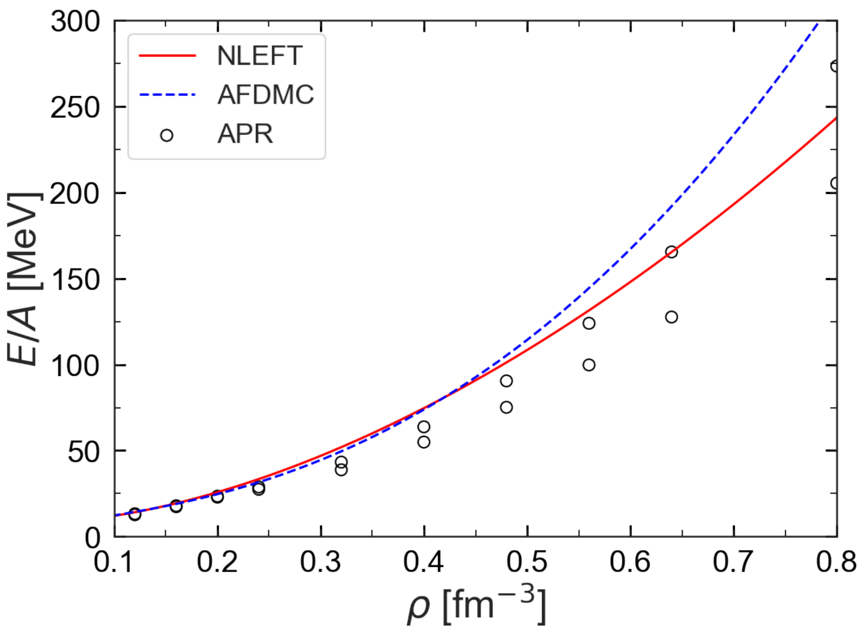
Tong, Elhatisari, UGM, Sci. Bull. **70** (2025) 825

- 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

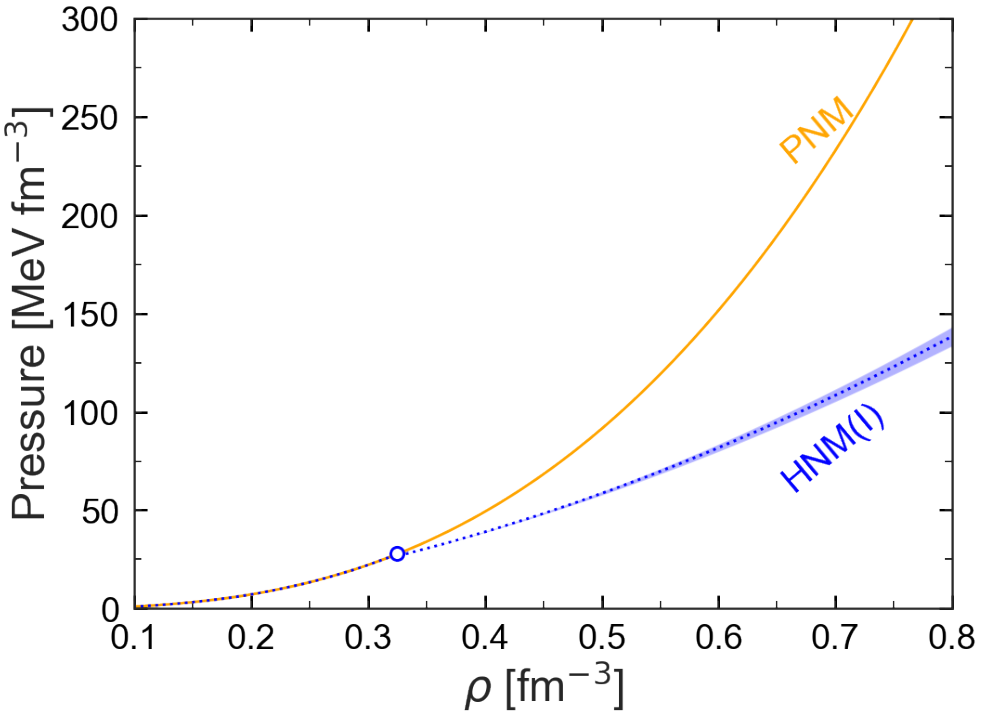
→ work out consequences for
neutron stars based on this PNM EoS

Neutron star properties

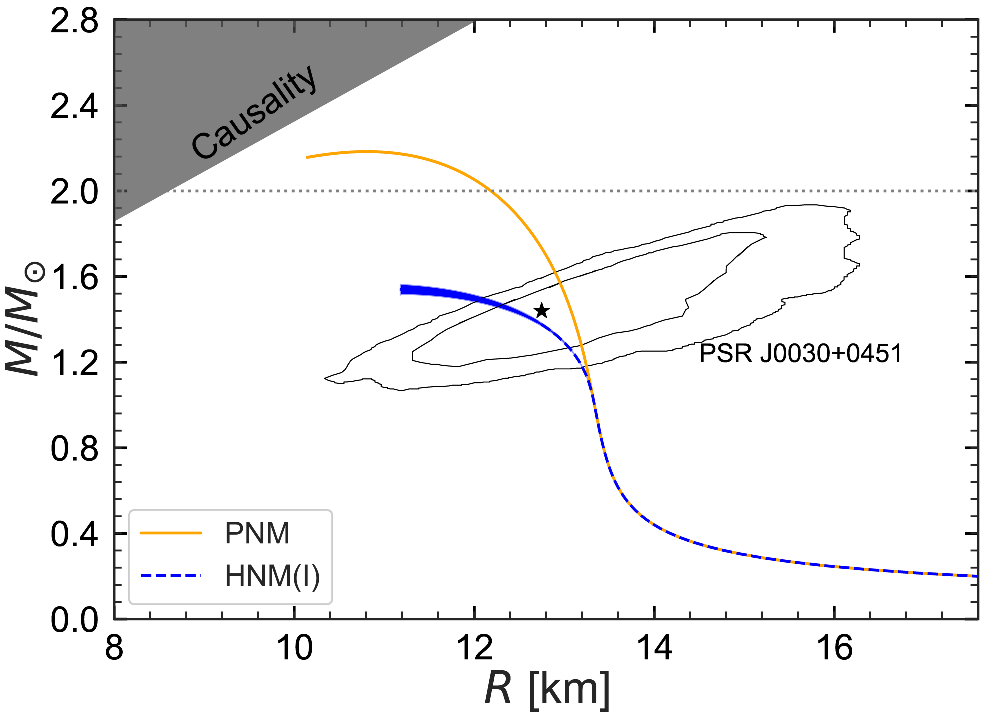
Tong, Elhatisari, UGM, Sci. Bull. **70** (2025) 825; Astrophys. J. **982** (2025) 164

- 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]

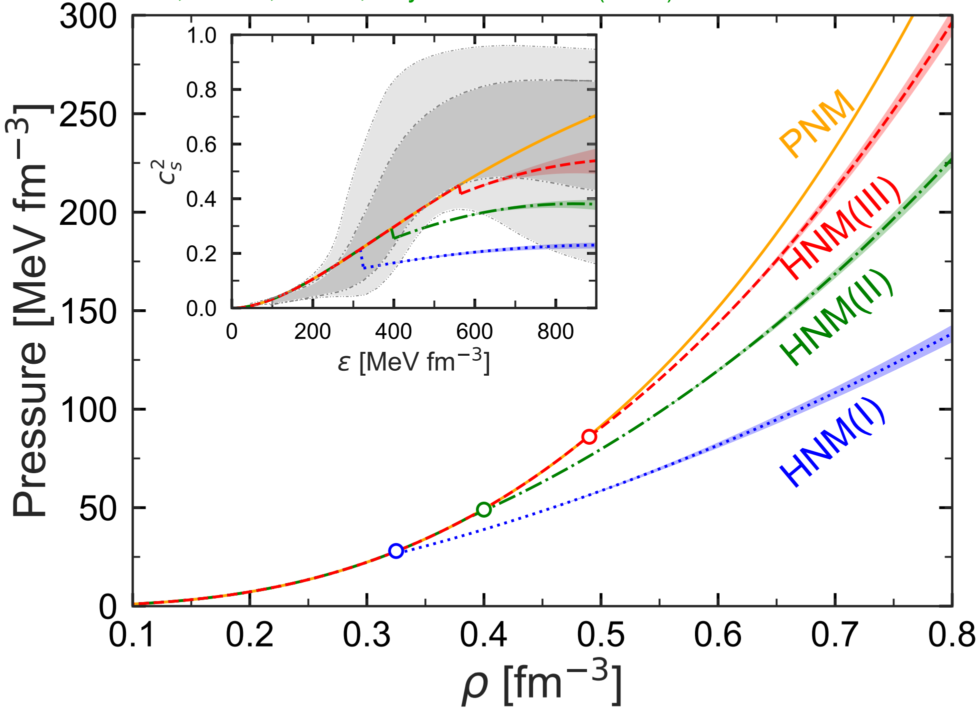
  ↪ this will move the threshold of $\mu_\Lambda = \mu_n$ up

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

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

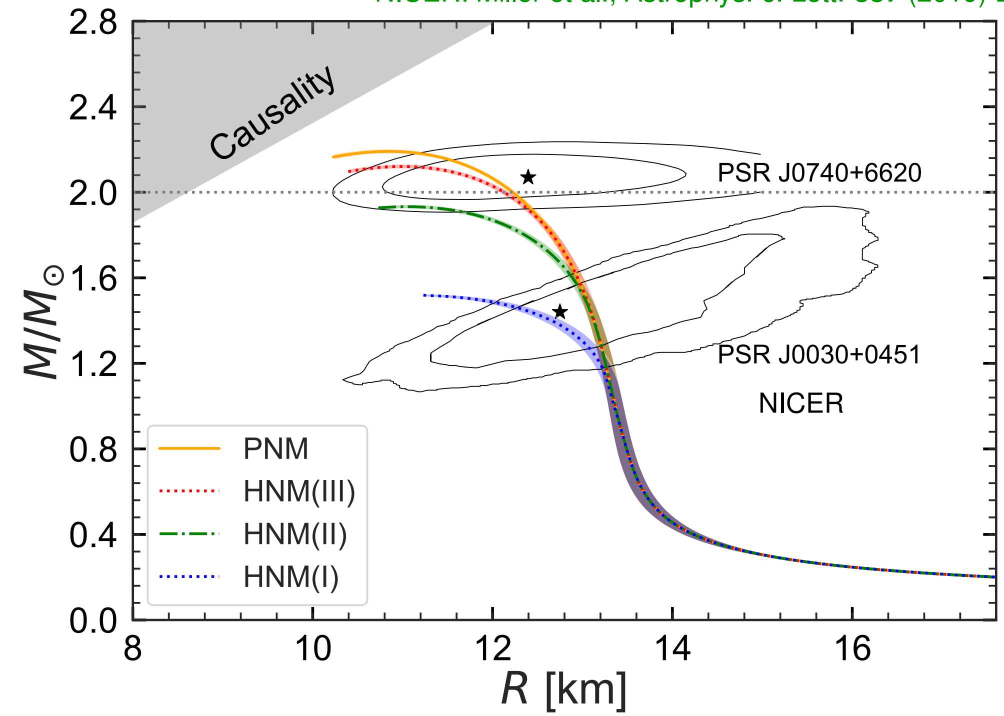
- EoS & speed of sound

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



- Mass-radius relation

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

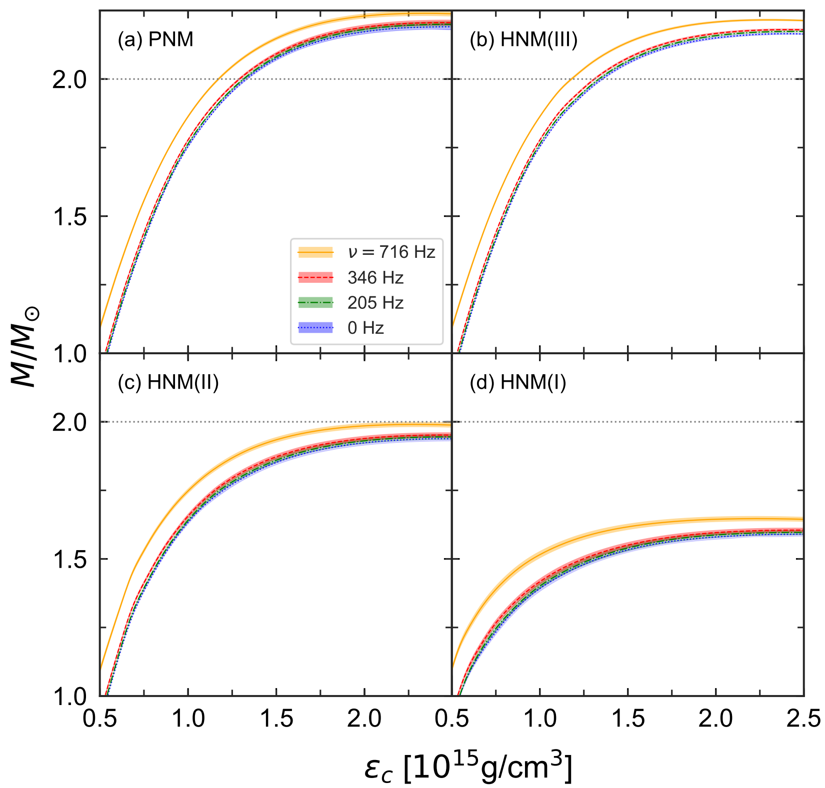


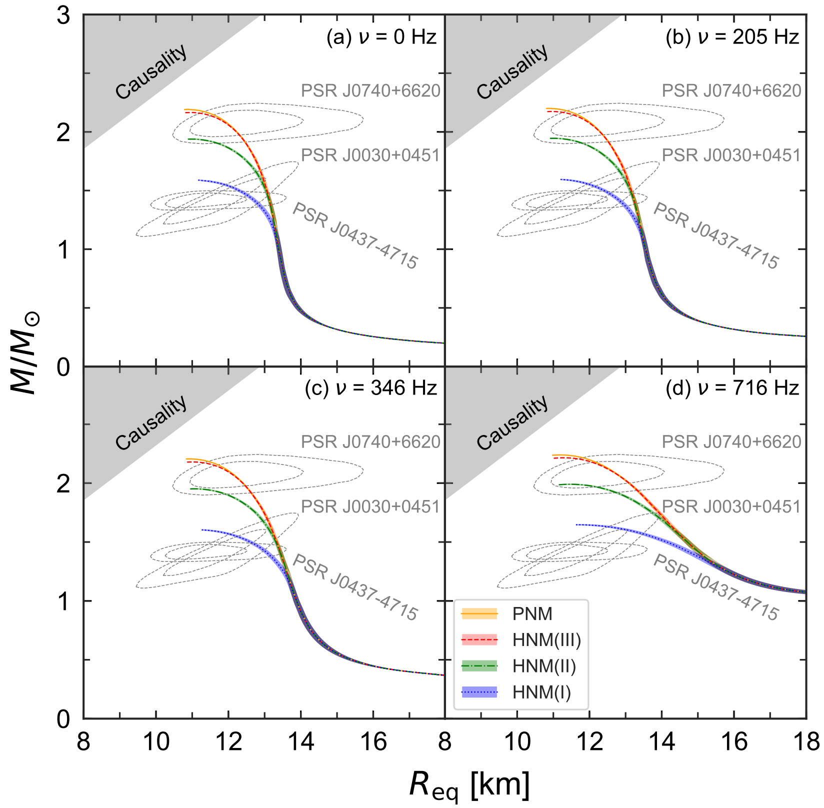
EoS for rotating neutron stars

Tong, Elhatisari, UGM, Astrophys. J. **982** (2025) 164

- Also rapidly rotating neutron stars observed: $\nu = 205, 346, 716$ Hz

Vinciguerra et al., Ap. J. **961** (2024) 62; Salmi et al., Ap. J. **974** (2024) 294; Hessels et al., Science **311** (2006) 1901





$\hookrightarrow$ impact of centrifugal forces visible

$\hookrightarrow$ mass-radius relations mostly consistent with the data

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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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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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.

- 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: 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

  $\hookrightarrow$ essentially done $\surd$ $\rightarrow$ CSB included in Wu, Wang, Lu, 2503.18017 [nucl-th]

  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) $\surd$

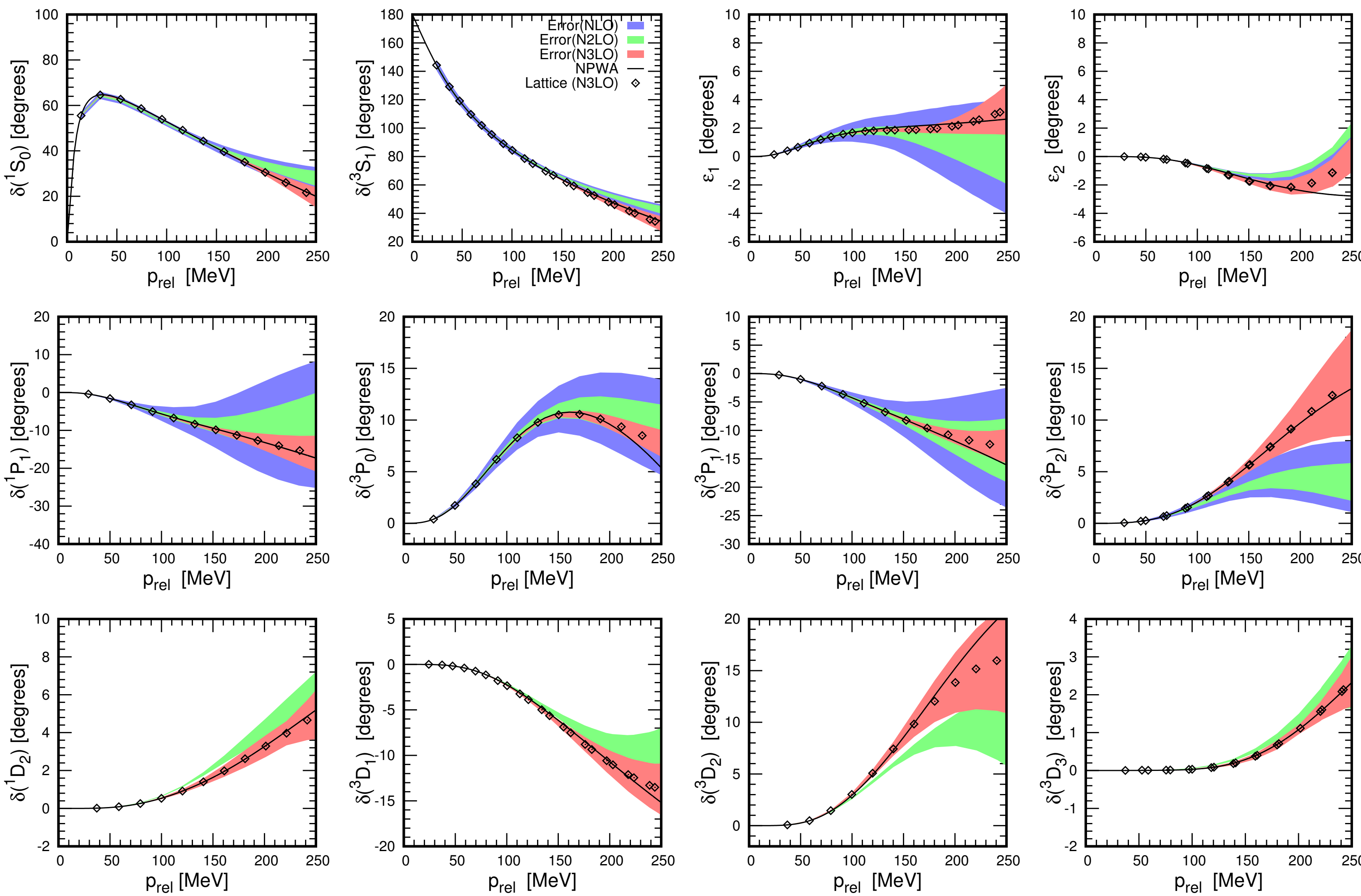
  $\hookrightarrow$ third for nuclear reactions/astrophysics (first results) $\surd$

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

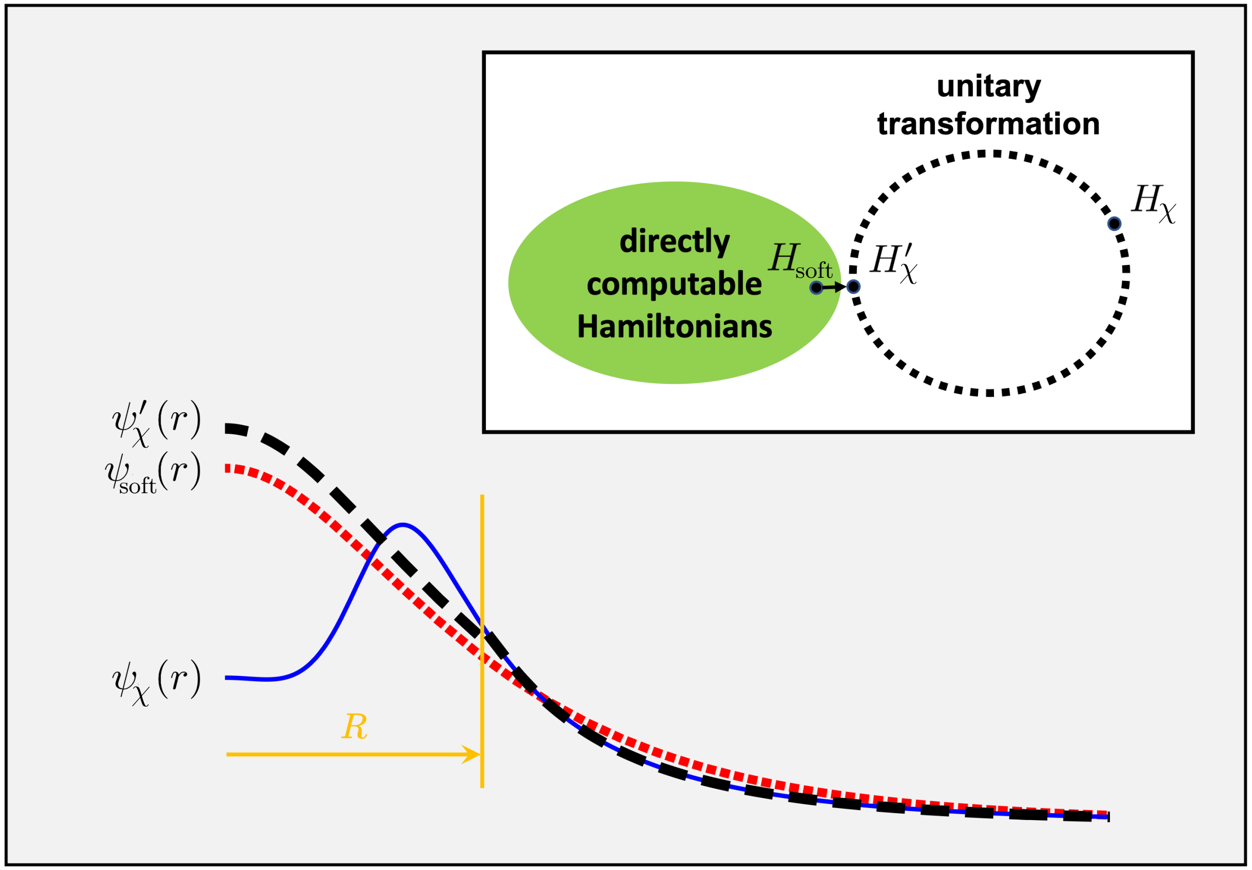


uncertainty estimates á la Epelbaum, Krebs, UGM,
Eur. Phys. J. A **51** (2015) 53

Wave function matching I

Elhatisari et al., Nature **630** (2024) 59 [arXiv:2210.17488 [nucl-th]]

- Graphical representation of w.f. matching



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

Wave function matching II

Elhatisari et al., Nature **630** (2024) 59 [arXiv:2210.17488 [nucl-th]

- $H_{\rm soft}$ has tolerable sign oscillations, good for many-body observables
- H_χ has severe sign oscillations, derived from the underlying theory

↪ can we find a unitary trafo, that creates a chiral H_χ that is pert. th'y friendly?

$$H'_\chi = U^\dagger \, H_\chi \, U$$

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

☐ Let $|\psi^0_\chi\rangle$ be the lowest eigenstate of H_χ

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

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

☐ Let $|\phi_\chi\rangle$ be the projected and normalized lowest eigenstate of H_χ

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

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

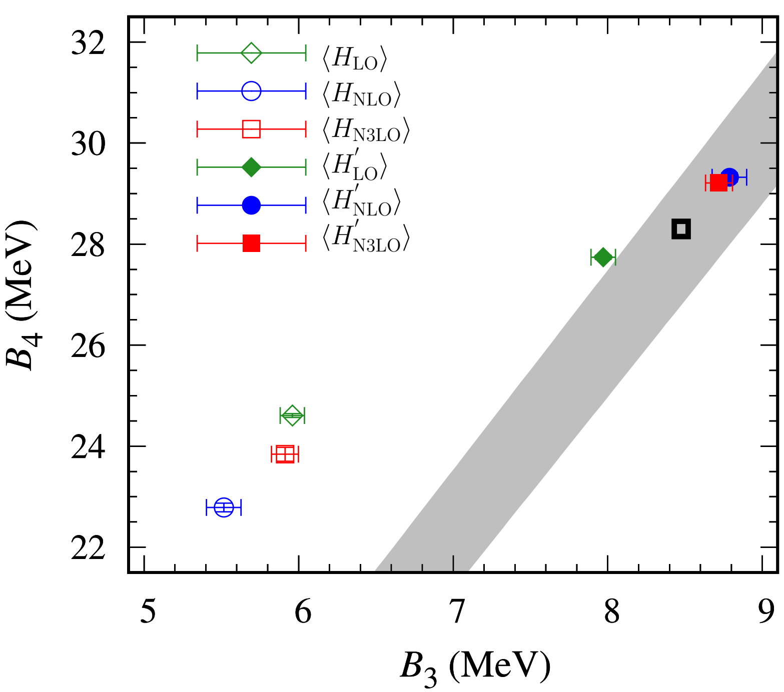
Chiral Interactions at N3LO: Applications to nuclear structure

Wave function matching for light nuclei

Elhatisari et al., Nature **630** (2024) 59 [arXiv:2210.17488 [nucl-th]]

- 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

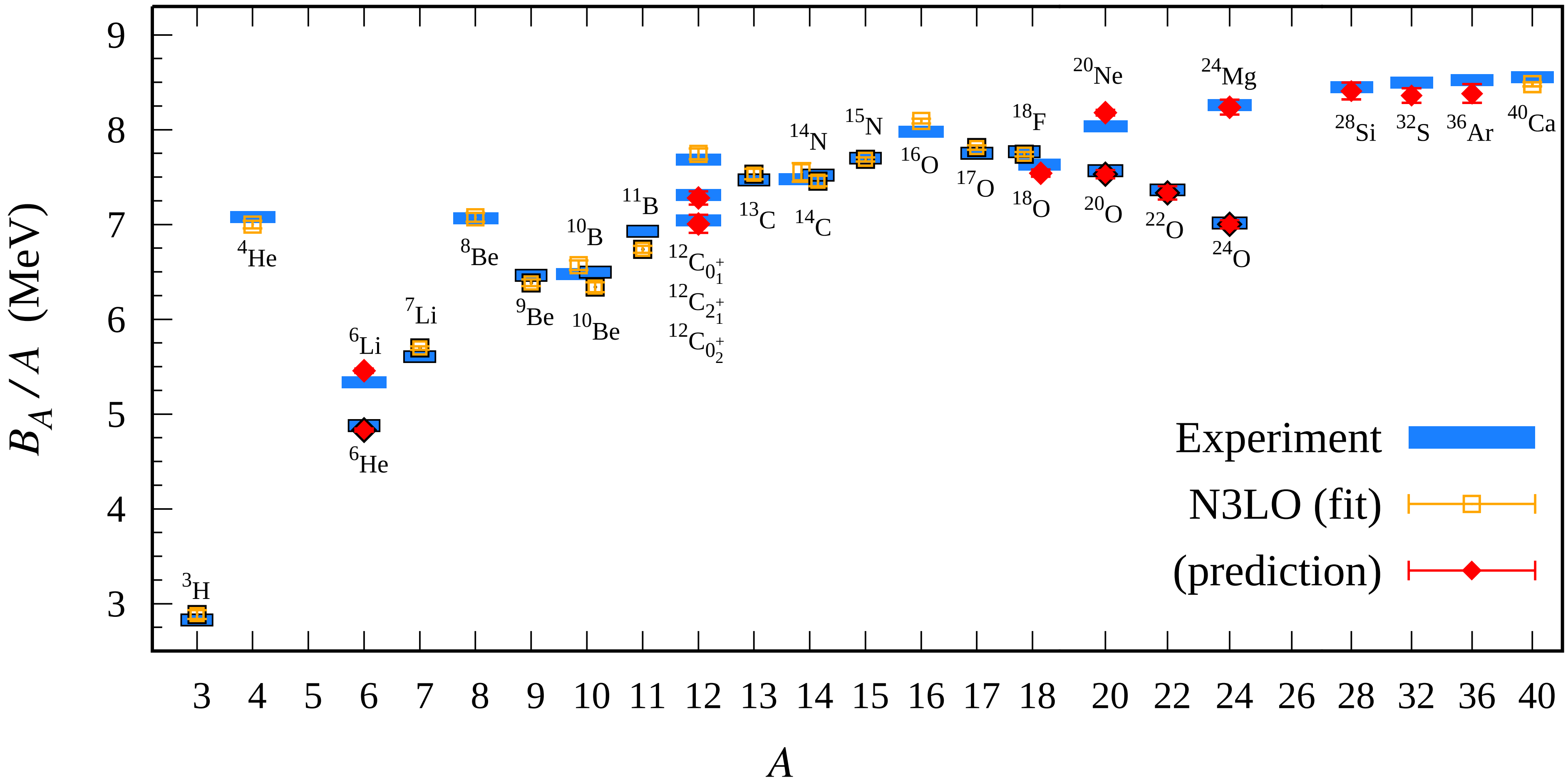
  Platter, Hammer, UGM, Phys. Lett. B **607** (2005) 254

$\hookrightarrow$ 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., Nature **630** (2024) 59 [arXiv:2210.17488 [nucl-th]]

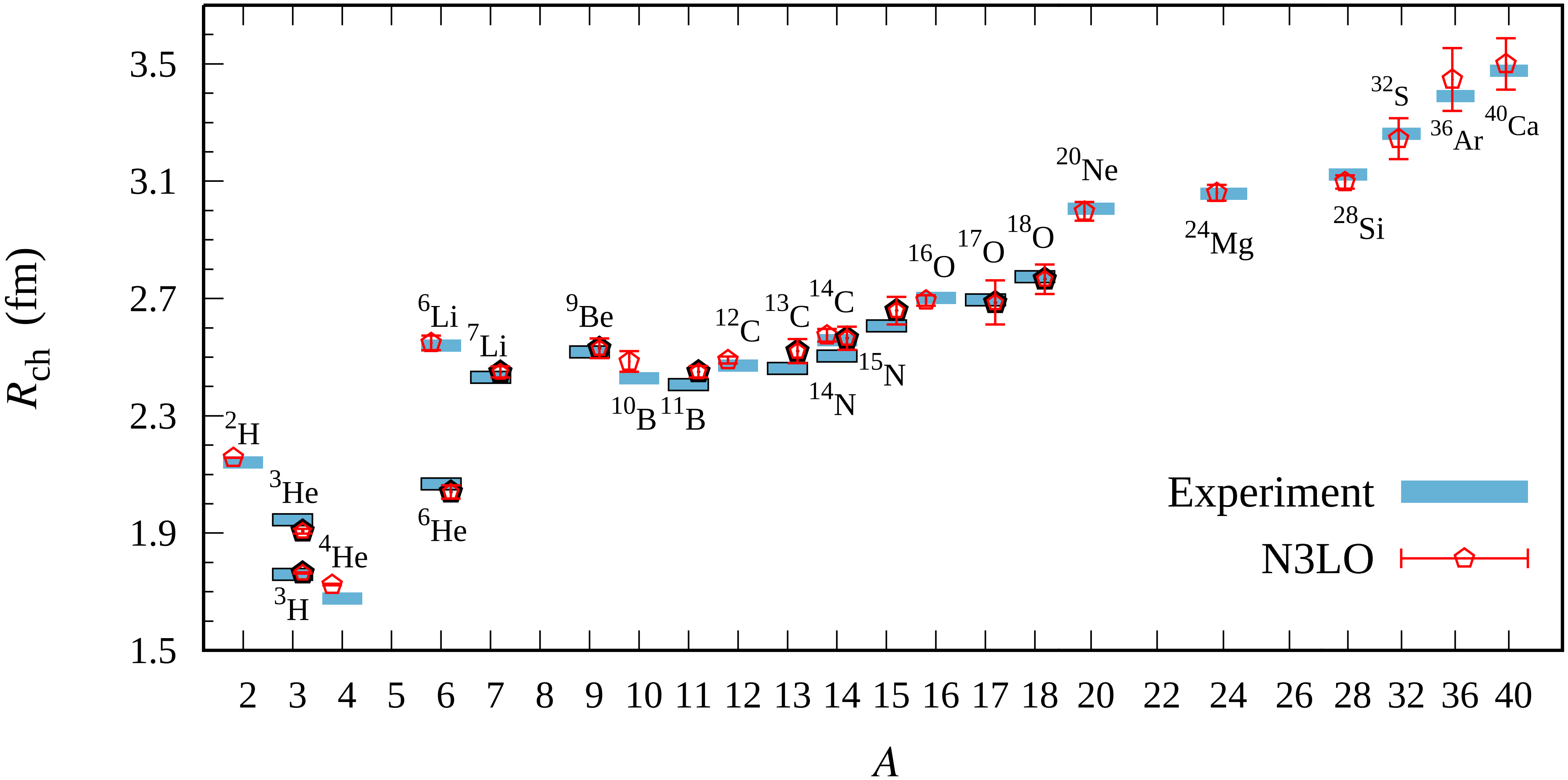


→ excellent starting point for precision studies

Prediction: Charge radii at N3LO

Elhatisari et al., Nature **630** (2024) 59 [arXiv:2210.17488 [nucl-th]]

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

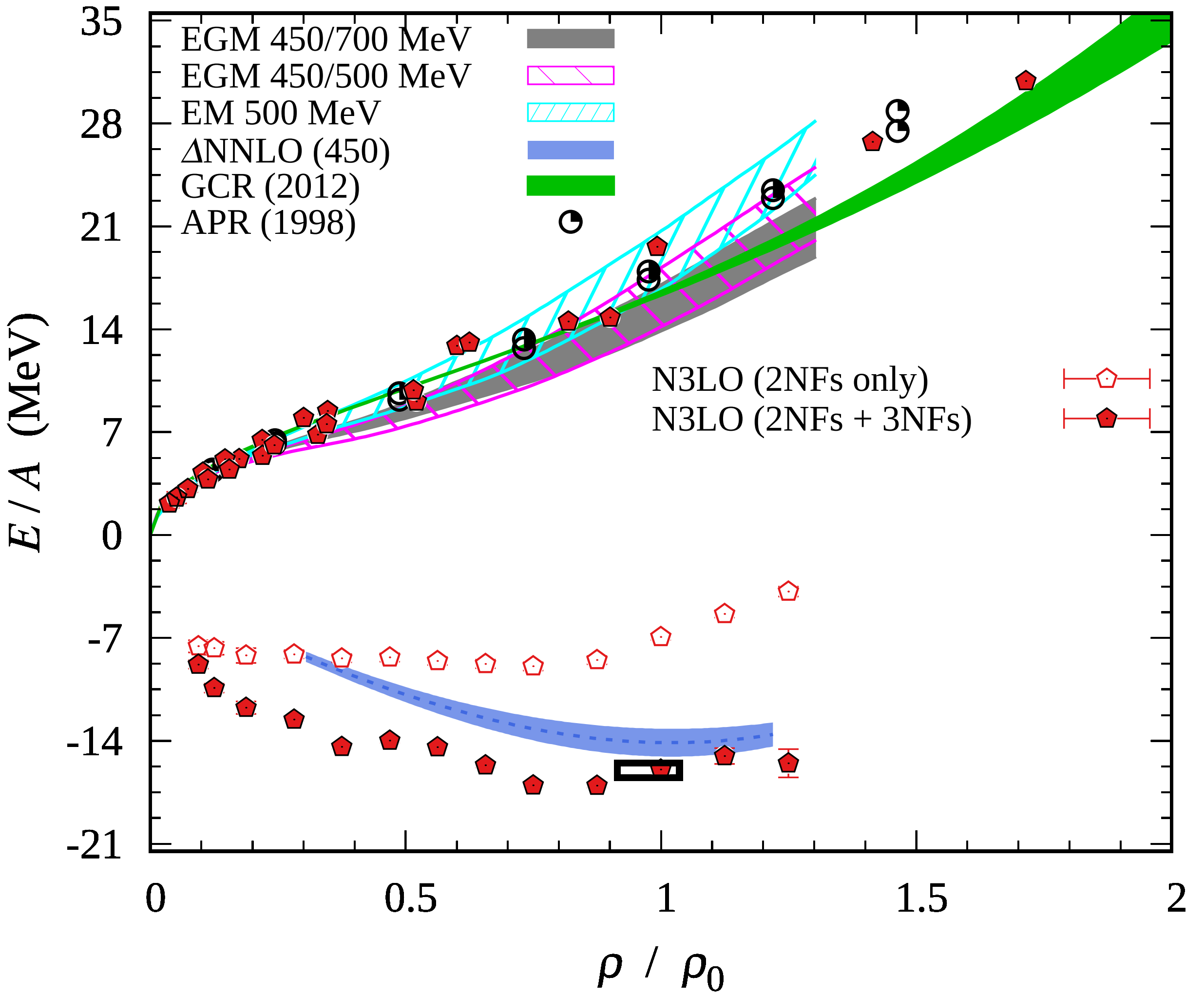


$\hookrightarrow$ no radius problem!

Prediction: Neutron & nuclear matter at N3LO

Elhatisari et al., Nature **630** (2024) 59 [arXiv:2210.17488 [nucl-th]]

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

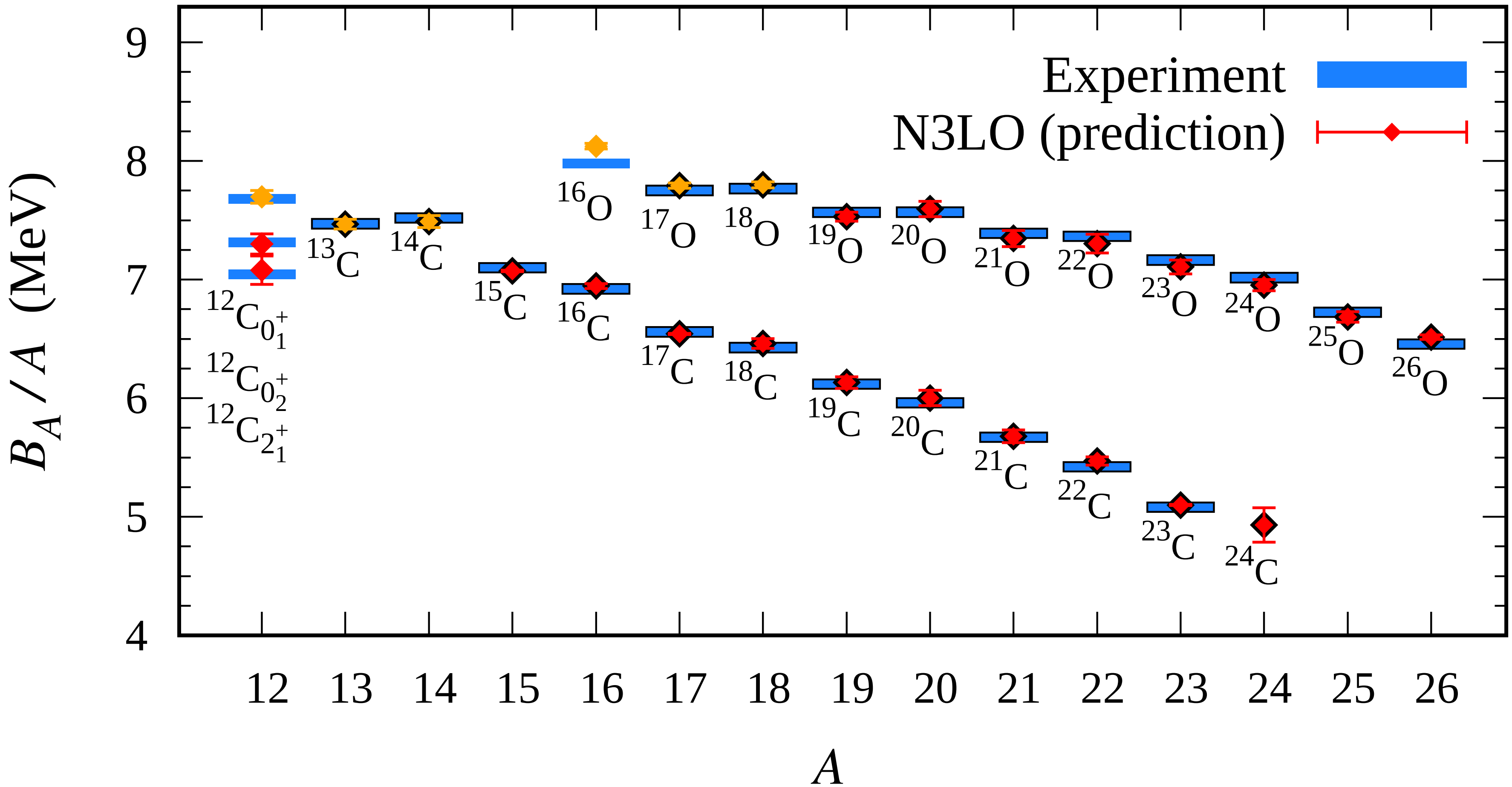


$\hookrightarrow$ can be improved using twisted b.c.'s

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!

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!]

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

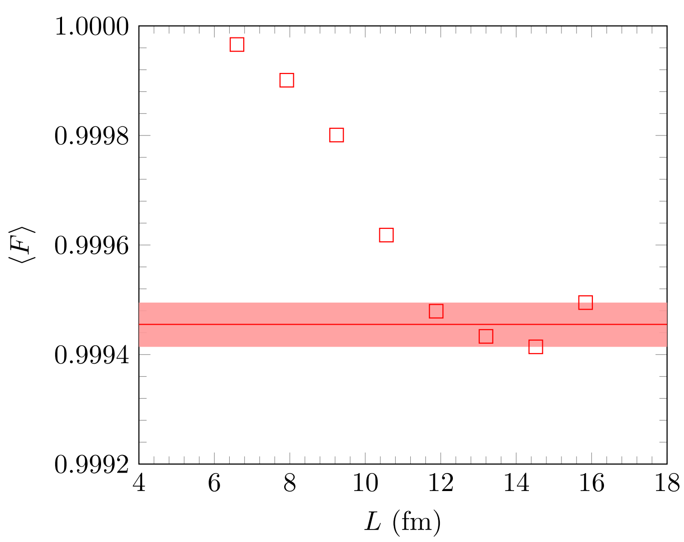
- NLEFT:

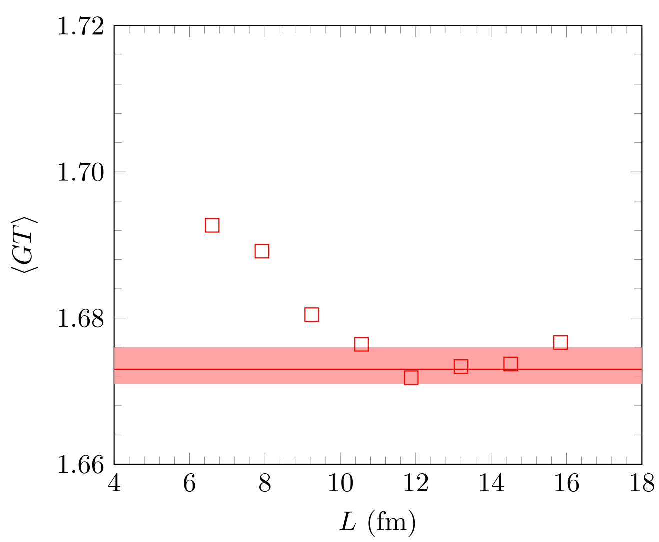
$$\langle \mathbf{F} \rangle_{\mathrm{N3LO}} = 0.99949(11)$$

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

$\hookrightarrow$ Important first step

$\hookrightarrow$ Larger nuclei underway...





Chiral Interactions at N3LO: Applications to scattering

Scattering: 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

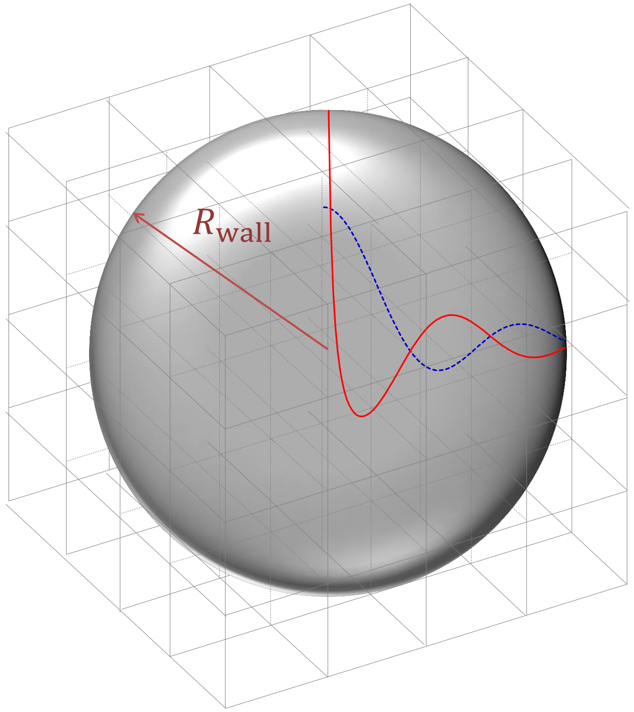
↪ works in many cases, problems w/ partial-wave mixing and cluster-cluster scattering

- 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

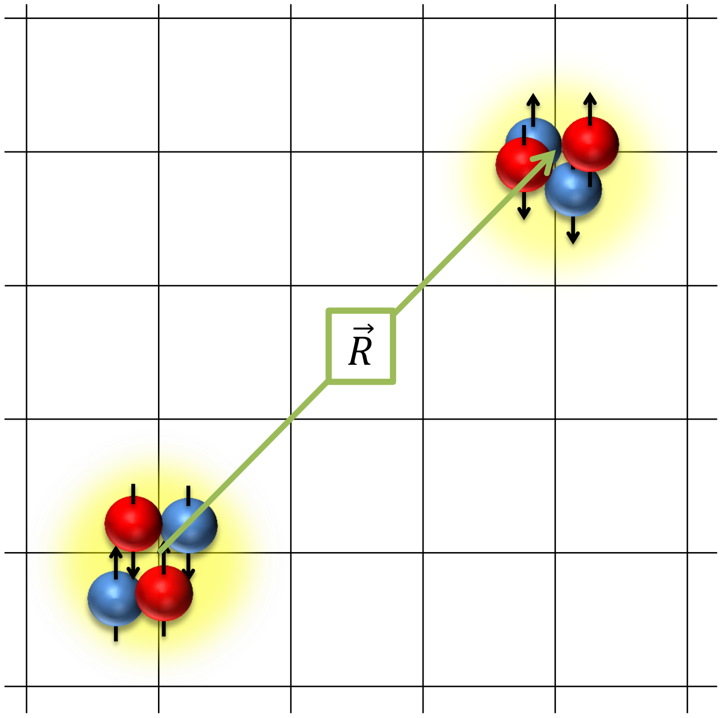
- Adiabatic projection method :

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 with the chiral EFT Hamiltonian H

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

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

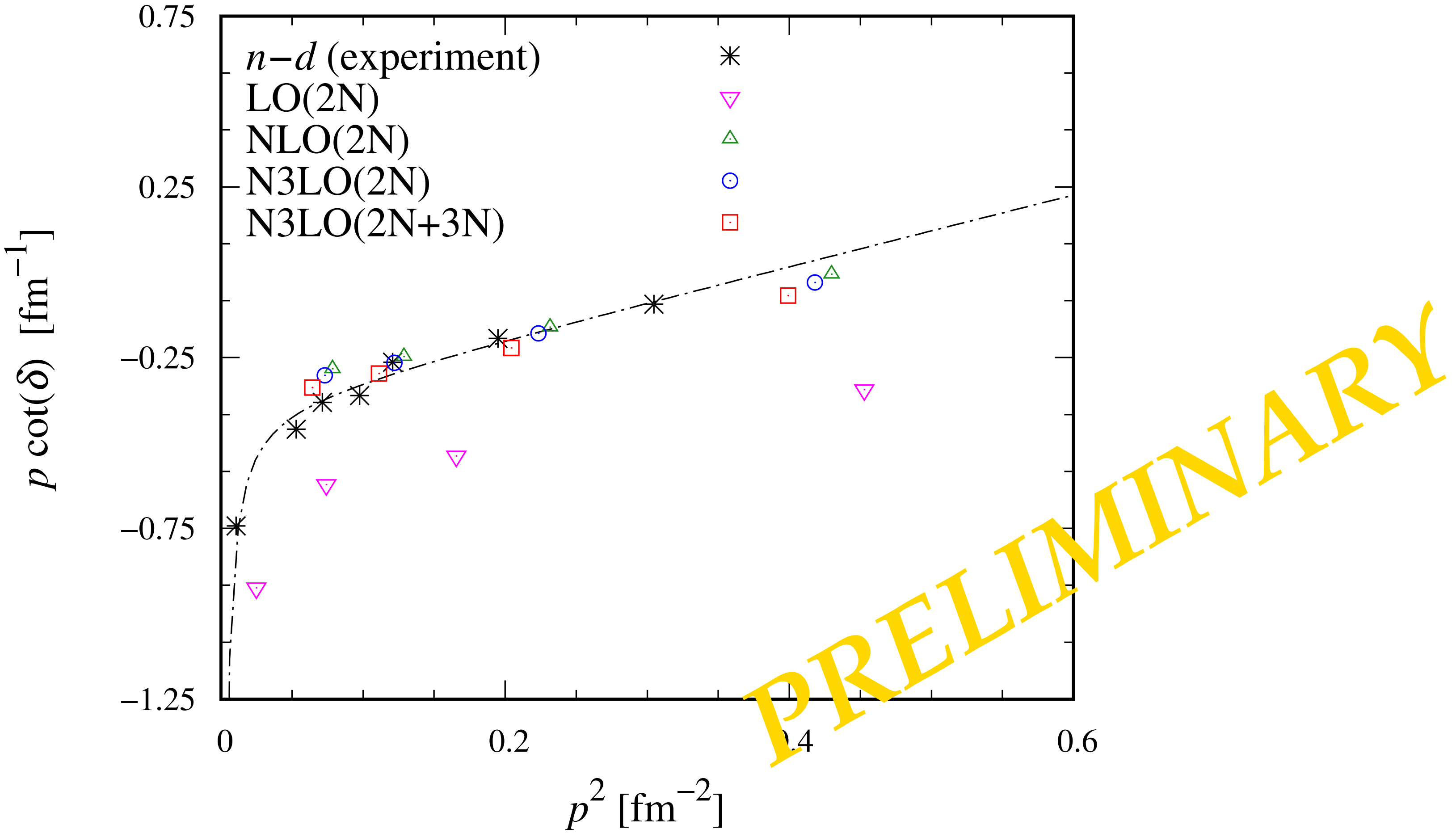
- Adiabatic Hamiltonian (requires norm matrices)

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

Scattering: Neutron-deuteron scattering at N3LO

Elhatisari, Hildenbrand, UGM, in progress

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

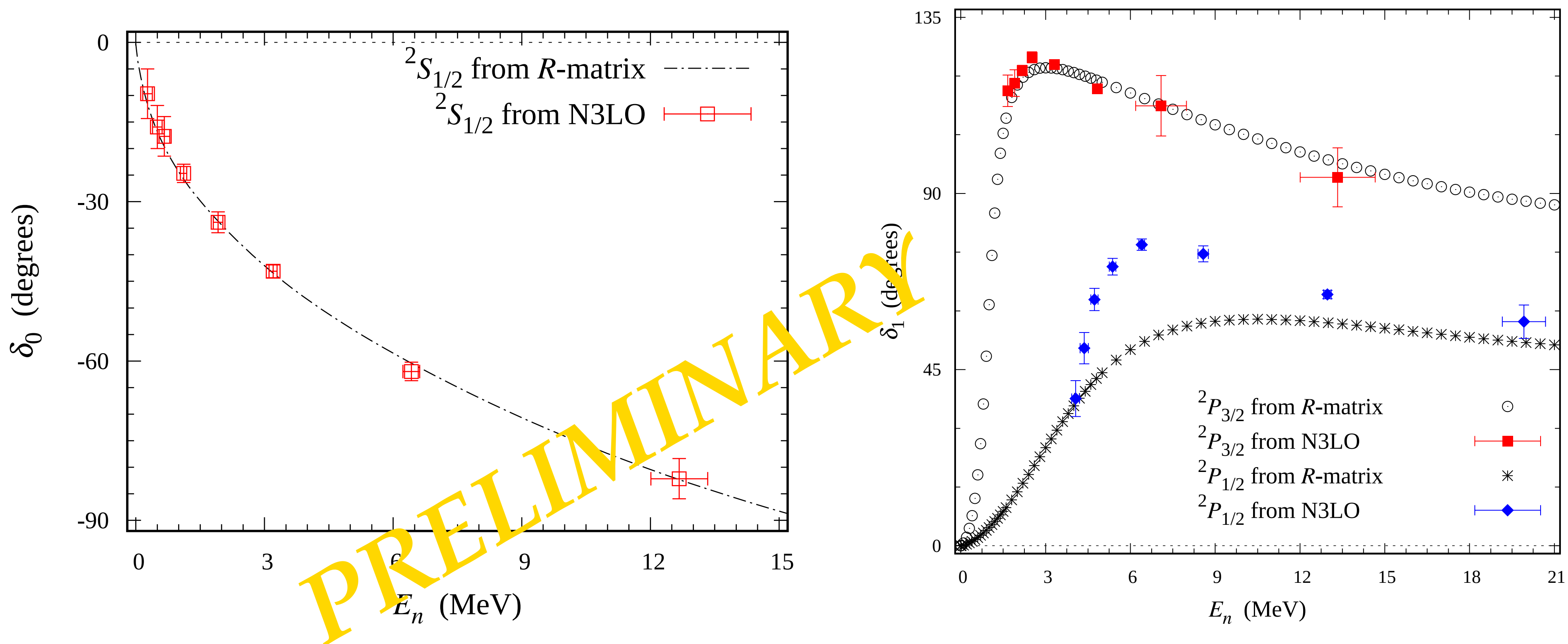


$\hookrightarrow$ shows good convergence

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

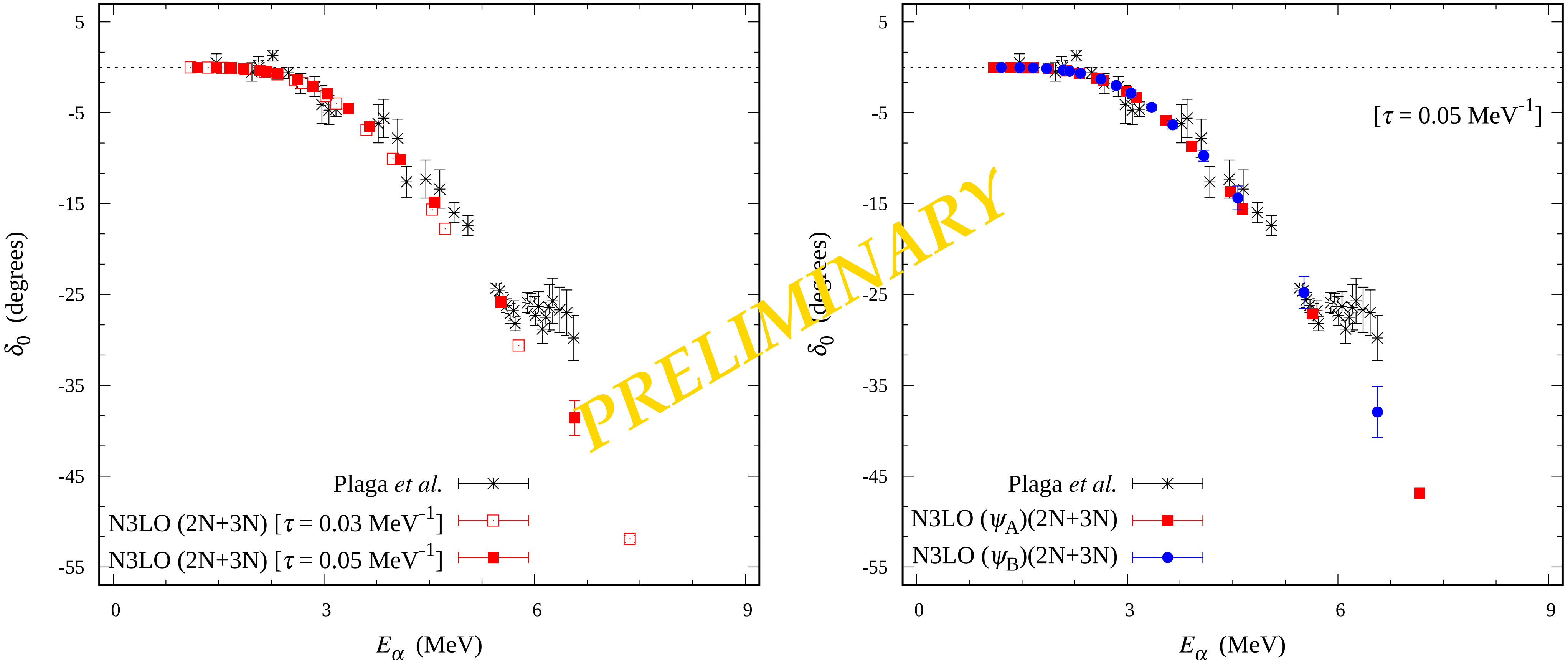
$\hookrightarrow$ Some fine-tuning of three-body forces for $^2P_{1/2}$ needed

Scattering: Alpha-carbon scattering at N3LO

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

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

  $\hookrightarrow$ different Euclidean times & different initial states



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

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

Summary & outlook

- Nuclear lattice simulations: a new quantum many-body approach
  - $\rightarrow$ based on the successful continuum nuclear chiral EFT
  - $\rightarrow$ a number of highly visible results already obtained

- Recent developments
  - $\rightarrow$ highly improved LO action based on SU(4)
    - $\hookrightarrow$ a number of interesting application (^{12}C, ^{4}He,...)
    - $\hookrightarrow$ towards the neutron matter EoS at high denstities (neutron stars)
  - $\rightarrow$ NN interaction at N3LO w/ wave function matching
    - $\hookrightarrow$ first promising results for nuclear structure, matter and scattering
    - $\hookrightarrow$ hyper-nuclei are under investigation

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

$\hookrightarrow$ stay tuned!

SPARES

The hidden spin-isospin exchange symmetry

Nucleon-nucleon interaction in large-N_C

Kaplan, Savage, Phys. Lett. **365B** (1996) 244; Kaplan, Manohar, Phys. Rev. **C 56** (1997) 96

- Performing the large-N_C analysis:

$$V^{\rm 2N}_{{\rm large}-N_c} = V_C + W_S\,\vec\sigma_1\cdot\vec\sigma_2\vec\tau_1\cdot\vec\tau_2 + W_T\,S_{12}\vec\tau_1\cdot\vec\tau_2 + \ldots$$

- Leading terms are $\sim N_C$
- First corrections are $1/N_C^2$ suppressed, fairly strong even for $N_C = 3$
- Velocity-dependent corrections can be incorporated
- Based on spin-isospin exchange symmetry of the nucleon w.f. $d_\uparrow \leftrightarrow u_\downarrow$ or on the nucleon level $n_\uparrow \leftrightarrow p_\downarrow$
- Constraints on 3NFs: Phillips, Schat, PRC **88** (2013) 034002; Epelbaum et al., EPJA **51** (2015) 26

Hidden spin-isospin symmetry: Basic ideas

Lee, Bogner, Brown, Elhatisari, Epelbaum, Hergert, Hjorth-Jensen, Krebs, Li, Lu, UGM, Phys. Rev. Lett. **127** (2021) 062501 [2010.09420 [nucl-th]]

- $V^{2N}_{\text{large}-N_c}$ is not renomalization group invariant: $\dfrac{dV_\mu(p,p')}{d\mu} \neq 0$

  $\simeq$ implicit setting of a preferred renormalization/resolution scale

- How does this happen?
  - **high energies**: corrections to the nucleon w.f. are $\sim v^2$

    $\to$ these high-energy modes must be $\mathcal{O}(1/N_C^2)$ in our low-energy EFT

    $\to$ momentum resolution scale $\Lambda \sim m_N/N_C \sim \mathcal{O}(1)$

    $\to$ consistent with the cutoff in a Δless th'y $\sim \sqrt{2m_N(m_\Delta - m_N)}$
  - **low energies:** the resolution scale must be large enough,

    so that orbital angular momentum and spin are fully resolved

    $\to$ as nucleon size is independent of N_C, so should be Λ $\surd$

- as will be shown, the optimal scale (where corrections are $\sim 1/N_C^2$) is:

$$\Lambda_{\text{large}-N_c} \simeq 500\,\text{MeV}$$

Nucleon-nucleon phase shifts – lattice

Lee, Bogner, Brown, Elhatisari, Epelbaum, Hergert, Hjorth-Jensen, Krebs, Li, Lu, UGM,
Phys. Rev. Lett. **127** (2021) 062501 [2010.09420 [nucl-th]]

- Use N3LO action (w/ TPE absorbed in contact interactions) at $a = 1.32$ fm

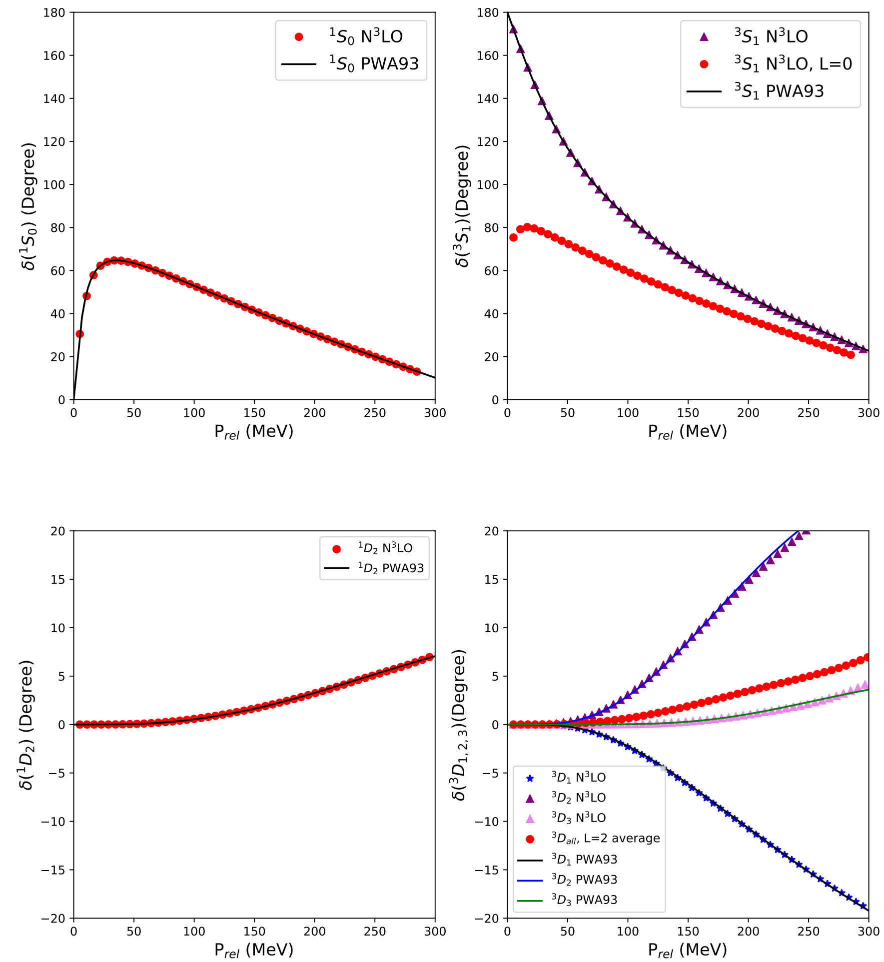
  $\hookrightarrow \Lambda = \pi/a = 470$ MeV

- compare $S = 0, T = 1$ w/ $S = 1, T = 0$
- S-waves: switch off the tensor force in $^3S_1$
- D-waves: average the spin-triplet channel

- NLEFT low-energy constants

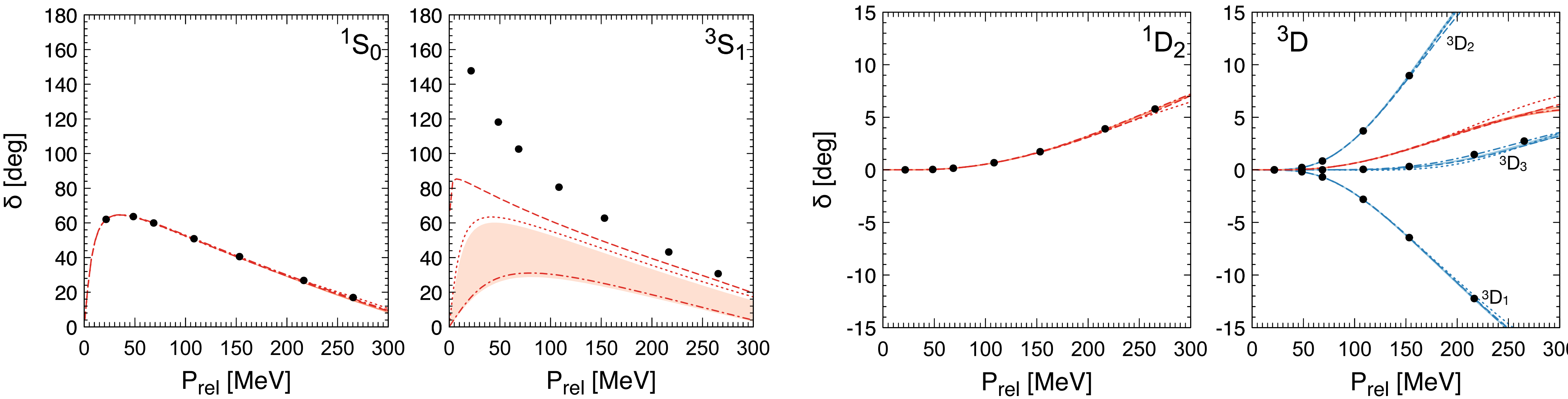
ch., order	LEC (l.u.)	ch., order	LEC (l.u.)
$^1\mathrm{S}_0, Q^0$	1.45(5)	$^3\mathrm{S}_1, Q^0$	1.56(3)
$^1\mathrm{S}_0, Q^2$	−0.47(3)	$^3\mathrm{S}_1, Q^2$	−0.53(1)
$^1\mathrm{S}_0, Q^4$	0.13(1)	$^3\mathrm{S}_1, Q^4$	0.12(1)
$^1\mathrm{D}_2, Q^4$	−0.088(1)	$^3\mathrm{D}_{\mathrm{all}}, Q^4$	−0.070(2)

$\Rightarrow$ works pretty well



Nucleon-nucleon phase shifts – continuum

- Consider various (chiral) continuum potentials → also works $\surd$



· · · · · ·	IDAHO N3LO	Entem, Machleidt, PRC **68** (2003) 041001
— — —	IDAHO N4LO ($\Lambda = 500$ MeV)	Entem, Machleidt, Nosyk PRC **96** (2017) 024004
· — ·—	CD-Bonn	Machleidt, PRC **63** (2001) 024001
(shaded band)	Bochum N4$^+$LO ($\Lambda = 400 - 550$ MeV)	Reinert, Krebs, Epelbaum, EPJA **54** (2018) 86
• • •	Nijmegen PWA	Wiringa, Stoks, Schiavilla, PRC **51** (1995) 38

Two-nucleon matrix elements

- Consider the ME between any two-nucleon states A and B. Both have total spin S and total isospin T. Then (for isospin-inv. H):

$$M(S,T) = \frac{1}{2S+1} \sum_{S_z=-S}^{S} \langle A; S, S_z; T, T_z | H | B; S, S_z; T, T_z \rangle$$

- Spin-isospin exchange symmetry: $\boxed{M(S,T) = M(T,S)}$

- Ex: ^{30}P has 1 proton + 1 neutron in the $1s_{1/2}$ orbitals (minimal shell model)

$\to$ if spin-isospin exchange symmetry were exact, the $S=0, T=1$ & $S=1, T=0$ states should be degenerate

- Data: The 1^+ g.s. is 0.677 MeV below the 0^+ excited state ($E_{g.s.} \simeq 220$ MeV)

$\to$ fairly good agreement, consistent w/ $1/N_C^2$ corrections

$\to$ explanation: interactions of the np pair with the ^{28}Si core are suppressing spatial correlations of the 1^+ w.f. caused by the tensor interaction

Two-nucleon matrix elements in the s-d shell

- Test the spin-isospin echange symmetry for general two-body MEs 1s-0d shell

- Use the spin-tensor analysis developed by Kirson, Brown et al.
  Kirson, PLB **47** (1973) 110; Brown et al., JPhysG **11** (1985) 1191; Ann. Phys. **182** (1988) 191

- Seven two-body MEs for $(S,T) = (1,0)$ and $(S,T) = (0,1)$

ME	L_1	L_2	L_3	L_4	L_{12}	L_{34}
1	2	2	2	2	0	0
2	2	2	2	2	2	2
3	2	2	2	2	4	4
4	2	2	2	0	2	2
5	2	2	0	0	0	0
6	2	0	2	0	2	2
7	0	0	0	0	0	0

L_1, L_2: orbital angular momenta of the outgoing orbitals of A

L_{12}: total angular momentum of state A

L_3, L_4: orbital angular momenta of the outgoing orbitals of B

L_{34}: total angular momentum of state A

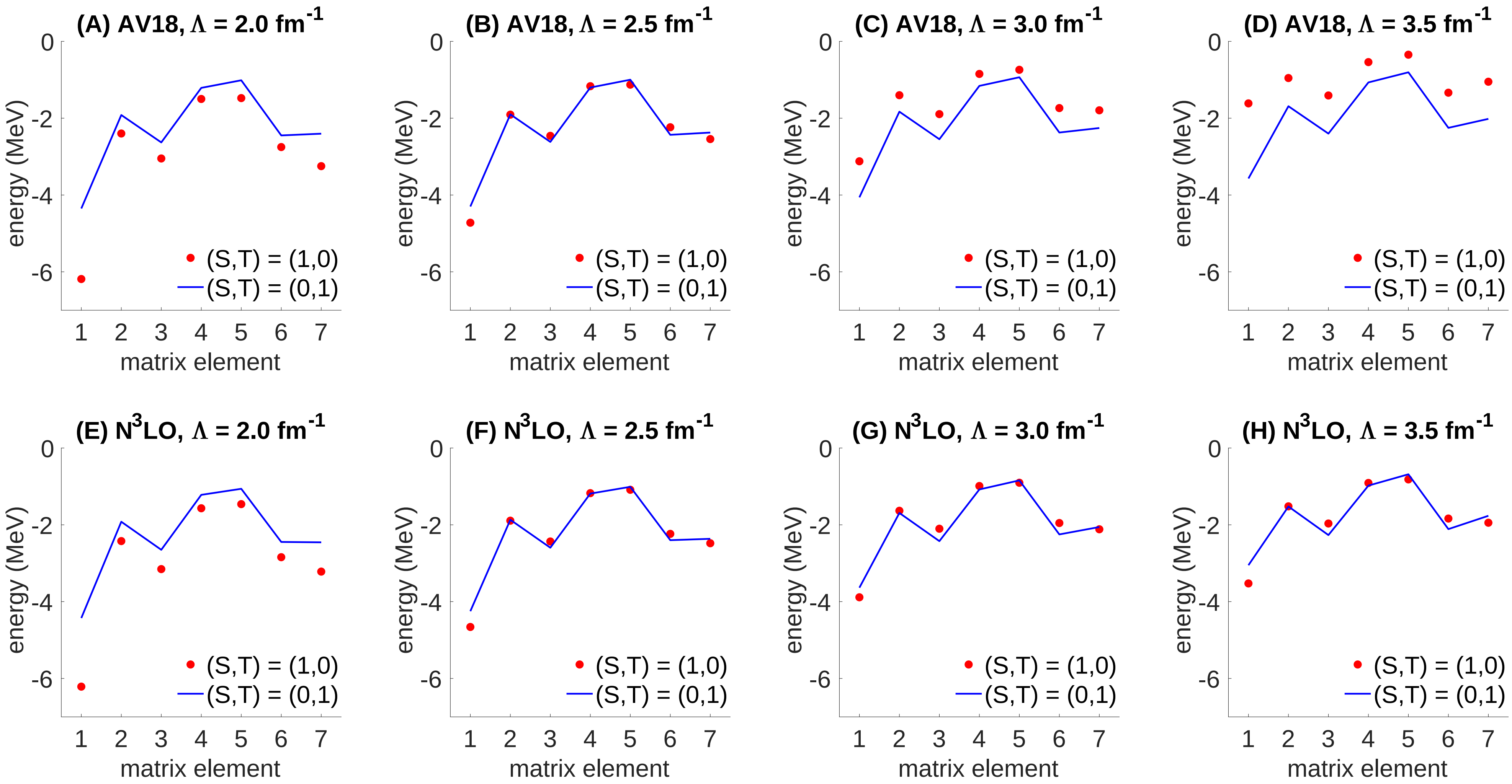
ME 7 corresponds to the $1s_{1/2}$ orbitals discussed before

set $L_Z = (L_{12})_z = (L_{34})_z$, average over L_z

$\rightarrow$ Work out $M(S,T)$ for various forces at $\Lambda = 2.0, 2.5, 3.0, 3.5$ fm^{-1}

Two-nucleon matrix elements in the s-d shell

- Results for the AV18 and N3LO chiral potentials



Two-nucleon matrix elements: Conclusions

- As anticipated:
  - The optimal resolution scale is obviously $\Lambda \sim 500$ MeV
  - For $\Lambda < \Lambda_{\text{large}-N_c}$, the $(S,T) = (1,0)$ channel is more attractive
  - For $\Lambda > \Lambda_{\text{large}-N_c}$, the $(S,T) = (0,1)$ channel is more attractive
  - These results do not depend on the type of interaction, while AV18 is local, chiral N3LO has some non-locality (and similar for more modern interactions like chiral N4$^+$LO)

$\hookrightarrow$ consistent with the results for NN scattering

$\Rightarrow$ **Validates Weinberg's power counting!** $\surd$

Three-nucleon forces

- Leading central three-nucleon force at the optimal resolution scale:

$$
\begin{aligned}
V^{\rm 3N}_{{\rm large}-N_c} &= V_C^{\rm 3N} + [(\vec\sigma_1 \times \vec\sigma_2)\cdot\vec\sigma_3][(\vec\tau_1 \times \vec\tau_2)\cdot\vec\tau_3] W_{123}^{\rm 3N} \\
&+ \vec\sigma_1\cdot\vec\sigma_2 \vec\tau_1\cdot\vec\tau_2 W_{12}^{\rm 3N} + \vec\sigma_2\cdot\vec\sigma_3 \vec\tau_2\cdot\vec\tau_3 W_{23}^{\rm 3N} \\
&+ \vec\sigma_3\cdot\vec\sigma_1 \vec\tau_3\cdot\vec\tau_1 W_{31}^{\rm 3N} + \ldots ,
\end{aligned}
$$

- Subleading central 3N interactions are of size $1/N_C$, of type

$$
\vec\sigma_1\cdot\vec\sigma_2[(\vec\tau_1\times\vec\tau_2)\cdot\vec\tau_3]\,, \qquad [(\vec\sigma_1\times\vec\sigma_2)\cdot\vec\sigma_3]\vec\tau_1\cdot\vec\tau_2
$$

⇒ helps in constraining the many short-range three-nucleon interactions that appear at higher orders in chiral EFT

- The spin-isospin exchange symmetry of the leading interactions also severely limits the isospin-dependent contributions of the 3N interactions to the nuclear EoS

⇒ relevant for calculations of the nuclear symmetry energy and its density dependence in dense nuclear matter

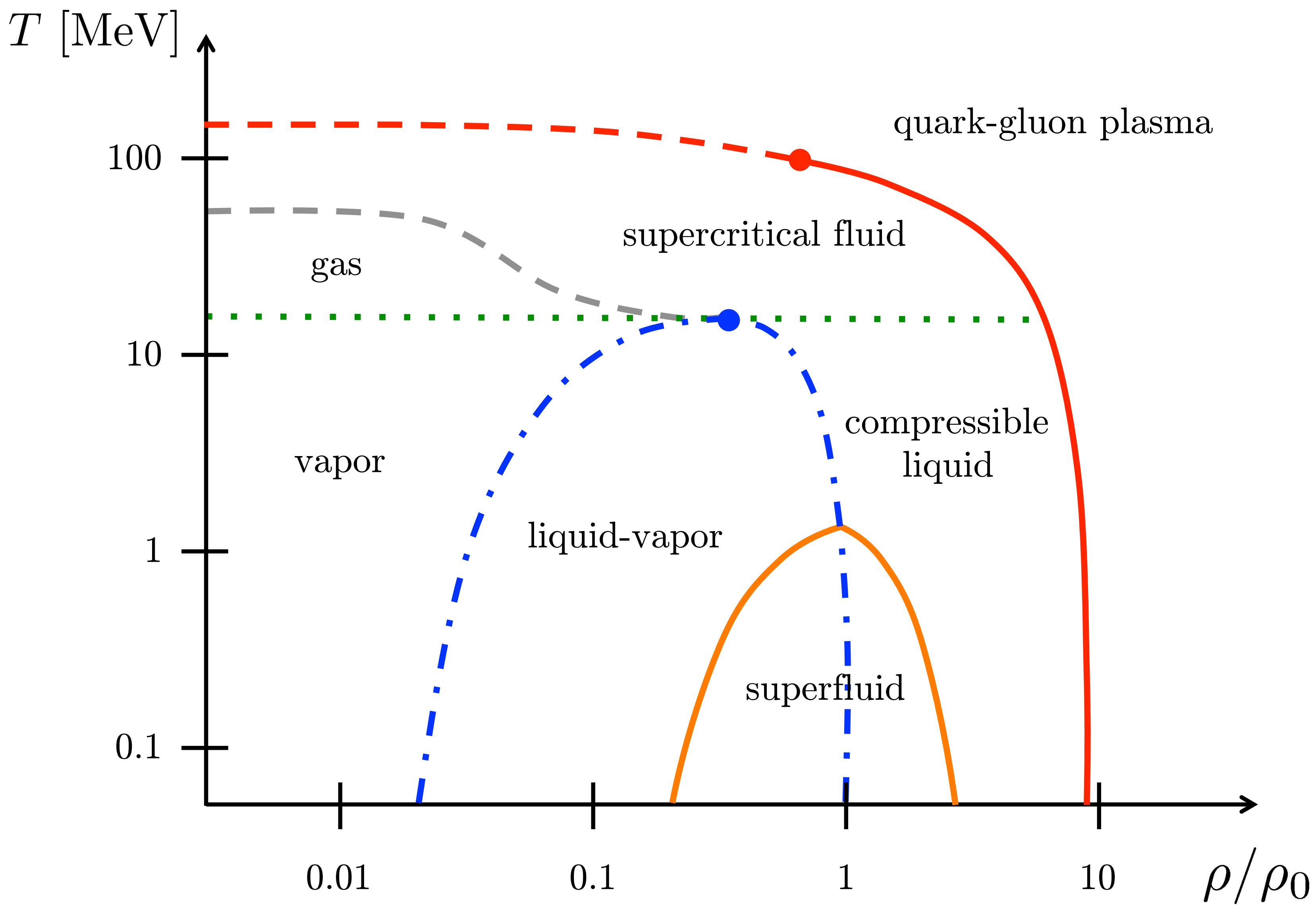
Ab Initio Nuclear Thermodynamics

B. N. Lu, N. Li, S. Elhatisari, D. Lee, J. Drut, T. Lähde, E. Epelbaum, UGM,
Phys. Rev. Lett. **125** (2020) 192502 [arXiv:1912.05105]

Phase diagram of strongly interacting matter

- Sketch of the phase diagram of strongly interacting matter

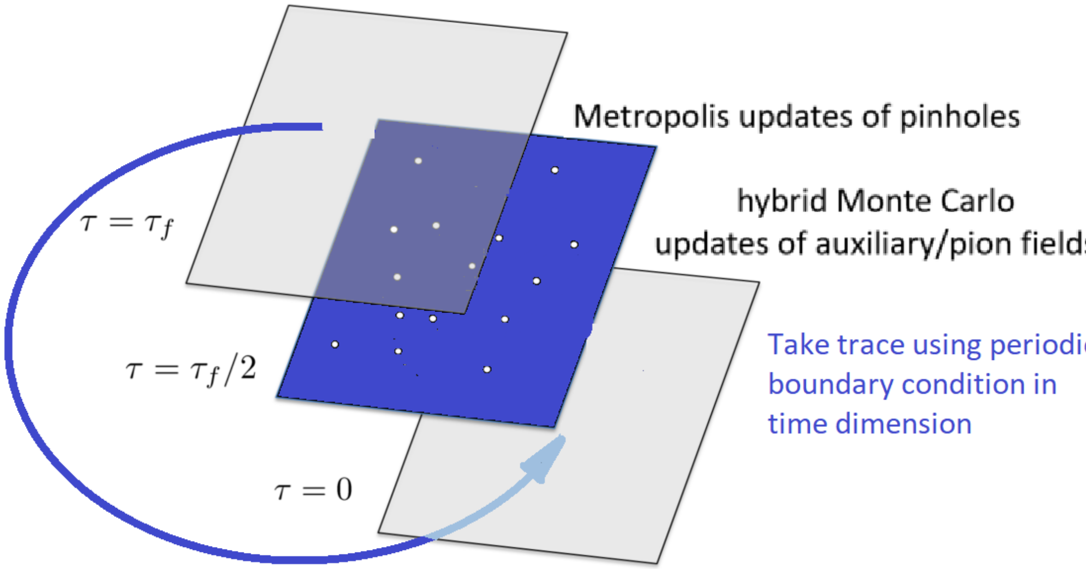
Fig. courtesy B.-N. Lu



Pinhole trace algorithm (PTA)

- The pinhole states span the whole A-body Hilbert space

- The canonical partition function can be expressed using pinholes:



$$Z_A = \mathrm{Tr}_A \left[\exp(-\beta H)\right] , \ \beta = 1/T$$

$$= \sum_{n_1,\cdots,n_A} \int \mathcal{D}s\mathcal{D}\pi \langle n_1, \cdots, n_A | \exp[-\beta H(s,\pi)] | n_1, \cdots, n_A \rangle$$

- allows to study: liquid-gas phase transition → this talk
  thermodynamics of finite nuclei
  thermal dissociation of hot nuclei
  cluster yields of dissociating nuclei

New paradigm for nuclear thermodynamics

- The PTA allows for simulations with fixed neutron & proton numbers at non-zero T

$\hookrightarrow$ thousands to millions times faster than existing codes using the grand-canonical ensemble ($t_{\rm CPU} \sim VN^2$ vs. $t_{\rm CPU} \sim V^3N^2$)

- Only a mild sign problem $\rightarrow$ pinholes are dynamically driven to form pairs

- Typical simulation parameters:

up to $N = 144$ nucleons in volumes $L^3 = 4^3, 5^3, 6^3$

$\hookrightarrow$ densities from 0.008 fm^{-3} ... 0.20 fm^{-3}

$a = 1.32$ fm $\rightarrow \Lambda = \pi/a = 470$ MeV , $a_t \simeq 0.1$ fm

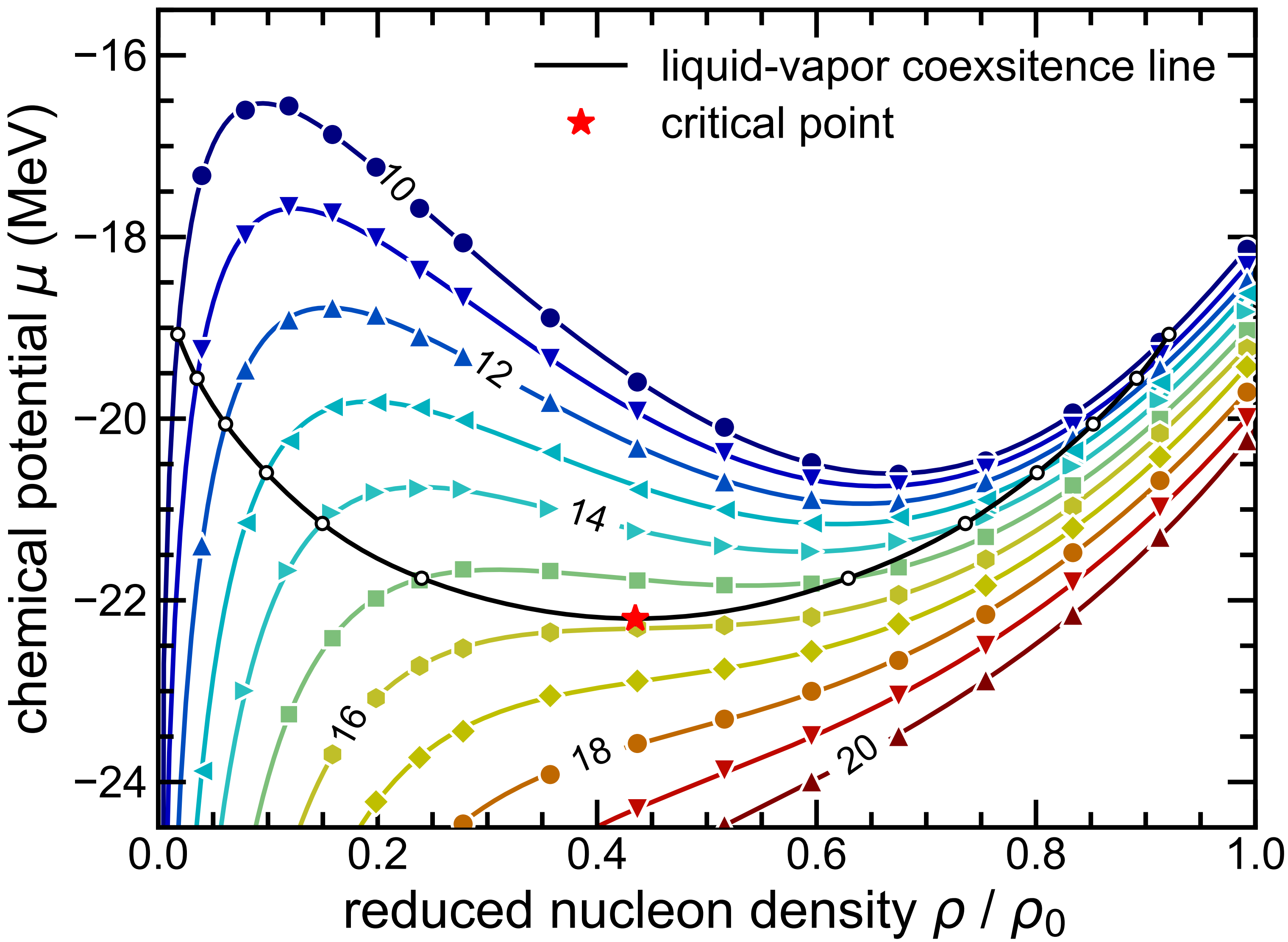
consider $T = 10\ldots 20$ MeV

- use twisted bc's, average over twist angles $\rightarrow$ acceleration to the td limit

- very favorable scaling for generating config's: $\Delta t \sim N^2 L^3$

Chemical potential

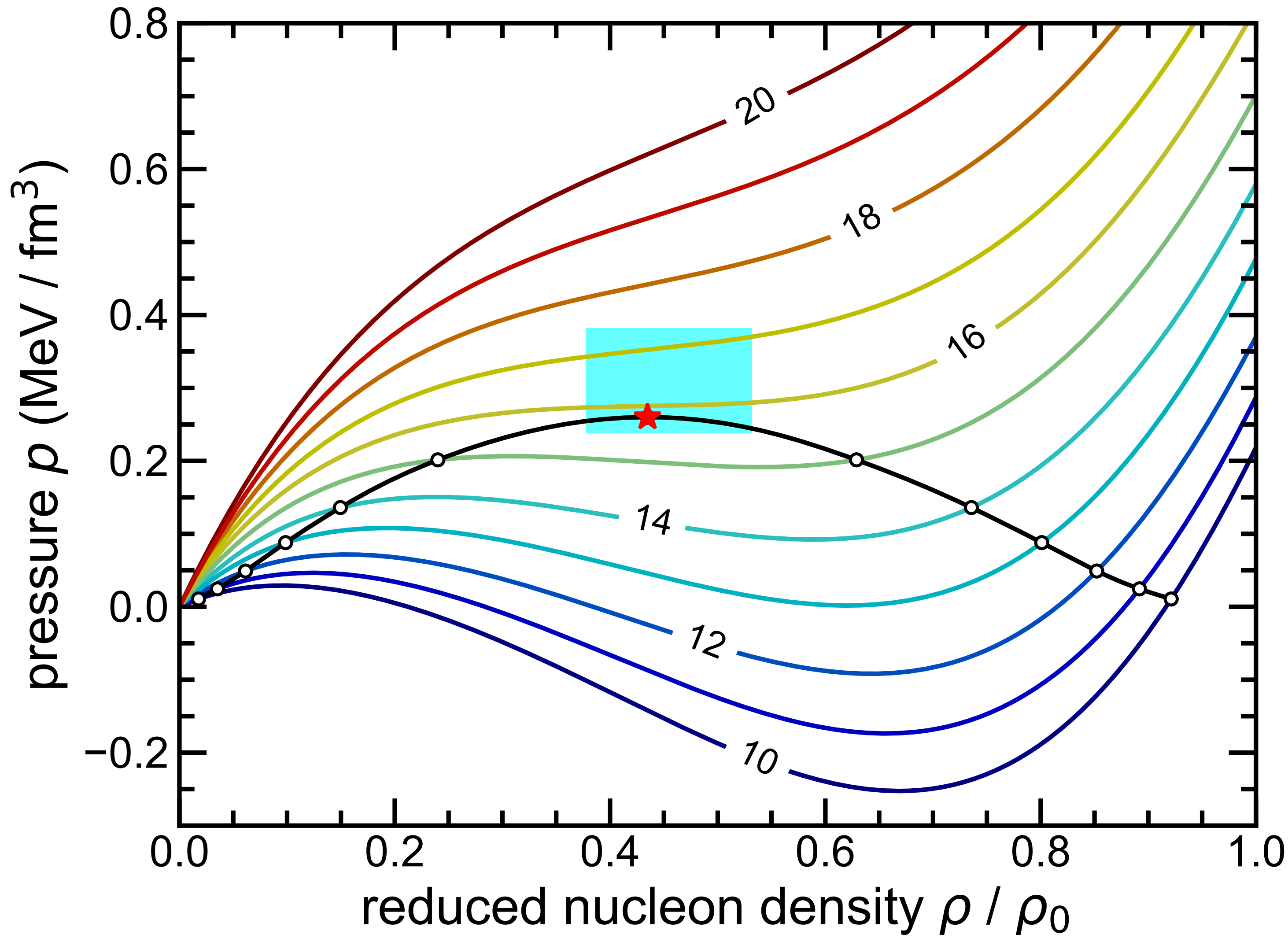
- Calculated from the free energy: $\mu = (F(N+1) - F(N-1))/2$



at very low densities like the ideal gas $\mu \propto \log(\rho)$

Equation of state

- Calculated by integrating: $dP = \rho\, d\mu$
- Crtitical point: $T_c = 15.8(1.6)$ MeV, $P_c = 0.26(3)$ MeV/fm^3, $\rho_c = 0.089(18)$ fm^{-3}

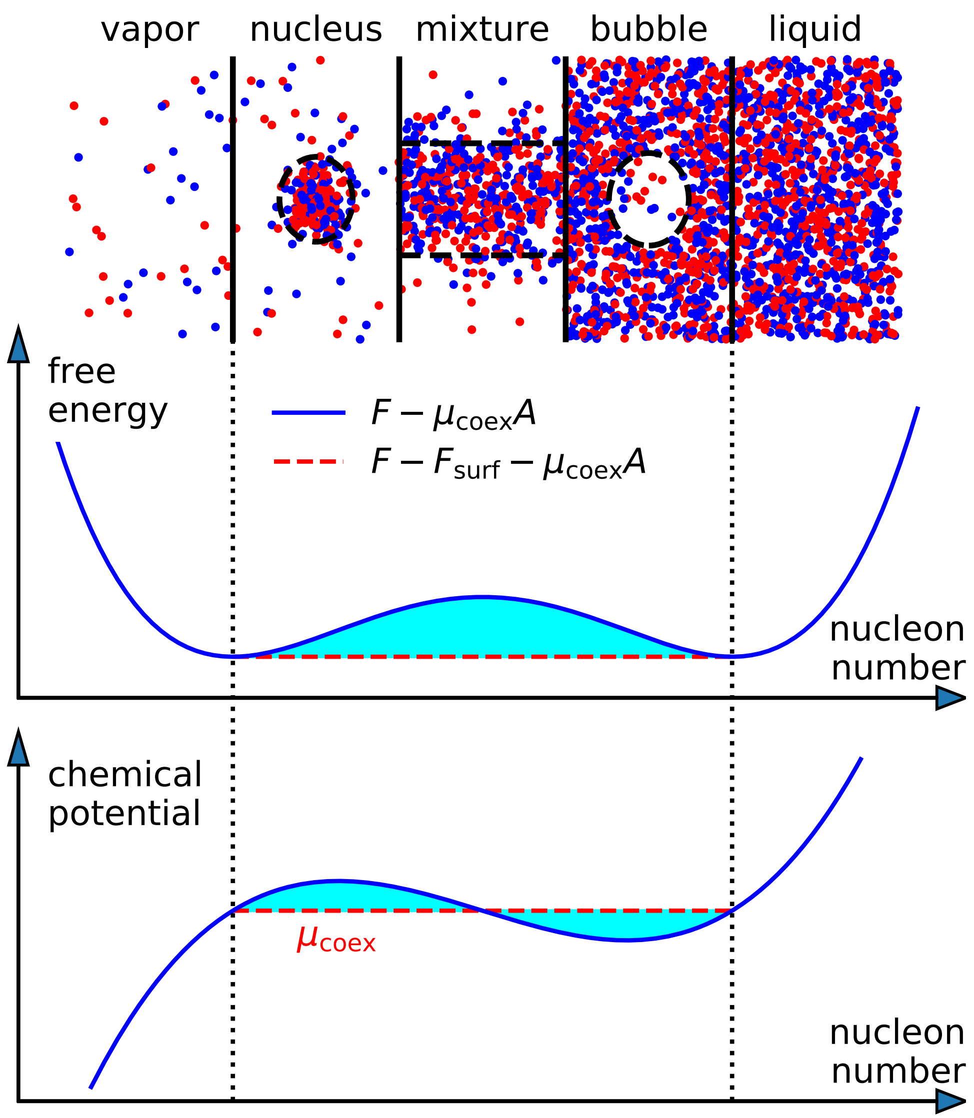


Experiment: $T_c = 15.0(3)$ MeV, $P_c = 0.31(7)$ MeV/fm^3, $\rho_c = 0.06(2)$ fm^{-3}

Vapor-liquid phase transition

- Vapor-liquid phase transition in a finite volume V & $T < T_c$

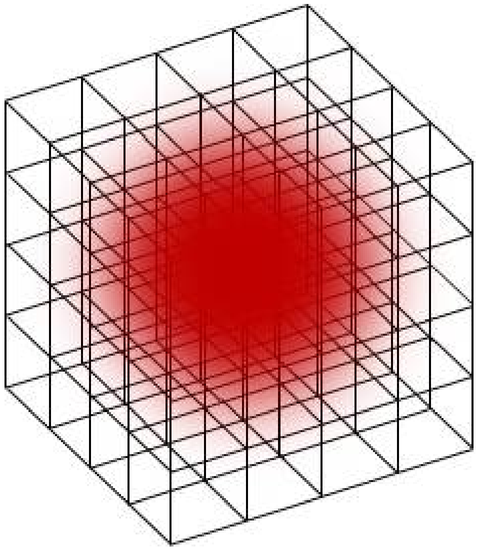
- the most probable configuration for different nucleon number A



- the free energy

- chemical potential $\mu = \partial F / \partial A$

CENTER-of-MASS PROBLEM



- AFQMC calculations involve states that are superpositions of many different center-of-mass (com) positions

$$Z_A(\tau) = \langle \Psi_A(\tau) | \Psi_A(\tau) \rangle$$
$$|\Psi_A(\tau)\rangle = \exp(-H\tau/2)|\Psi_A\rangle$$

- but: translational invariance requires summation over all transitions

$$Z_A(\tau) = \sum_{i_{\rm com}, j_{\rm com}} \langle \Psi_A(\tau, i_{\rm com}) | \Psi_A(\tau, j_{\rm com}) \rangle \,, \;\; {\rm com} = {\rm mod}((i_{\rm com} - j_{\rm com}), L)$$

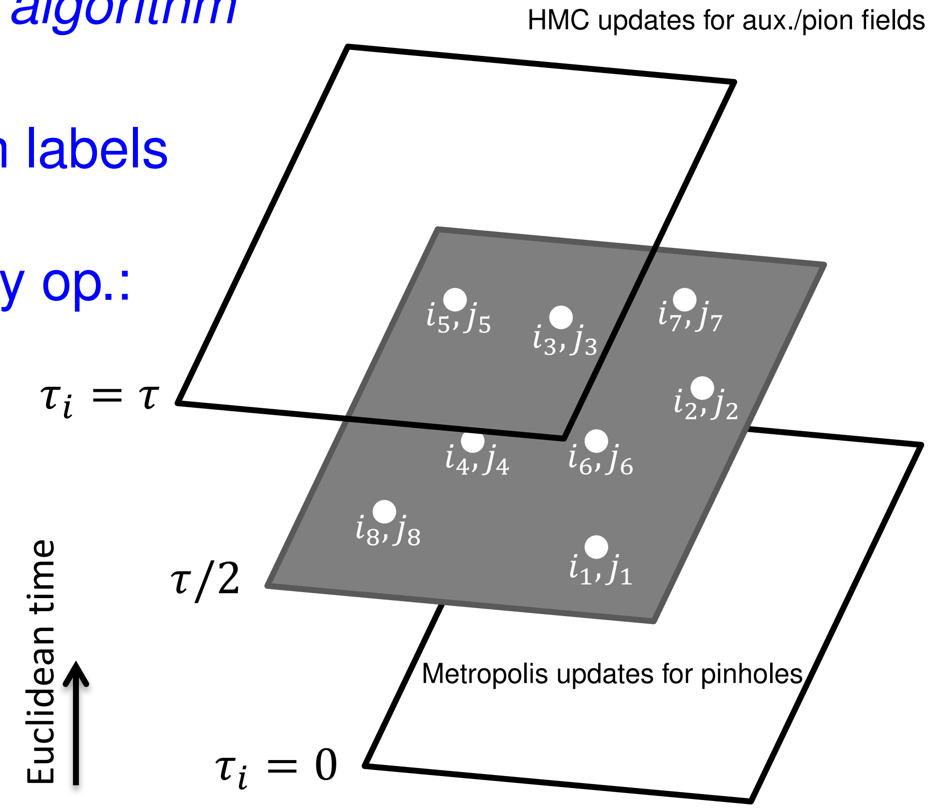
$i_{\rm com}$ $(j_{\rm com})$ = position of the center-of-mass in the final (initial) state

→ density distributions of nucleons can not be computed directly, only moments

→ need to overcome this deficieny

PINHOLE ALGORITHM

- Solution to the CM-problem:
  track the individual nucleons using the *pinhole algorithm*



- Insert a screen with pinholes with spin & isospin labels that allows nucleons with corresponding spin & isospin to pass = insertion of the A-body density op.:

$$\boldsymbol{\rho}_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots\mathbf{n}_A) = :\boldsymbol{\rho}_{i_1,j_1}(\mathbf{n}_1)\cdots\boldsymbol{\rho}_{i_A,j_A}(\mathbf{n}_A):$$

- MC sampling of the amplitude:

$$\boldsymbol{A}_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\ldots,\mathbf{n}_A,\boldsymbol{L}_t) = \langle\boldsymbol{\Psi}_A(\boldsymbol{\tau}/2)|\boldsymbol{\rho}_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\ldots,\mathbf{n}_A)|\boldsymbol{\Psi}_A(\boldsymbol{\tau}/2)\rangle$$

- Allows to measure proton and neutron distributions

- Resolution scale $\sim \boldsymbol{a}/\boldsymbol{A}$ as cm position $\mathbf{r}_{\mathbf{cm}}$ is an integer $\mathbf{n}_{\mathbf{cm}}$ times $\boldsymbol{a}/\boldsymbol{A}$