UNIVERSITÄT BONN   bctp   CENTER FOR SCIENCE & THOUGHT   JÜLICH Forschungszentrum

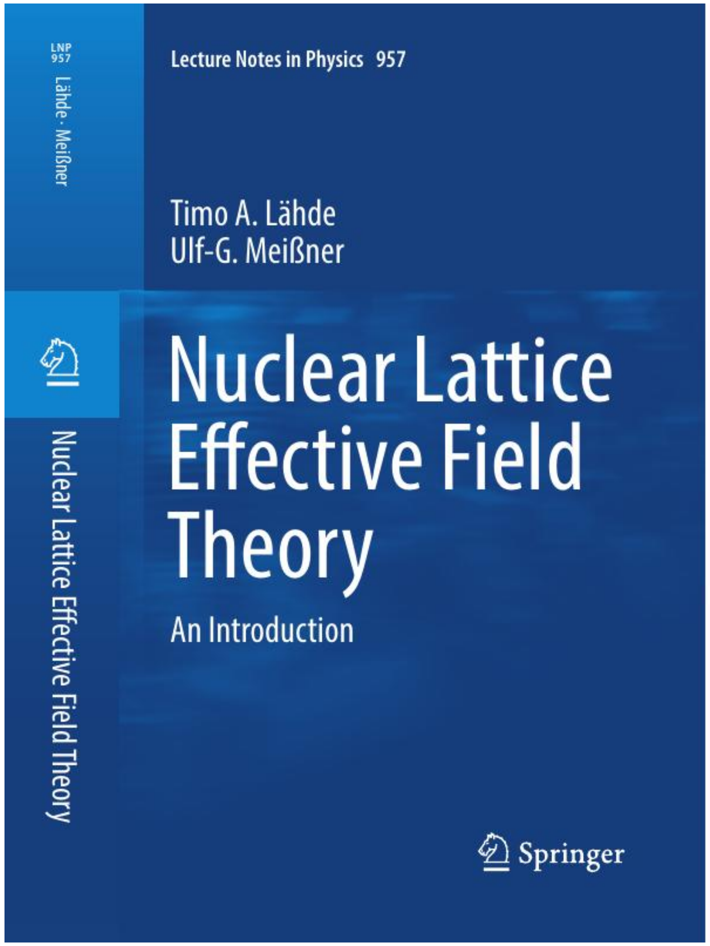
Recent Progress in Nuclear Lattice EFT (B.9)

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

supported by DFG, SFB/TR-110   by CAS, PIFI   by VolkswagenStftung   by ERC, EXOTIC   by NRW-FAIR

Contents

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

AUTHORS:
Ulf-G Meißner, Rheinische Friedrich-Wilhelms-Universität Bonn and Forschungszentrum Jülich
Akaki Rusetsky, Rheinische Friedrich-Wilhelms-Universität Bonn

DATE PUBLISHED: August 2022
AVAILABILITY: Available
FORMAT: Hardback
ISBN: 9781108476980

Rate & review

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

Nuclear lattice effective field theory

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

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

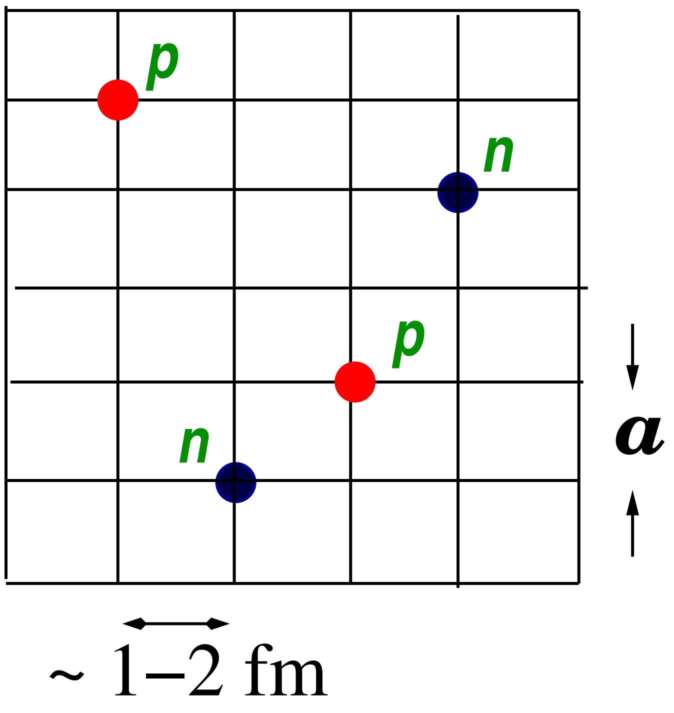
- discretize space-time $V = L_s \times L_s \times L_s \times L_t$:
  nucleons are point-like particles on the sites

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

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

- typical lattice parameters

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



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

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

- physics independent of the lattice spacing for $a = 1 \ldots 2$ fm

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

Transfer matrix method

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

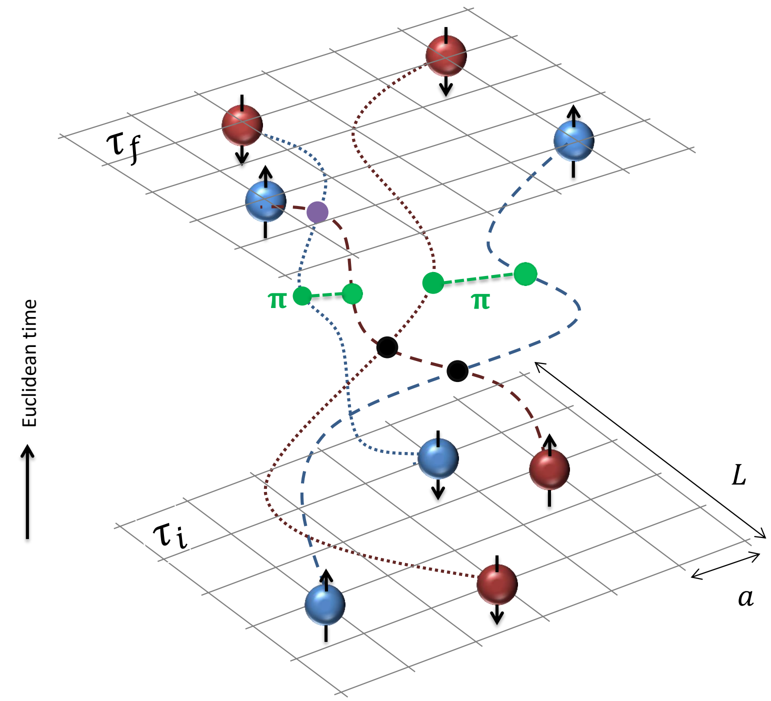
  with Ψ_A a Slater determinant for A free nucleons
  [or a more sophisticated (correlated) initial/final state]

  Euclidean time

- Transient energy

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

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

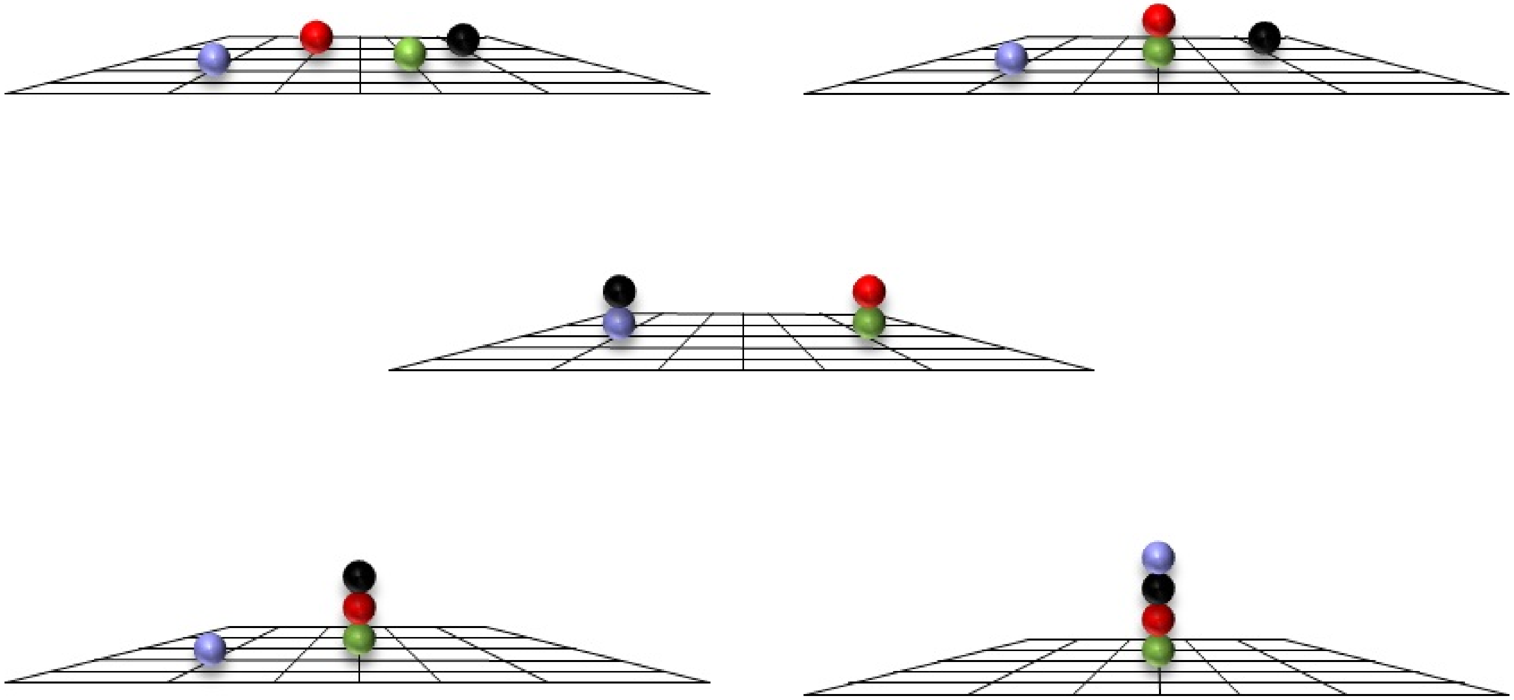


- Exp. value of any normal–ordered operator $\mathcal{O}$

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

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

Configurations



⇒ all *possible* configurations are sampled

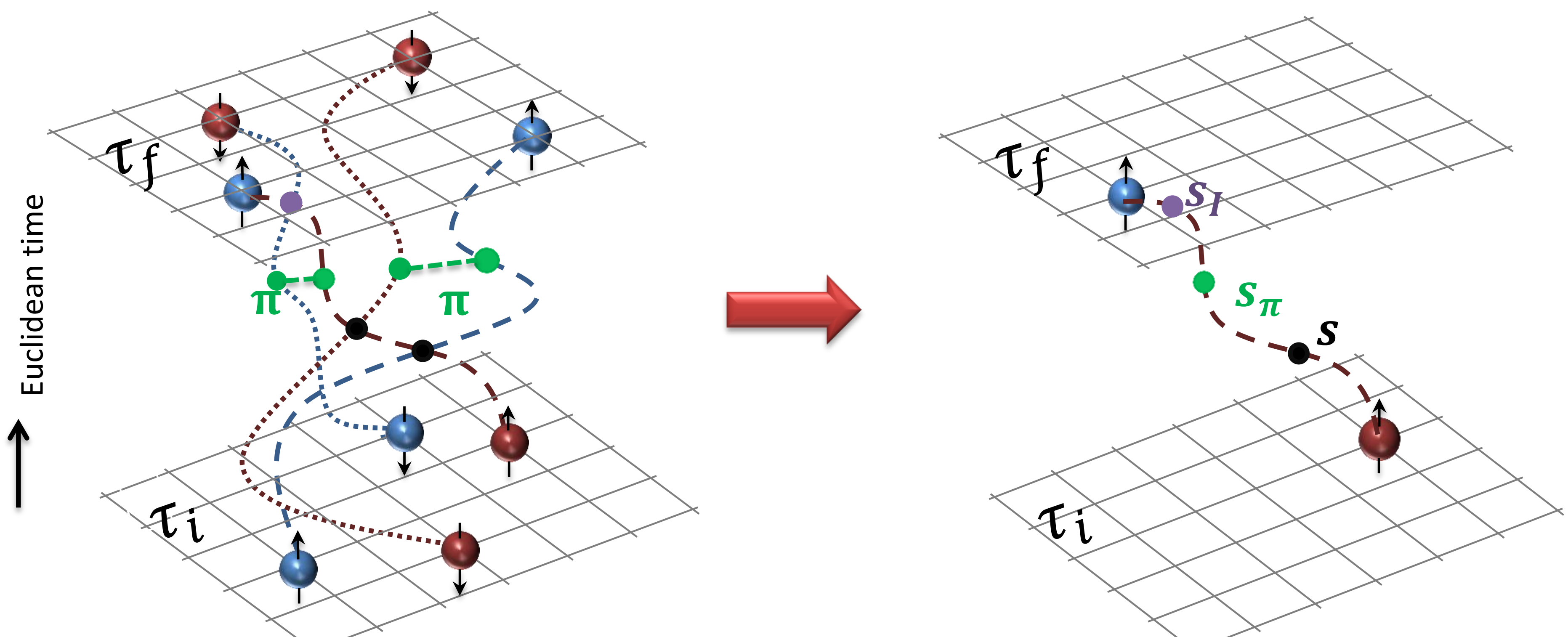
⇒ preparation of *all possible* initial/final states

⇒ *clustering* emerges *naturally*

Auxiliary field method

- Represent interactions by auxiliary fields:

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



optimally suited for parallel computing!

Computational equipment

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

Emergent geometry and duality in the carbon nucleus

Short reminder of Wigner SU(4) 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 $U(4) = U(1) \times SU(4)$]:

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

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

- LO pionless EFT: $\mathcal{L}_{\not\pi} = N^\dagger \left(i\partial_t + \frac{\vec{\nabla}^2}{2m_N} \right) N - \frac{1}{2} \left(C_S (N^\dagger N)^2 + C_T (N^\dagger \vec{\sigma} N)^2 \right)$

Mehen, Stewart, Wise, Phys. Rev. Lett. **83** (1999) 931

- Partial wave LECs: $C(^1S_0) = C_S - 3C_T\ , \quad C(^3S_1) = C_S + C_T$

⇒ The operator $(N^\dagger N)^2$ is invariant under Wigner SU(4), but $(N^\dagger \vec{\sigma} N)^2$ is not

⇒ In the Wigner SU(4) limit, one finds: $C(^1S_0) = C(^3S_1) \ \to a_{np}^{S=0} = a_{np}^{S=1} \to \infty$

⇒ The exact symmetry limit corresponds to a scale invariant non-relativistic system

Remarks on Wigner's SU(4) symmetry

- 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

  $\hookrightarrow$ related to the unitary limit
  König, Griesshammer, Hammer, van Kolck, Phys. Rev. Lett. **118** (2017) 202501

- 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

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

- Study of the spectrum of ^{12}C Shen, Lähde, Lee, UGM, Eur. Phys.J. A **57** (2021) 276

  $\hookrightarrow$ 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 $\rightarrow$ next slide

- Locally and non-locally smeared SU(4) invariant interaction:

$$V = C_2 \sum_{\mathbf{n}',\mathbf{n},\mathbf{n}''} : \rho_{\rm NL}(\mathbf{n}') f_{s_{\rm L}}(\mathbf{n}'-\mathbf{n}) f_{s_{\rm L}}(\mathbf{n}-\mathbf{n}'') \rho_{\rm NL}(\mathbf{n}'') : , \quad f_{s_{\rm L}}(\mathbf{n}) = \begin{cases} 1, & |\mathbf{n}| = 0, \\ s_{\rm L}, & |\mathbf{n}| = 1, \\ 0, & \text{otherwise} \end{cases}$$

$$\rho_{\rm NL}(\mathbf{n}) = a^\dagger_{\rm NL}(\mathbf{n}) a_{\rm NL}(\mathbf{n})$$

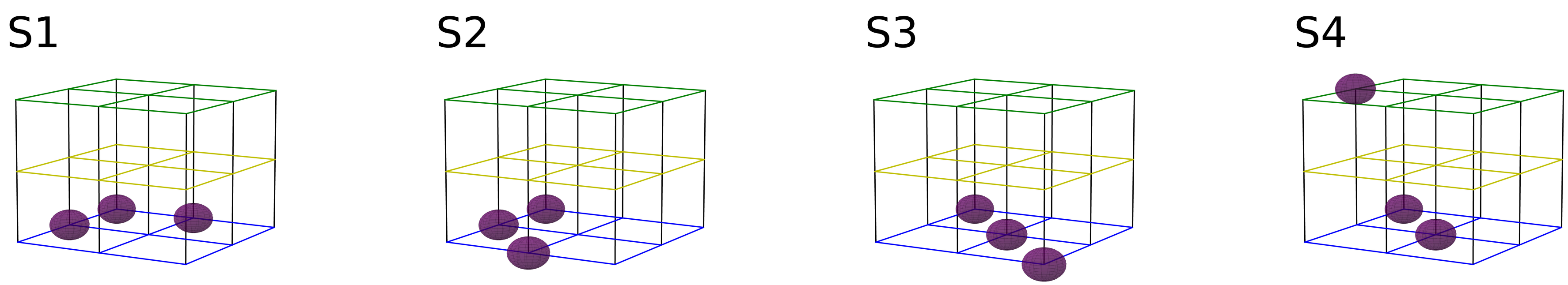
$$a^{(\dagger)}_{\rm NL}(\mathbf{n}) = a^{(\dagger)}(\mathbf{n}) + s_{\rm NL} \sum_{|\mathbf{n}'|=1} a^{(\dagger)}(\mathbf{n}+\mathbf{n}') , \quad s_{\rm NL} = 0.2$$

$\hookrightarrow$ only two adjustable parameters (C_2, s_L) fitted to $E_{^4\rm He}$ & $E_{^{12}\rm C}$

$\hookrightarrow$ investigate the spectrum for $a = 1.64$ fm and $a = 1.97$ fm

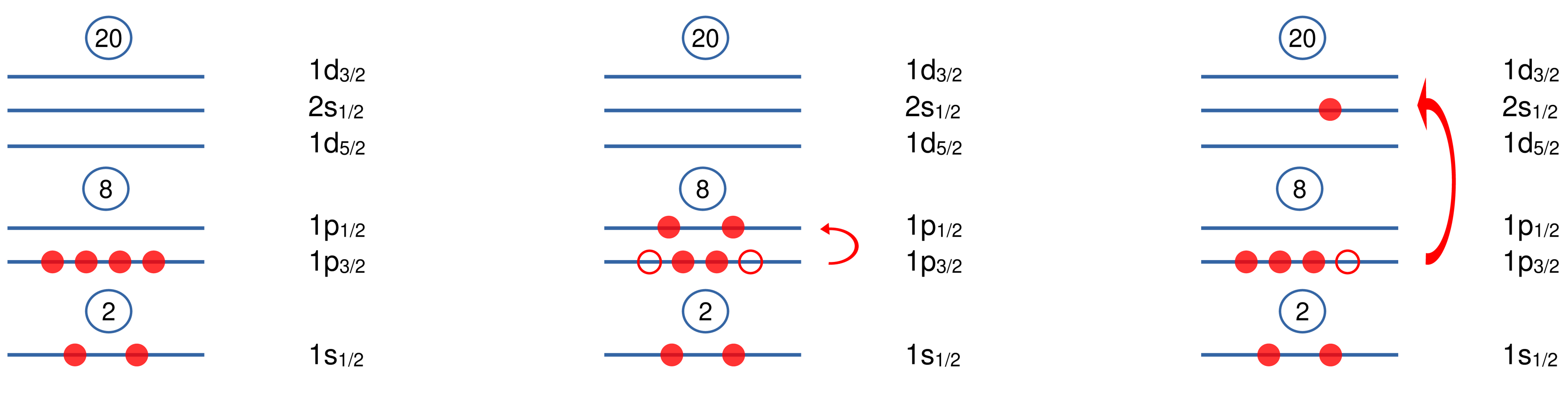
Configurations

- Cluster and shell model configurations



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

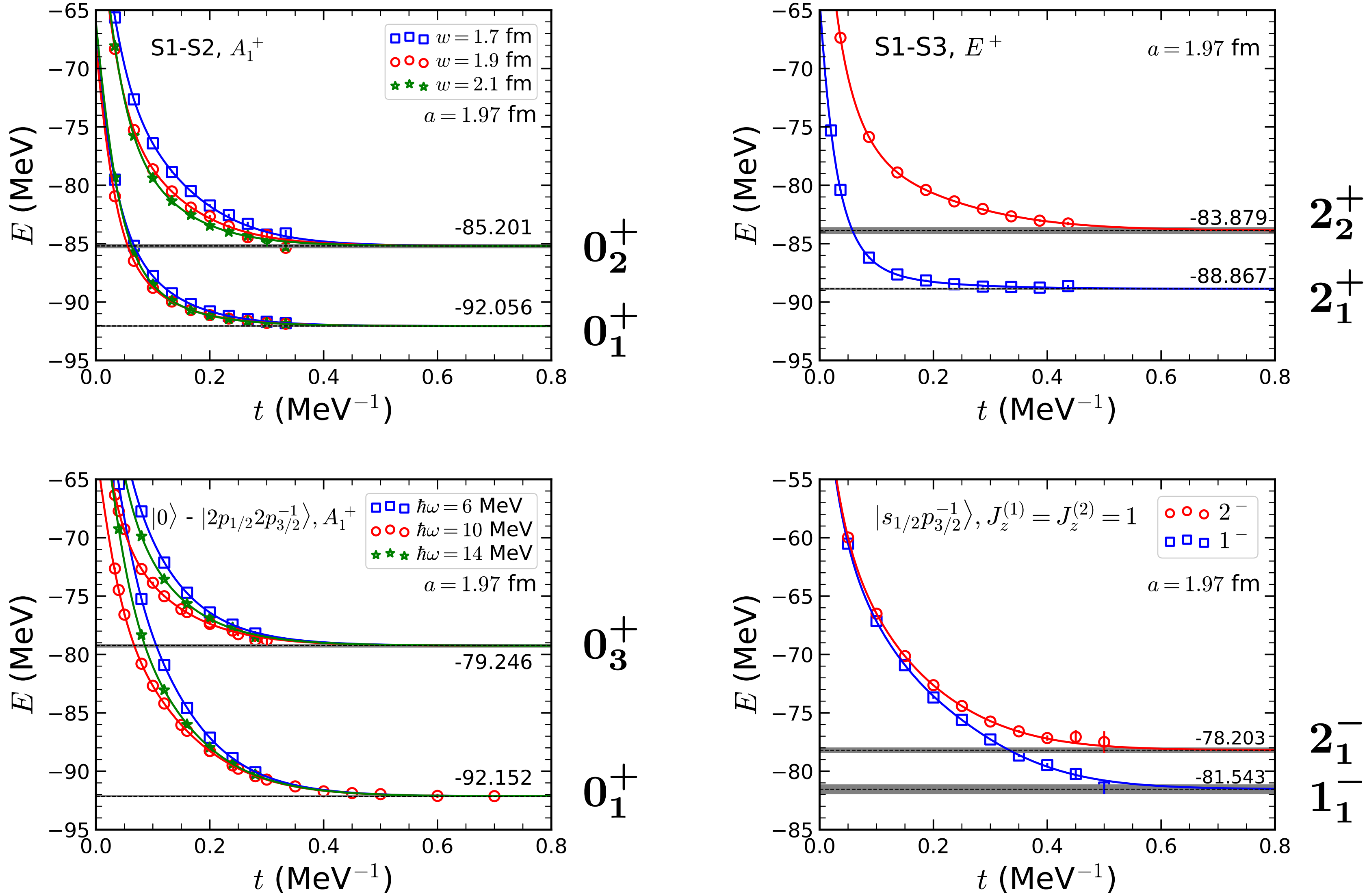
Gaussian wave packets
$w = 1.7 - 2.1$ fm



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

Transient energies

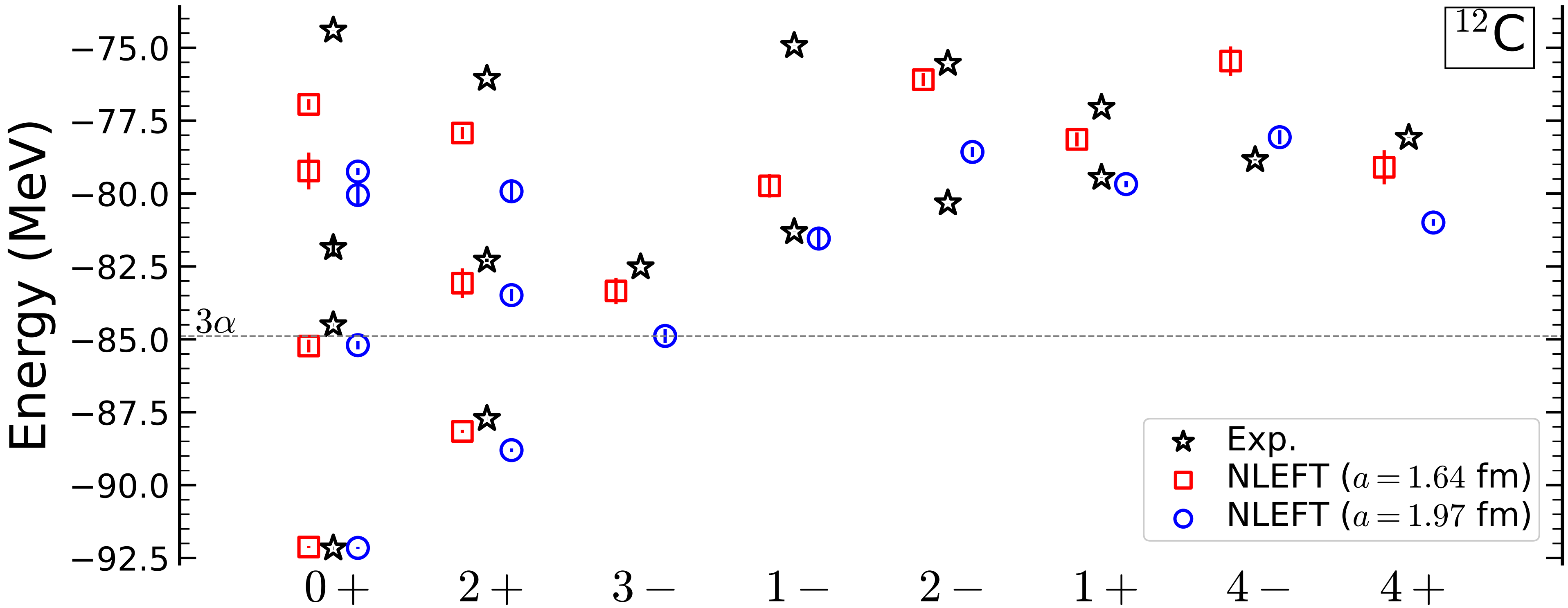
- Transient energies from cluster and shell-model configurations



Spectrum of ^{12}C

Shen, Lähde, Lee, UGM, Eur. Phys.J. A **57** (2021) 276 [arXiv:2106.04834]

- Amazingly precise description $\longrightarrow$ great starting point



Gives all states, other than NCSM

$\longrightarrow$ solidifies earlier NLEFT statements about the structure of the $\mathbf{0_2^+}$ and $\mathbf{2_2^+}$ states

A closer look at the spectrum of ^{12}C

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

- Include also 3NFs: $V = \frac{C_2}{2!}\sum_{\mathbf{n}} \tilde{\rho}(\mathbf{n})^2 + \frac{C_3}{3!}\sum_{\mathbf{n}} \tilde{\rho}(\mathbf{n})^3$

- Fit the four parameters:

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

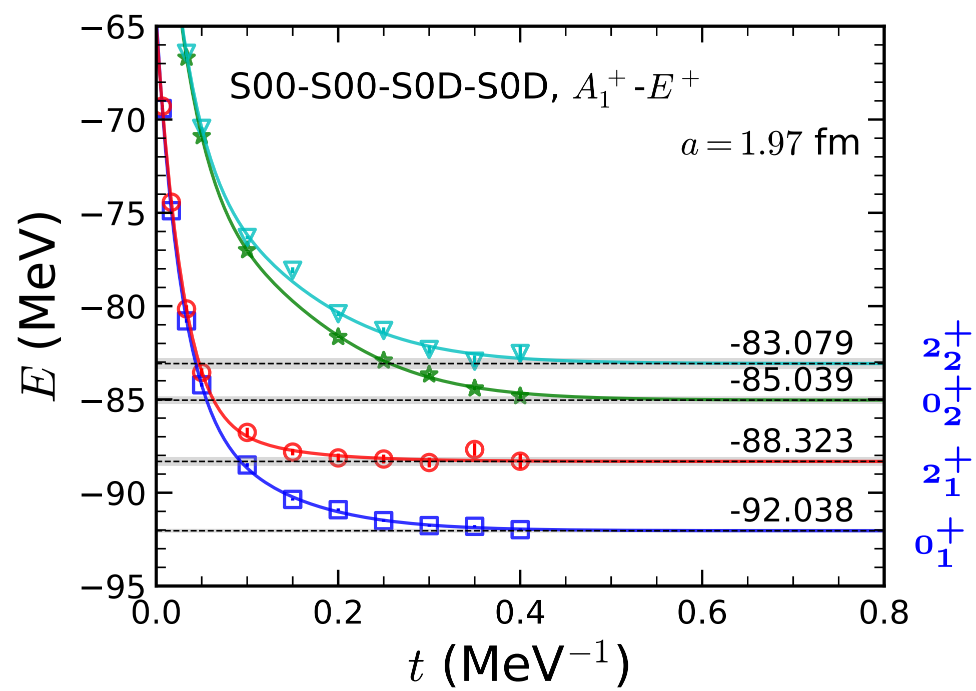
  s_L – radius of ^{12}C around 2.4 fm

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

- Calculation of em transitions

  requires coupled-channel approach

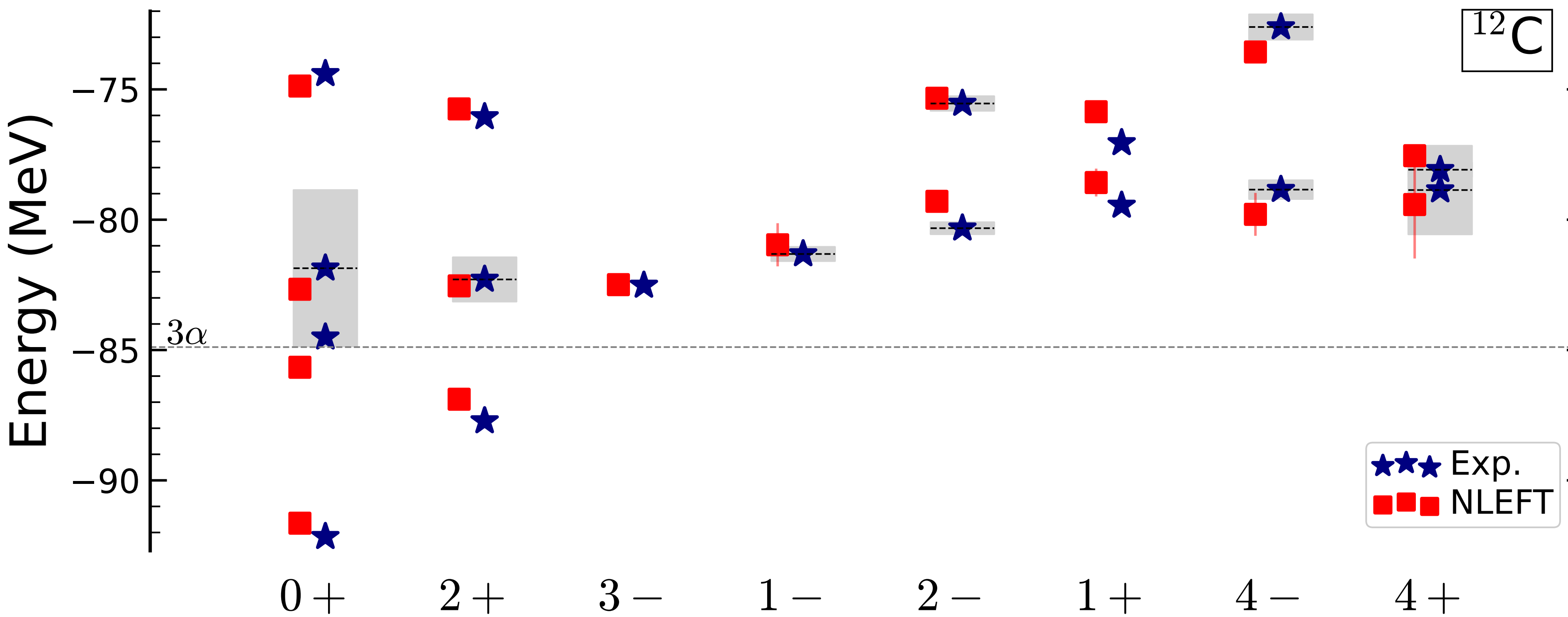
  e.g. 0^+ and 2^+ states



Spectrum of ^{12}C reloaded

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

- Improved description when 3NFs are included, amazingly good



$\rightarrow$ solidifies earlier NLEFT statements about the structure of the $\mathbf{0_2^+}$ and $\mathbf{2_2^+}$ states

Electromagnetic properties

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

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

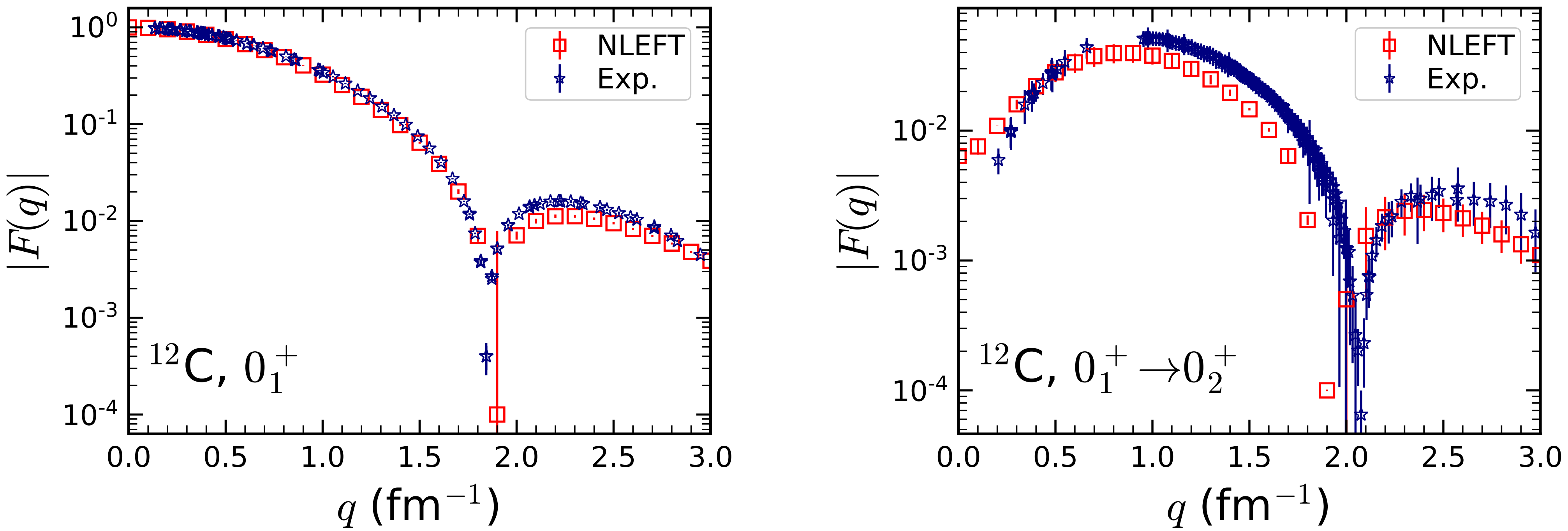
	NLEFT	FMD	α cluster	BEC	RXMC	Exp.
$r_c(0_1^+)$ [fm]	$\mathbf{2.53(1)}$	2.53	2.54	2.53	2.65	$\mathbf{2.47(2)}$
$r(0_2^+)$ [fm]	$\mathbf{3.45(2)}$	3.38	3.71	3.83	4.00	–
$r(0_3^+)$ [fm]	$\mathbf{3.47(1)}$	4.62	4.75	–	4.80	–
$r(2_1^+)$ [fm]	$\mathbf{2.42(1)}$	2.50	2.37	2.38	–	–
$r(2_2^+)$ [fm]	$\mathbf{3.30(1)}$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

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

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

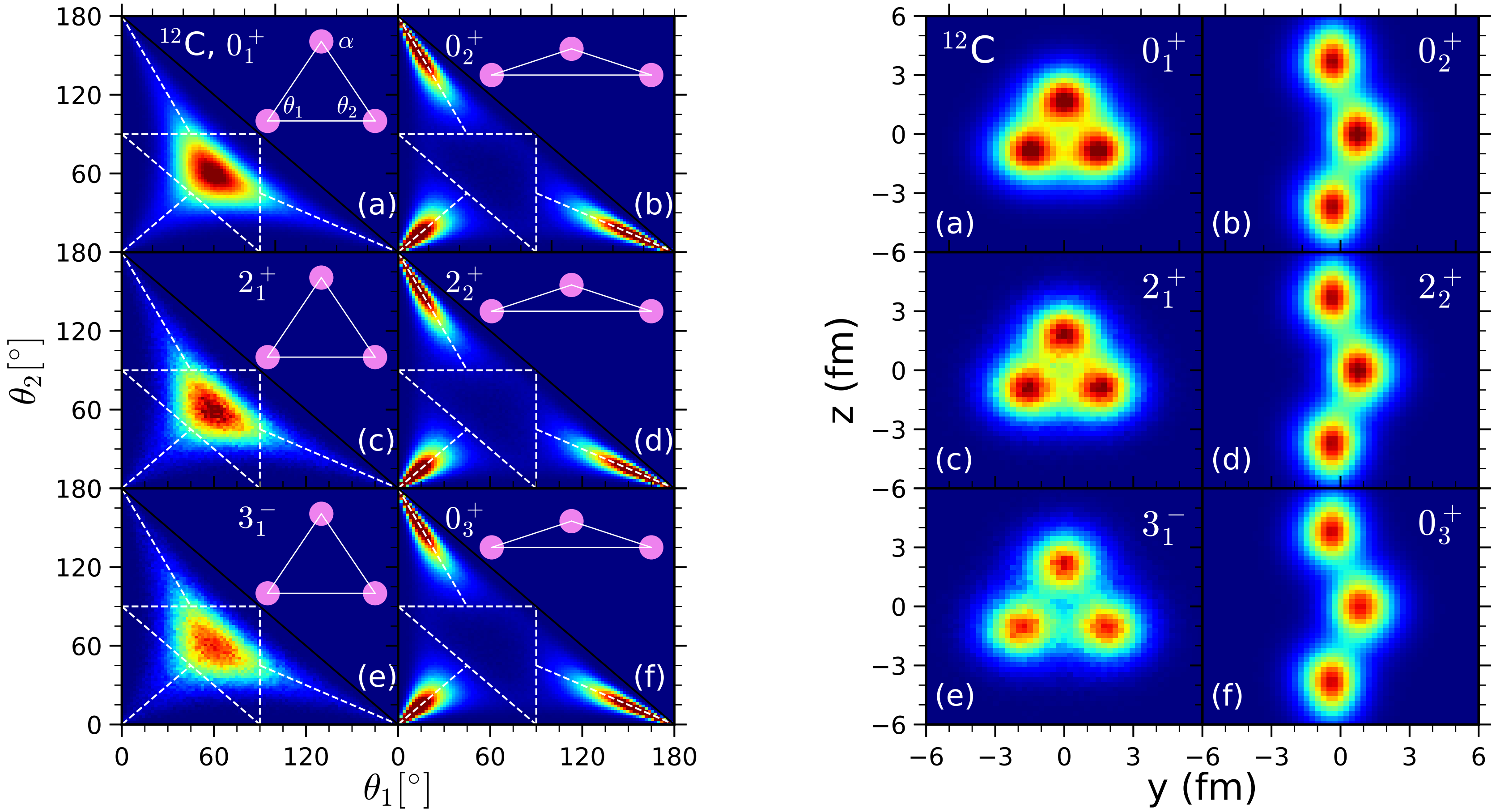


Sick, McCarthy, Nucl. Phys. A 150 (1970) 631
Strehl, Z. Phys. 234 (1970) 416
Crannell et al., Nucl. Phys. A 758 (2005) 399

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

Emergence of geometry

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

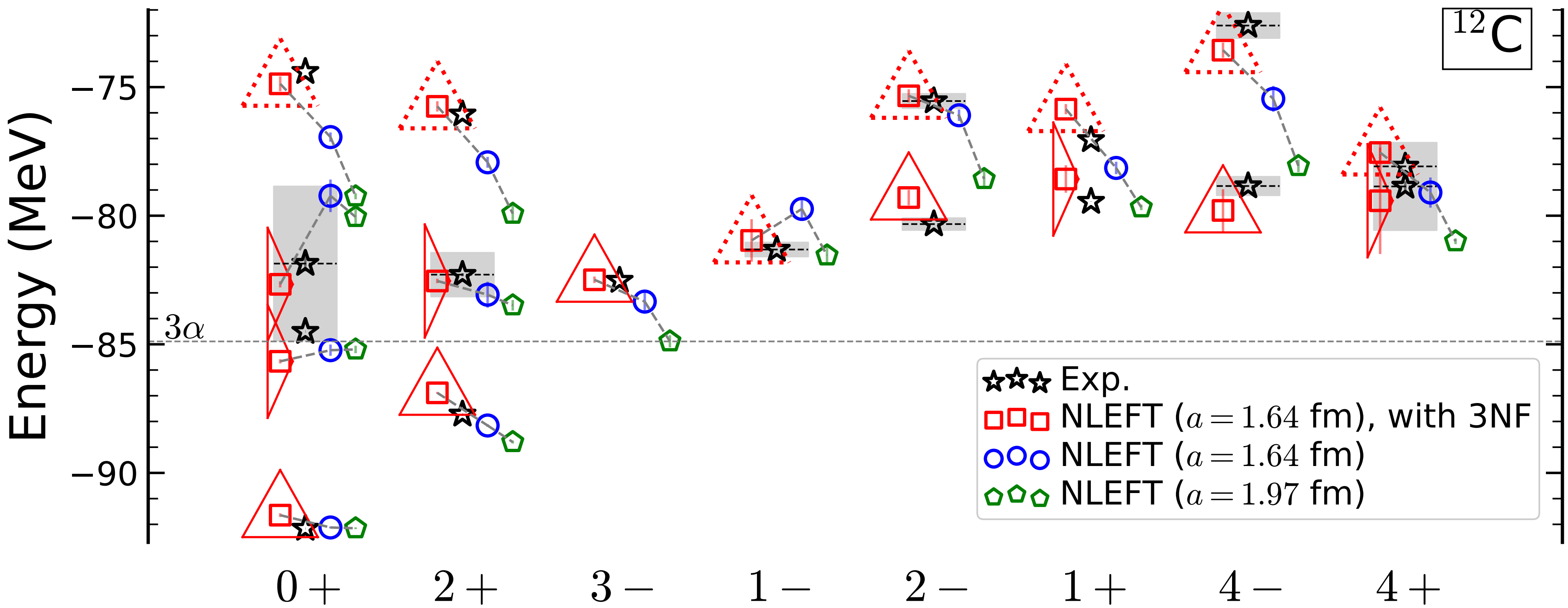


- equilateral & obstuse triangles $\rightarrow$ $\mathbf{2}^+$ states are excitations of the $\mathbf{0}^+$ states

Emergence of duality

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

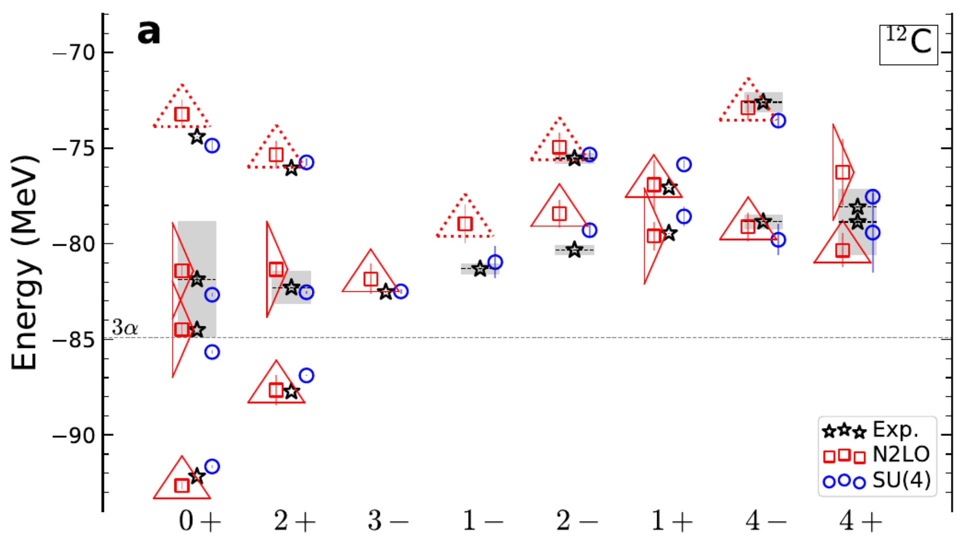
- ^{12}C spectrum shows a cluster/shell-model duality

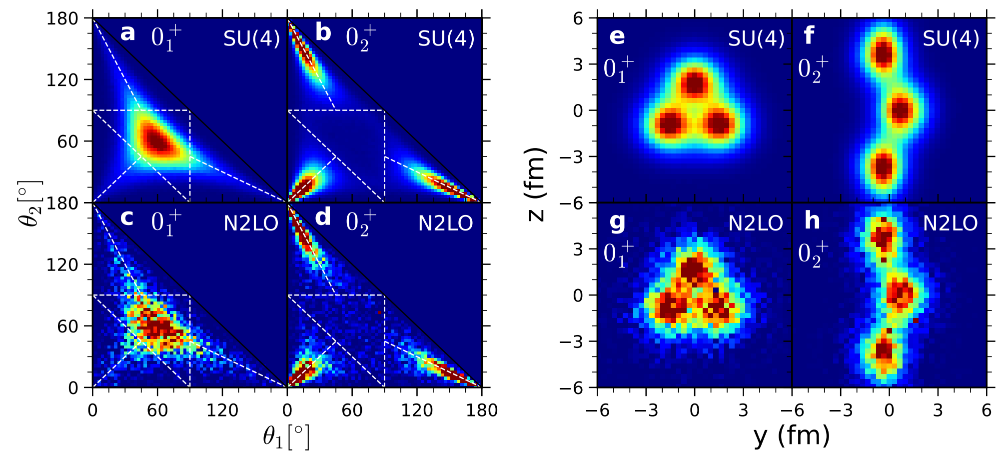


- dashed triangles: strong 1p-1h admixture in the wave function

Sanity check

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





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

Towards heavy nuclei and nuclear matter in NLEFT

Towards heavy nuclei in NLEFT

- Two step procedure:

  1) Further improve the LO action

  $\hookrightarrow$ minimize the sign oscillations

  $\hookrightarrow$ minimize the higher-body forces

  $\hookrightarrow$ gain an understanding of the essentials of nuclear binding

  $\hookrightarrow$ essentially done $\surd$ $\to$ next slide

  2) Work out the corrections to N3LO

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

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

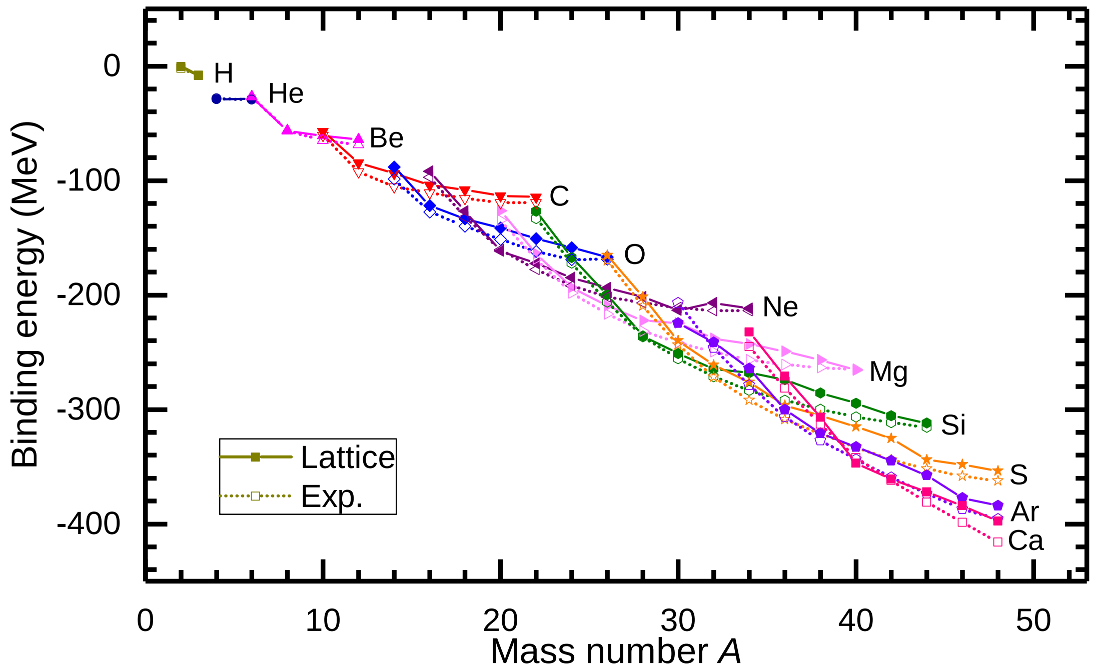
  $\hookrightarrow$ second for the spectra/radii/... of nuclei (first results) $\surd$

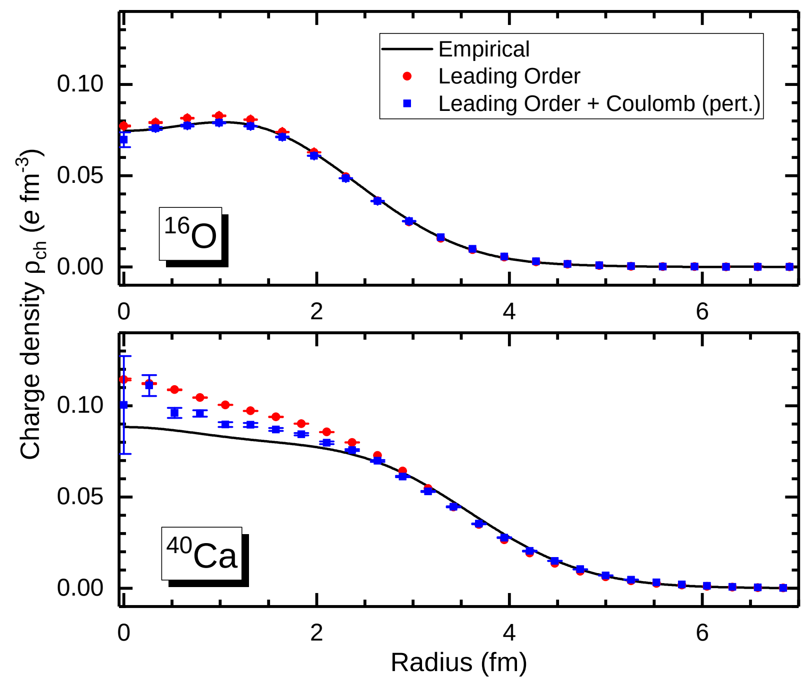
  $\hookrightarrow$ third for nuclear reactions (nuclear astrophysics)

Essential elements of nuclear binding

Lu, Li, Elhatisari, Lee, Epelbaum, UGM, Phys. Lett. B **797** (2019) 134863

- LO smeared SU(4) symmetric action with 2NFs and 3NFs:





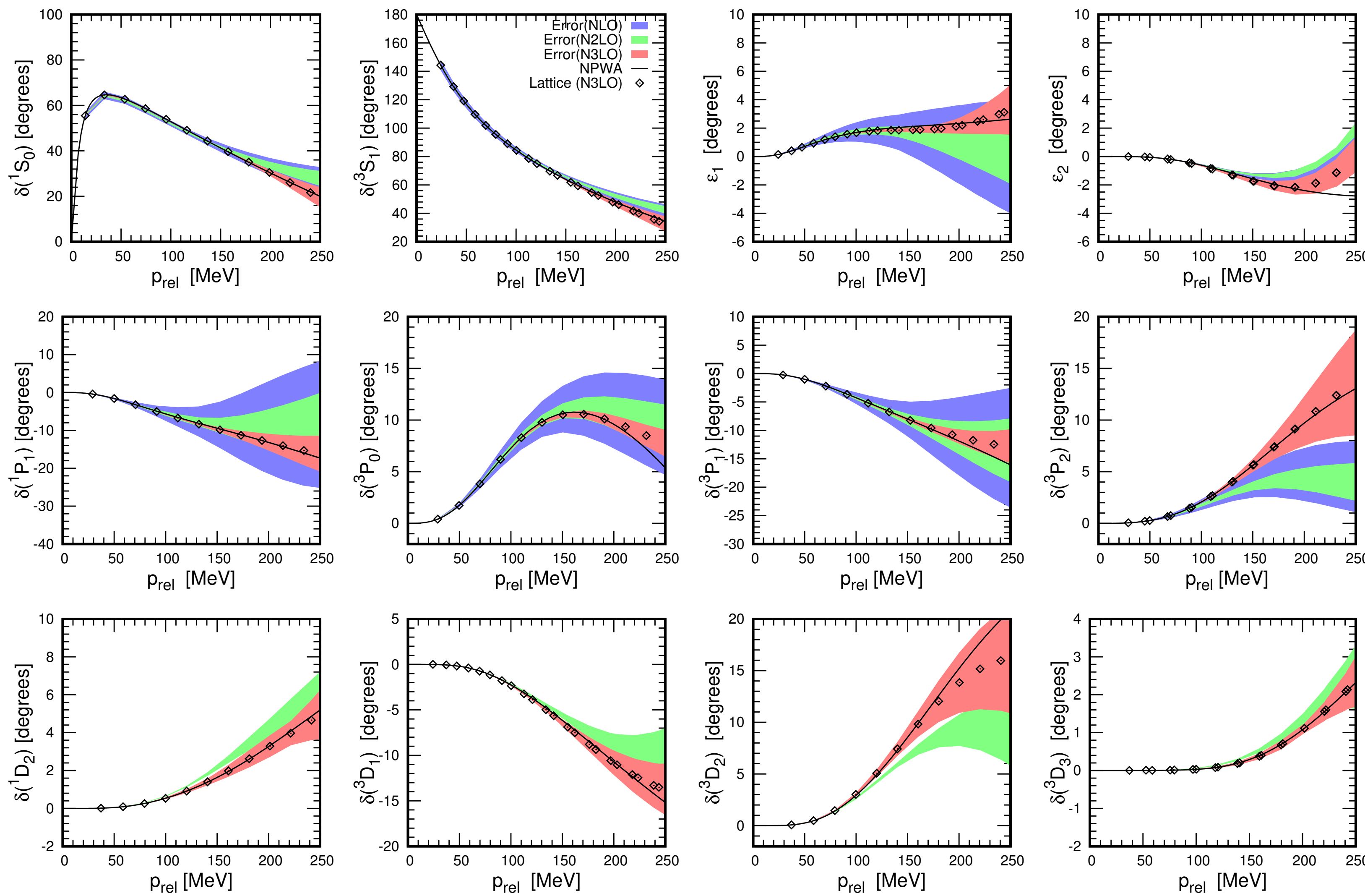
- Masses of 88 nuclei up to $A = 48$, largest deviation about 4%
- Charge radii deviate by at most 5% (expect ^{3}H)
- Neutron matter EoS also consistent w/ other calculations (APR, GCR, ...)

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., [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

$\hookrightarrow$ 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

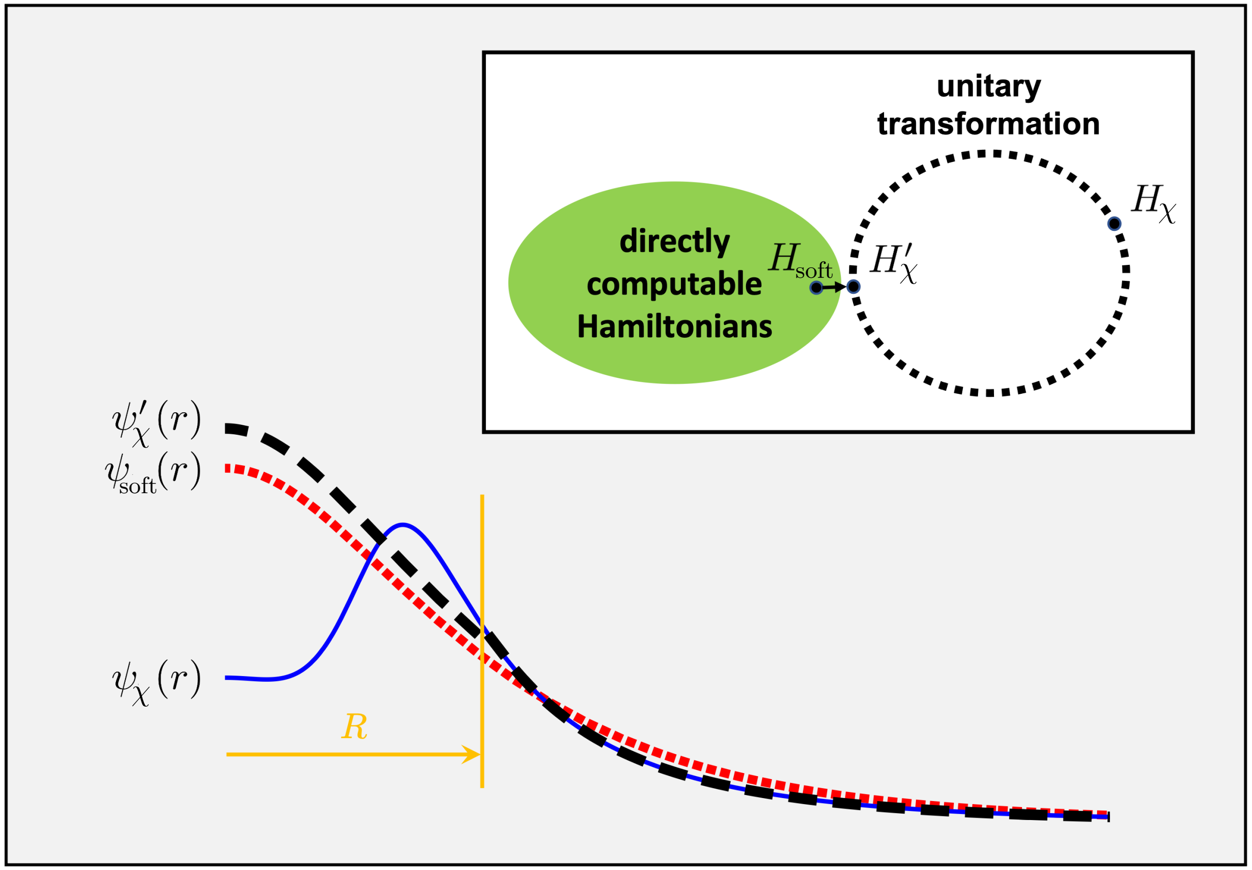
$$|\phi_\chi\rangle = \mathcal{P}\,|\psi^0_\chi\rangle / ||\psi^0_\chi\rangle||$$

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

Wave function matching II

Elhatisari et al., [arXiv:2210.17488 [nucl-th]]

- Graphical representation of w.f. matching



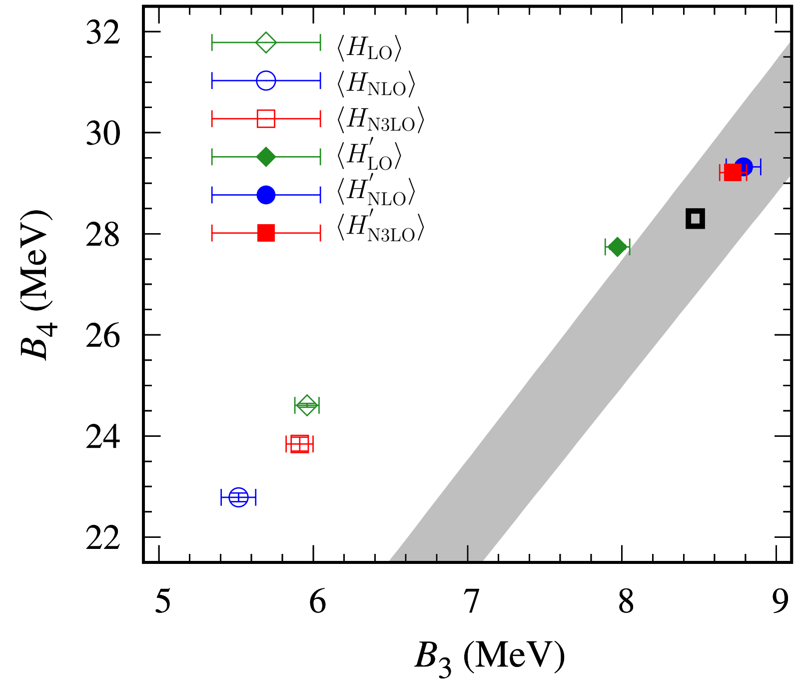
- W.F. matching is a “Hamiltonian translator”:
  eigenenergies from H_1 but w.f. from $H_2 = U^\dagger H_1 U$

Wave function matching III

Elhatisari et al., [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
$\langle\psi^0_{\rm soft}\vert\, H_{\chi,{\rm d}}\,\vert\psi^0_{\rm soft}\rangle$	0.45	0.62	
$\langle\psi^0_{\rm soft}\vert\, H'_{\chi,{\rm d}}\,\vert\psi^0_{\rm soft}\rangle$	1.65	2.01	
$\langle\psi^0_{\rm soft}\vert\, H_{\chi,{\rm t}}\,\vert\psi^0_{\rm soft}\rangle$	5.96(8)	5.91(9)	8.48
$\langle\psi^0_{\rm soft}\vert\, H'_{\chi,{\rm t}}\,\vert\psi^0_{\rm soft}\rangle$	7.97(8)	8.72(9)	
$\langle\psi^0_{\rm soft}\vert\, H_{\chi,\alpha}\,\vert\psi^0_{\rm soft}\rangle$	24.61(4)	23.84(14)	28.30
$\langle\psi^0_{\rm soft}\vert\, H'_{\chi,\alpha}\,\vert\psi^0_{\rm soft}\rangle$	27.74(4)	29.21(14)	



- reasonable accuracy for the light nuclei

- Tjon-band recovered with H'_χ

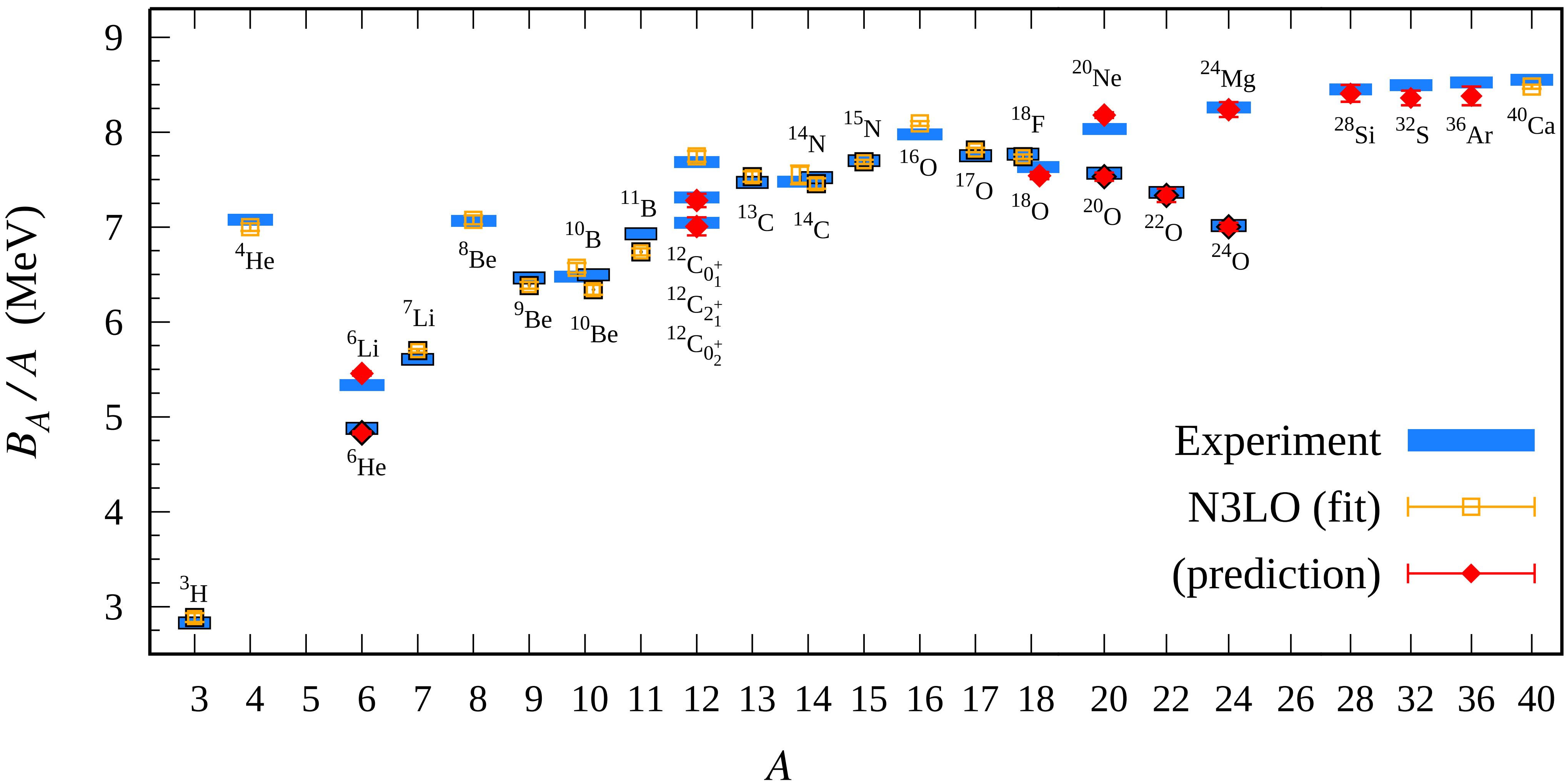
  Platter, Hammer, UGM, Phys. Lett. B **607** (2005) 254

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

Nuclei at N3LO

- Binding energies of nuclei for $a = 1.32$ fm ($p_{\max} = 470$ MeV)

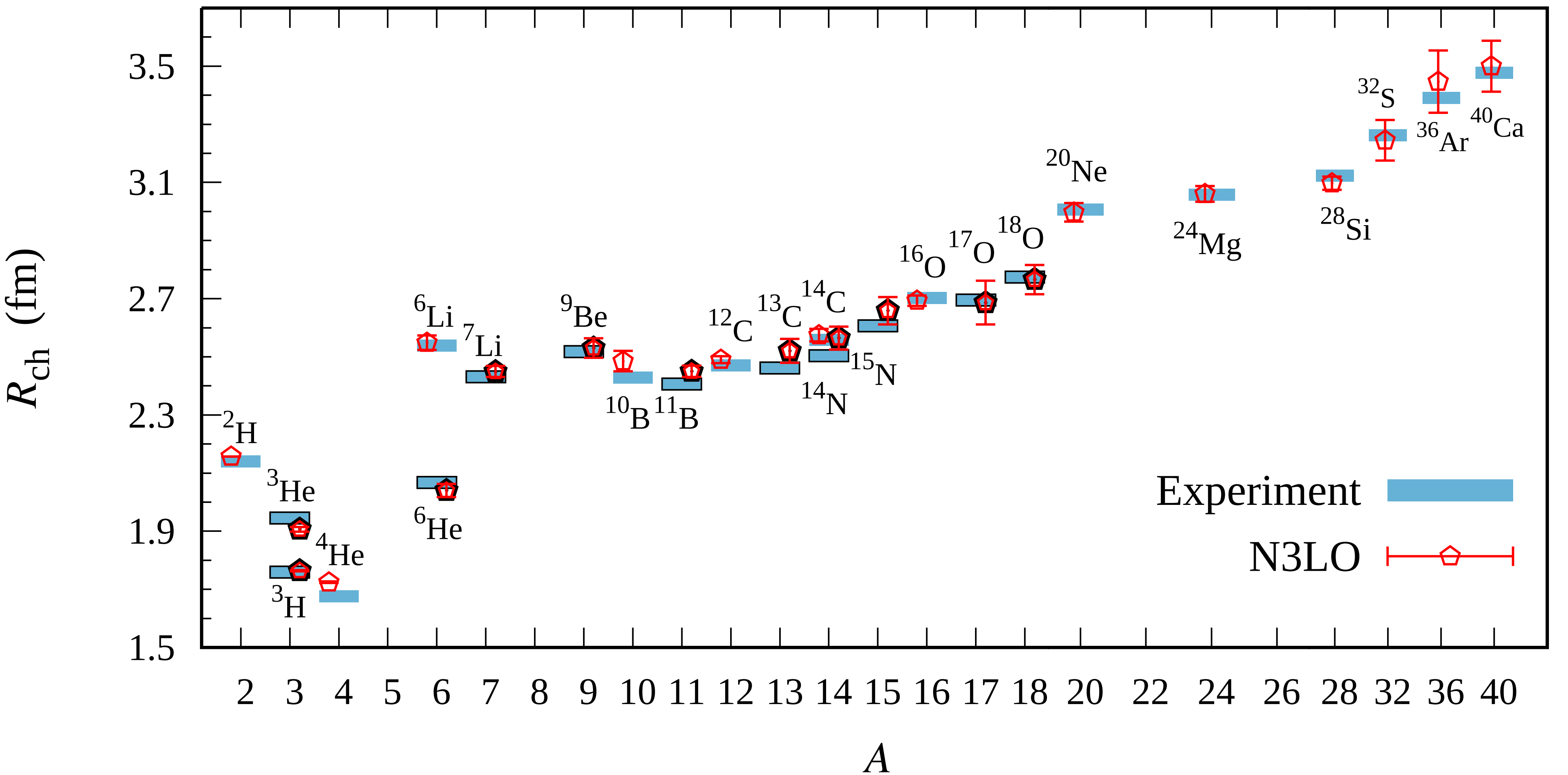
$\rightarrow$ systematic errors via history matching Elhatisari et al., [arXiv:2210.17488 [nucl-th]]



Charge radii at N3LO

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

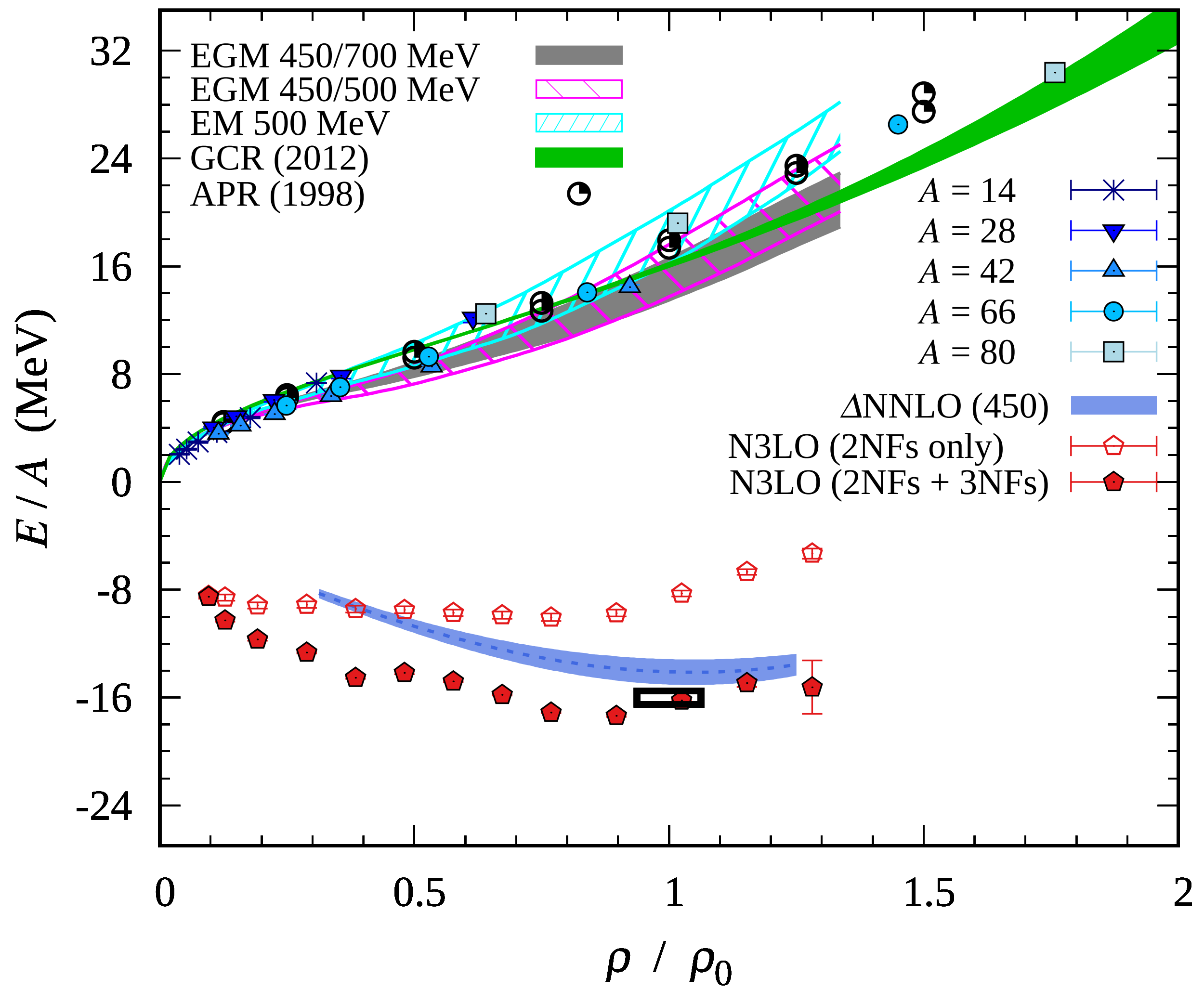
Elhatisari et al., [arXiv:2210.17488 [nucl-th]]



Neutron & nuclear matter at N3LO

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

Elhatisari et al., [arXiv:2210.17488 [nucl-th]]



Sanity check

- One referee asked us to do calculations outside the history matching interval

$\hookrightarrow$ so let us look at ^{50}Cr and ^{58}Ni:

Nucleus	$E_{\rm N3LO}$ [MeV]	$E_{\rm exp}$ [MeV]	$R_{\rm N3LO}$ [fm]	$R_{\rm exp}$ [fm]
^{50}Cr	$-425.32(943)$	-435.05	$3.6469(229)$	3.6588
^{58}Ni	$-493.13(661)$	-506.46	$3.7754(202)$	3.7752

$\hookrightarrow$ Energies within 2-3%, uncertainties on the 1-2% level

$\hookrightarrow$ Radii smack on, uncertainties can be improved

$\hookrightarrow$ Test passed $\surd$

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
  - $\rightarrow$ hidden spin-isospin exchange symmetry — Lee et al., PRL **127** (2021) 062501
    - $\hookrightarrow$ optimal cut-off $\Lambda \simeq 500$ MeV, validates Weinberg counting
  - $\rightarrow$ Wigner SU(4) symmetry in nuclear structure
    - $\hookrightarrow$ emergence of geometry and duality in the ^{12}C spectrum

- Towards heavier nuclei & higher precision
  - $\rightarrow$ highly improved LO action based on SU(4)
  - $\rightarrow$ NN interaction at N3LO, first promosing results for nuclei at N3LO
    - $\hookrightarrow$ requires the new wave function matching technique

- Ab initio nuclear thermodynamics — Lu et al., PRL **125** (2020) 192502
  - $\rightarrow$ partition function via the pinhole trace algorithm
    - $\hookrightarrow$ first promising results for the phase diagram of nuclear matter at finite temperature
    - $\hookrightarrow$ prediction of the vapor-liquid phase transition within reasonable accuracy

Summary & outlook

- Strangeness nuclear physics
  - $\rightarrow$ treat hyperons as impurities, ILMC algorithm — Bour et al., PRL **115** (2015) 185301
  - $\hookrightarrow$ first exploratory study, $t_{\rm CPU} \sim A$ — Frame et al., Eur. Phys. J. A **56** (2020) 248
  - $\hookrightarrow$ developed the two-impurity formalism — Hildenbrand et al., Eur. Phys. J. A **58** (2022) 167
  - $\hookrightarrow$ hypernuclear landscape up to $A = 20$ in the works

- Studies of the oxygen and calcium isotopic chains
  - $\rightarrow$ first results for oxygen from $A = 16$ to $A = 26$ $\surd$
  - $\hookrightarrow$ calcium isotopes from $A = 40$ to $A = 72$
  - $\hookrightarrow$ driplines, proton and neutron density distributions

- Studies of alpha cluster states
  - $\rightarrow$ detailed studies of the four α-clusters in ^{16}O
  - $\hookrightarrow$ compute the spectrum & possible em transitions
  - $\hookrightarrow$ map out all geometries of the cluster states, duality?

- and . . .

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

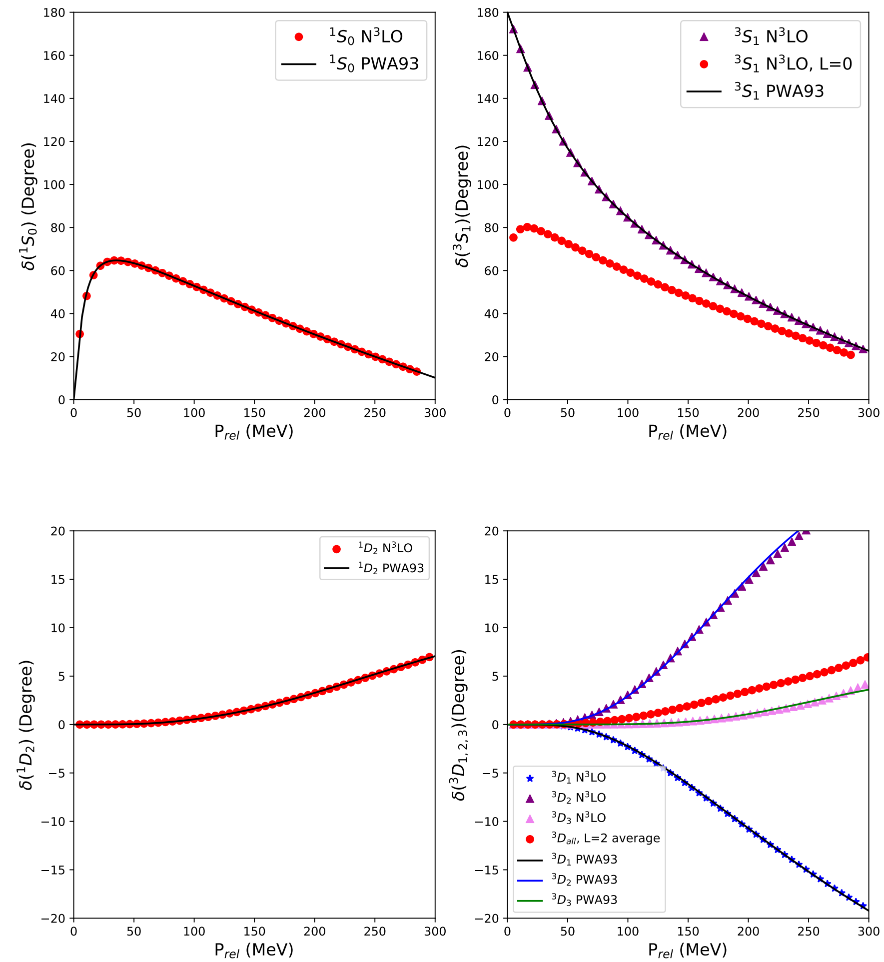
  $\hookrightarrow \Lambda = \pi/a = 470$ MeV

- 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

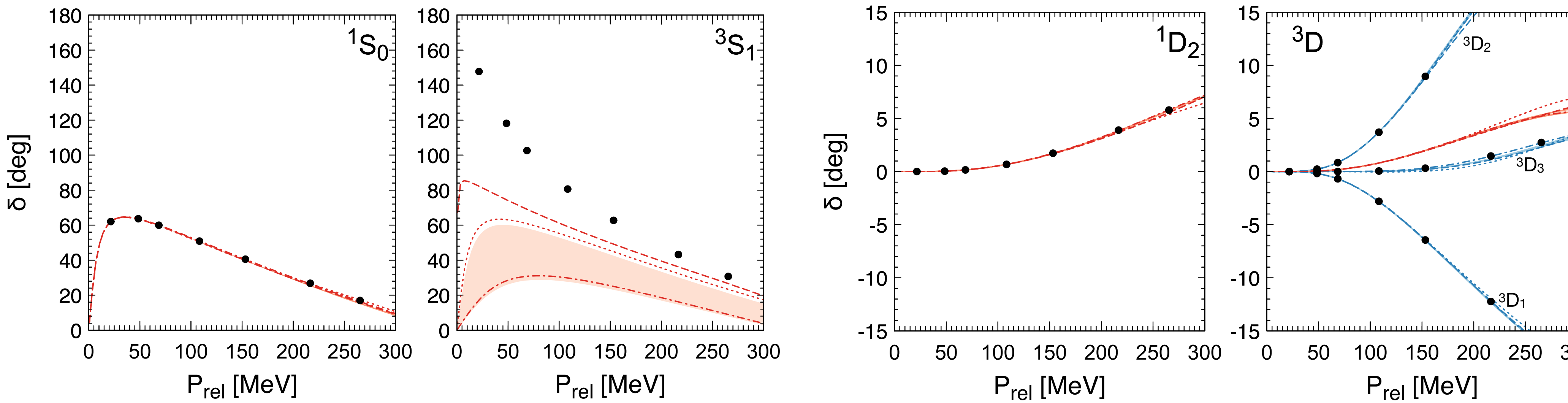
ch., order	LEC (l.u.)	ch., order	LEC (l.u.)
${}^1\mathrm{S}_0, Q^0$	1.45(5)	${}^3\mathrm{S}_1, Q^0$	1.56(3)
${}^1\mathrm{S}_0, Q^2$	−0.47(3)	${}^3\mathrm{S}_1, Q^2$	−0.53(1)
${}^1\mathrm{S}_0, Q^4$	0.13(1)	${}^3\mathrm{S}_1, Q^4$	0.12(1)
${}^1\mathrm{D}_2, Q^4$	−0.088(1)	${}^3\mathrm{D}_{\mathrm{all}},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

$\Rightarrow$ works pretty well



Nucleon-nucleon phase shifts – continuum

- Consider various (chiral) continuum potentials $\rightarrow$ 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

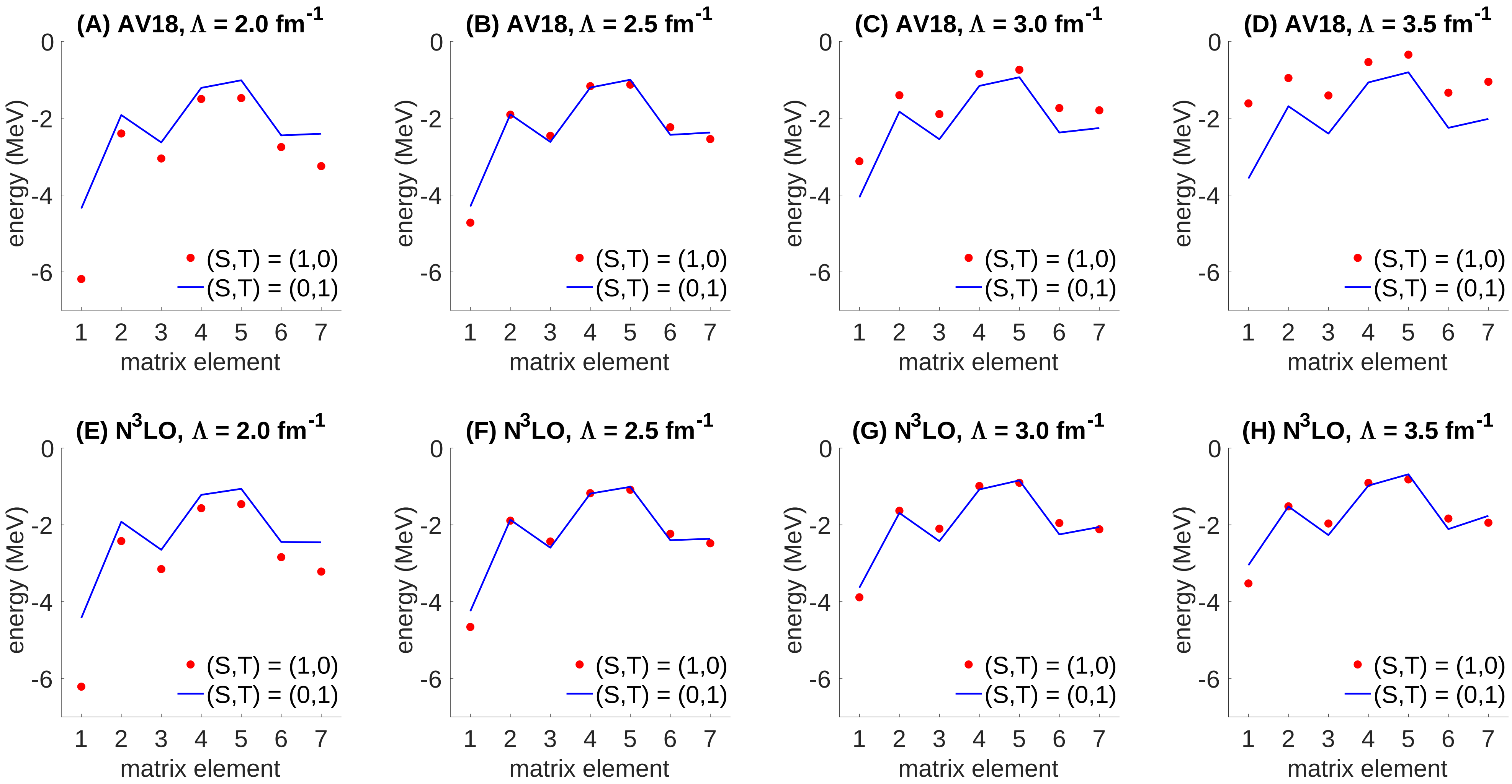
ME 7 corresponds to the $1s_{1/2}$ orbitals discussed before

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

→ 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 $\Lambda < \Lambda_{\mathrm{large}-N_c}$, the $(S,T) = (1,0)$ channel is more attractive
  - For $\Lambda > \Lambda_{\mathrm{large}-N_c}$, 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:

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

- 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

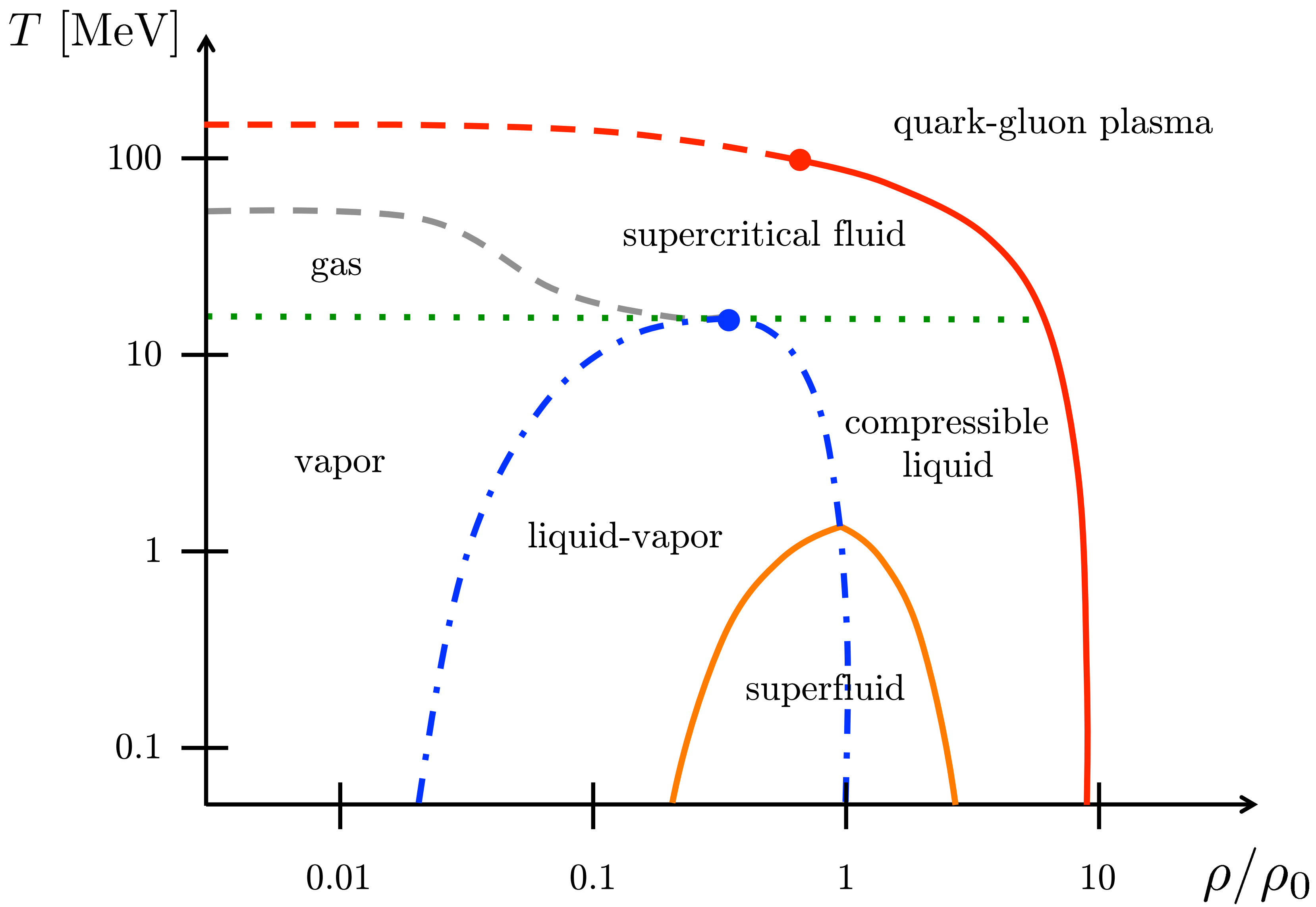
Ab Initio Nuclear Thermodynamics

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

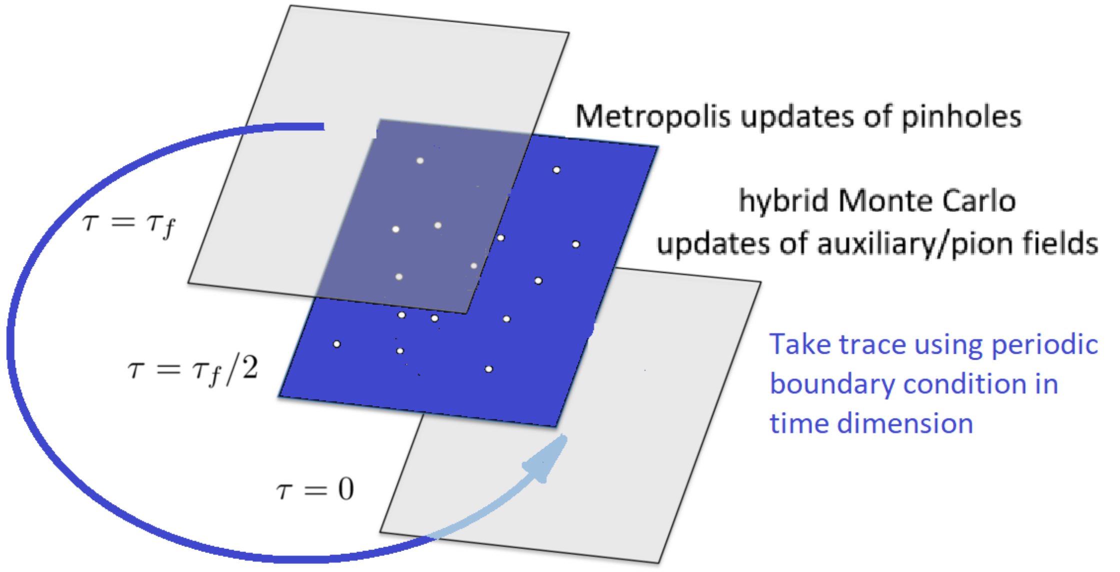
Fig. courtesy B.-N. Lu



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

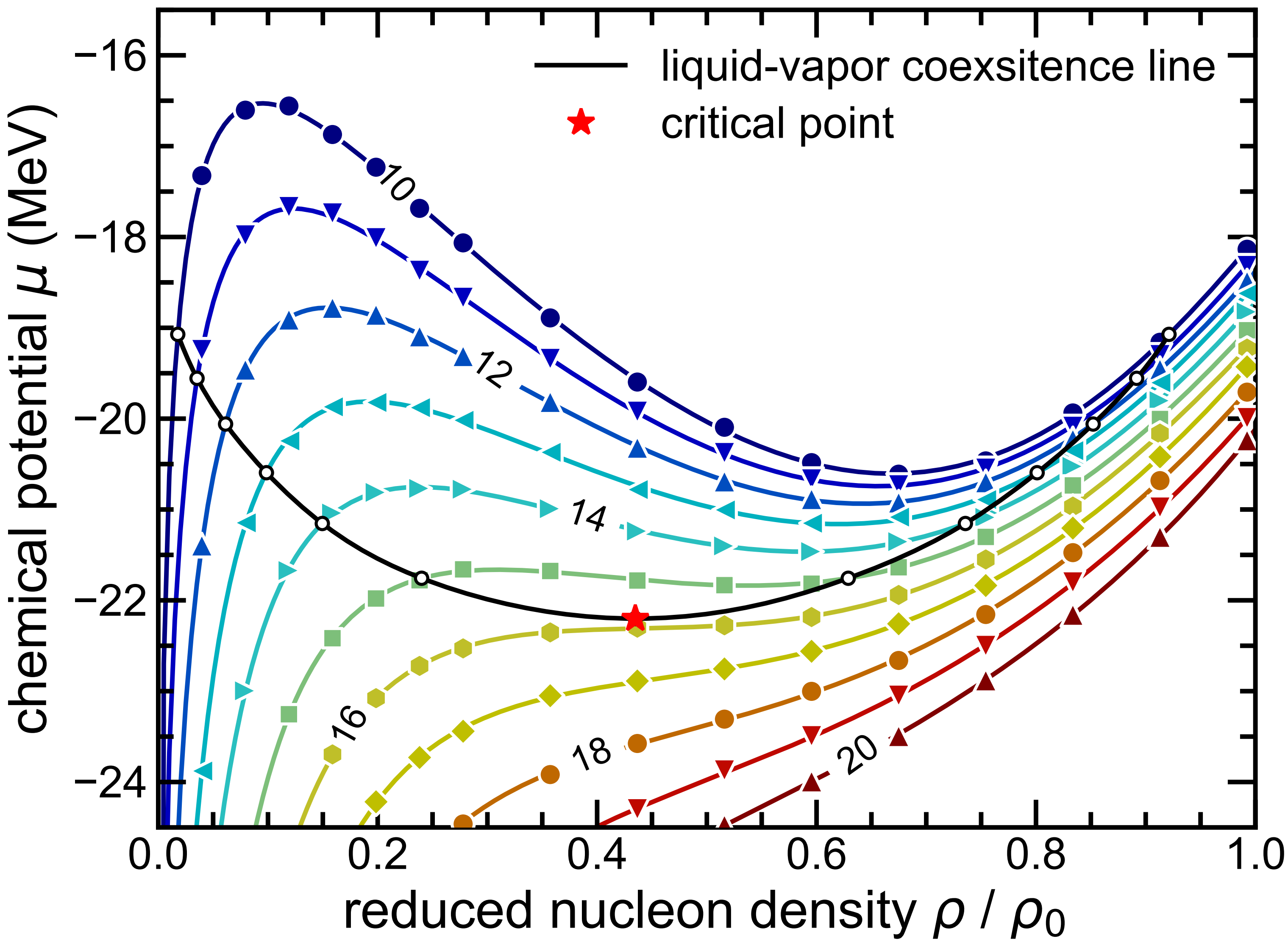
consider $T = 10 \ldots 20$ MeV

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

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

Chemical potential

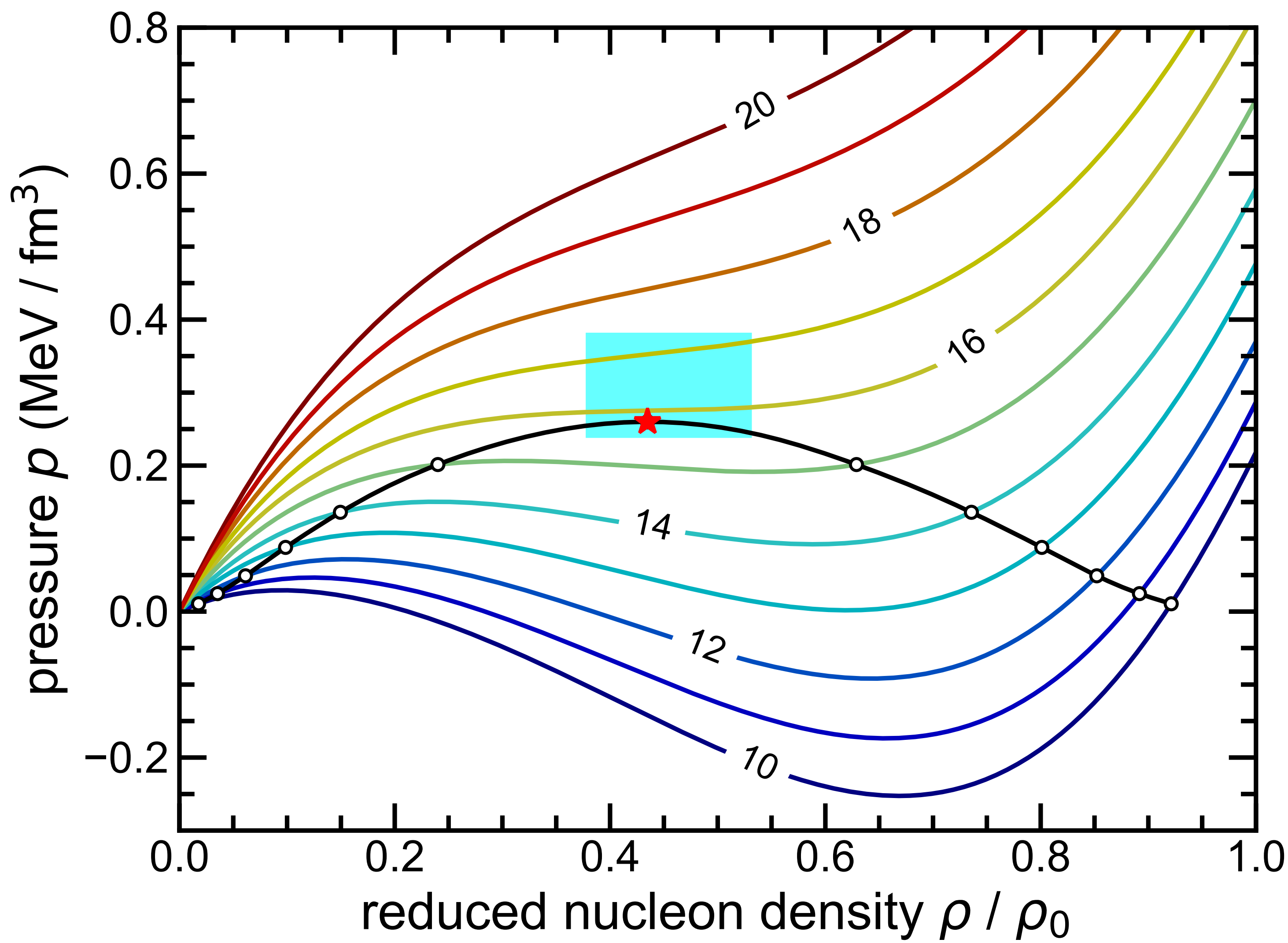
- Calculated from the free energy: $\mu = (F(N+1) - F(N-1))/2$



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}

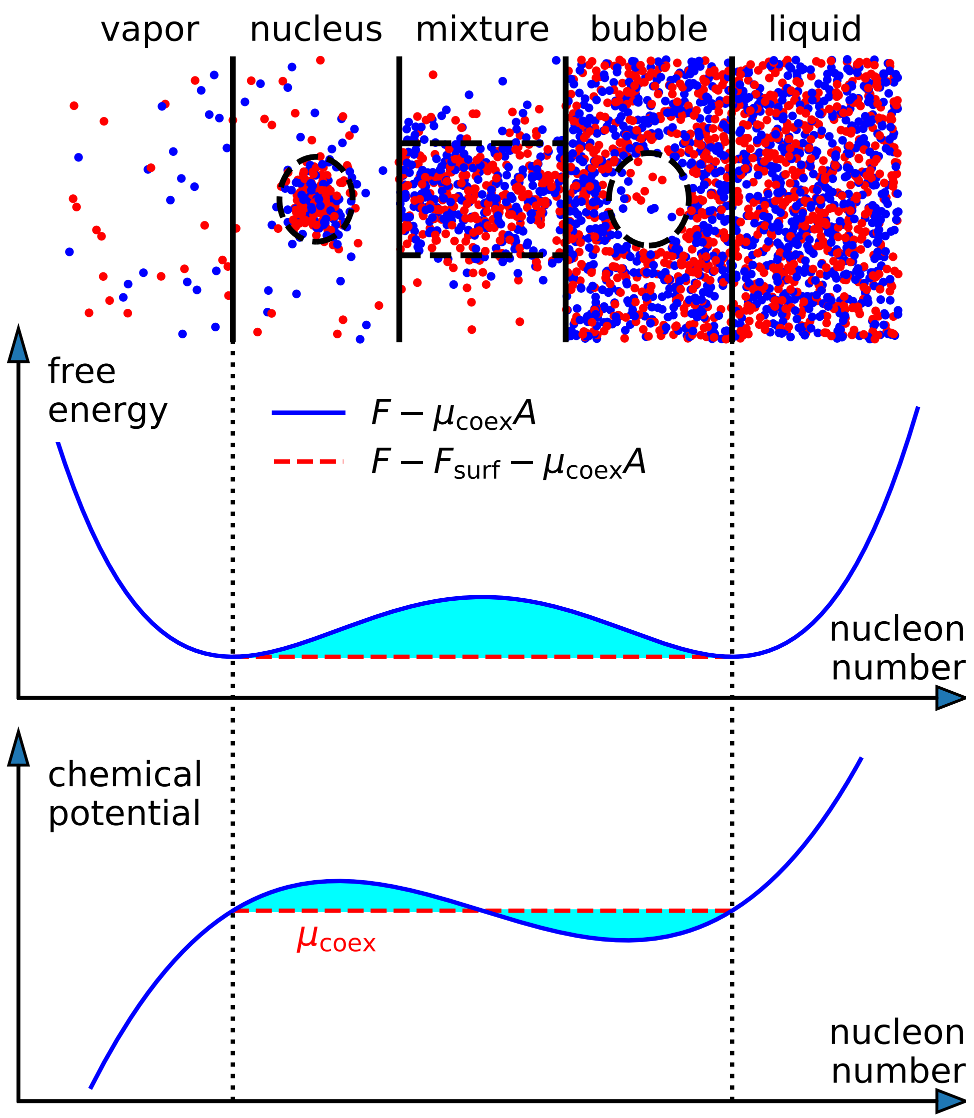
Vapor-liquid phase transition

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

- the most probable configuration
  for different nucleon number A

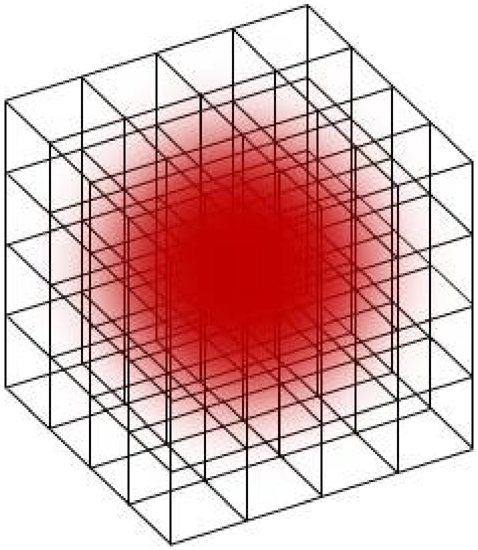
- the free energy

- 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

$\rightarrow$ density distributions of nucleons can not be computed directly, only moments

$\rightarrow$ need to overcome this deficieny

PINHOLE ALGORITHM

- Solution to the CM-problem:

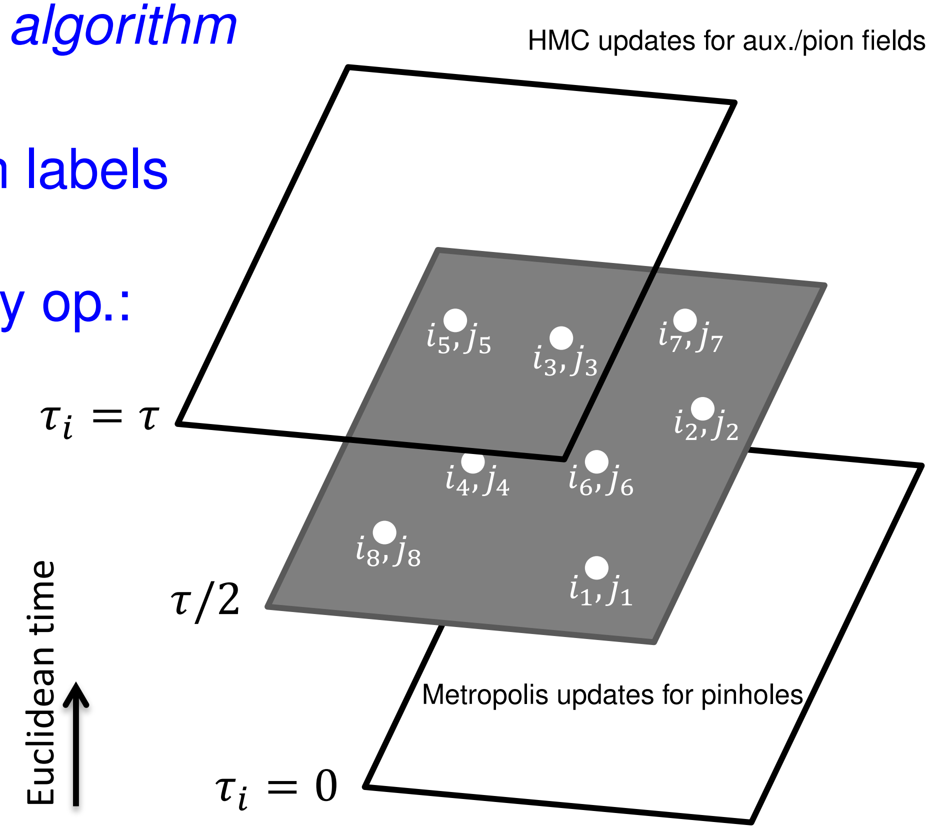
  track the individual nucleons using the *pinhole algorithm*

- 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.:

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

- MC sampling of the amplitude:

$$A_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\ldots,\mathbf{n}_A,L_t) = \langle\Psi_A(\tau/2)|\rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\ldots,\mathbf{n}_A)|\Psi_A(\tau/2)\rangle$$



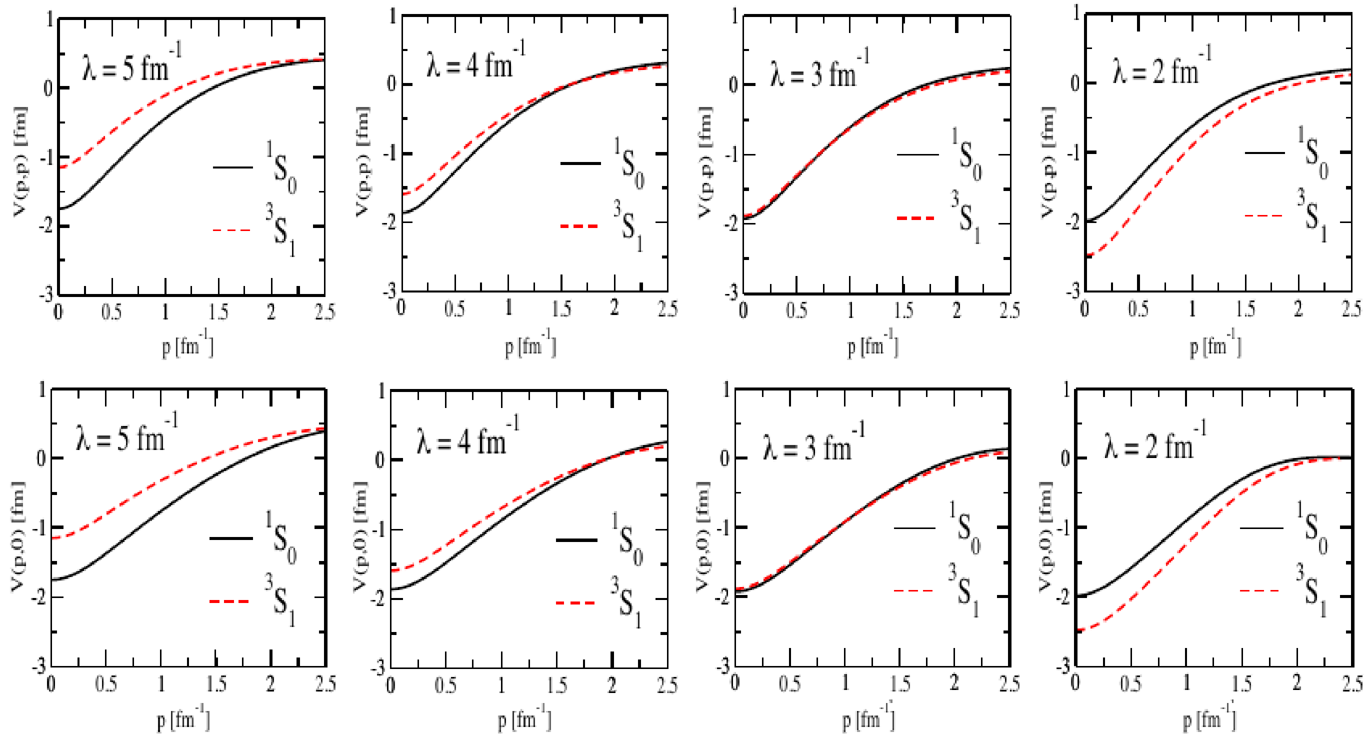
- Allows to measure proton and neutron distributions

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

Similarity renormalization group studies

Timoteo, Szpigel, Ruiz Arriola, Phys. Rev. C **86** (2012) 034002

- Investigation of Wigner SU(4) symmetry using the SRG, use AV18:



- At the scale $\lambda_{\rm Wigner} \simeq 3\,{\rm fm}^{-1}$ one has $V_{^1S_0,{\rm Wigner}}(p',p) \approx V_{^3S_1,{\rm Wigner}}(p',p)$