Recent Developments in Nuclear Lattice EFT

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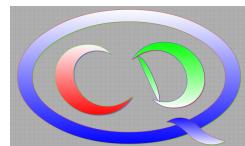
CONTENTS

- Chiral EFT on a lattice

- The hidden spin-isospin exchange symmetry

- Wigner SU(4) symmetry and the emergence of duality

- Towards heavy nuclei in NLEFT

- *Ab initio* nuclear thermodynamics

- Summary & outlook

Chiral EFT on a lattice

T. Lähde & UGM

Nuclear Lattice Effective Field Theory - An Introduction

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

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

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

• typical lattice parameters

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

p

n

p

n

a
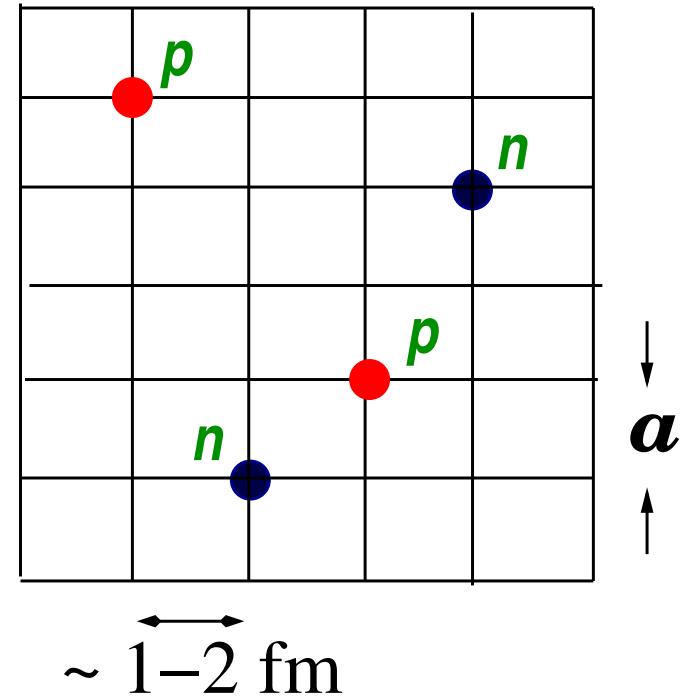
$\sim \overleftrightarrow{1-2} \, \text{fm}$

• 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

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

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

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

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

$$\lim_{\tau \to \infty} \frac{Z_A^{\mathcal{O}}(\tau)}{Z_A(\tau)} = \langle \Psi_A | \mathcal{O} | \Psi_A \rangle$$
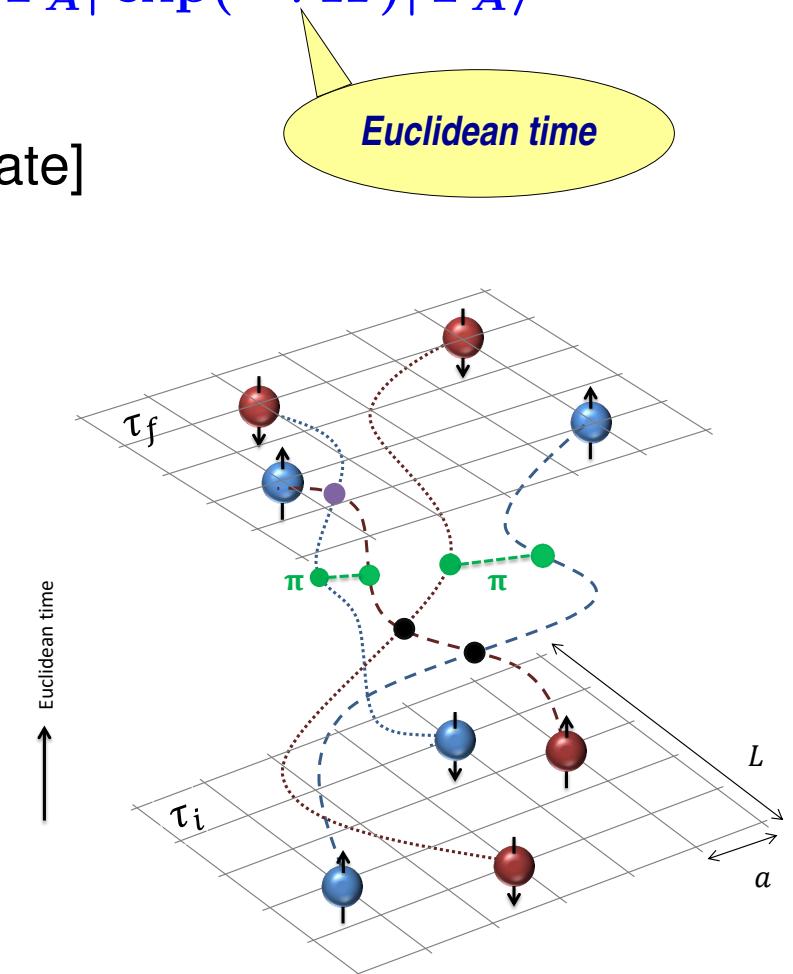
Configurations
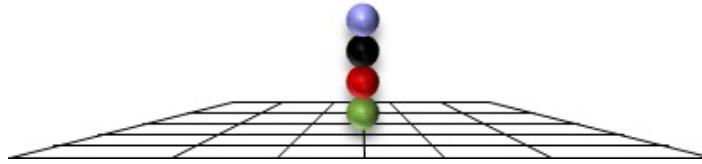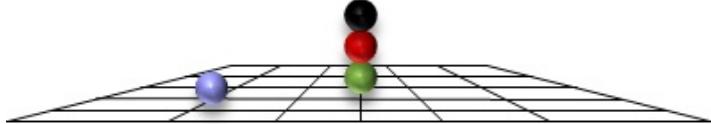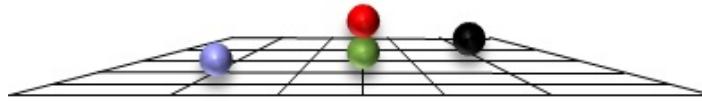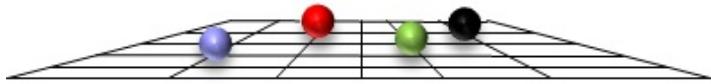
⇒ all *possible* configurations are sampled

⇒ preparation of *all possible* initial/final states

⇒ *clustering* emerges *naturally*

Auxiliary field method

- Represent interactions by auxiliary fields:

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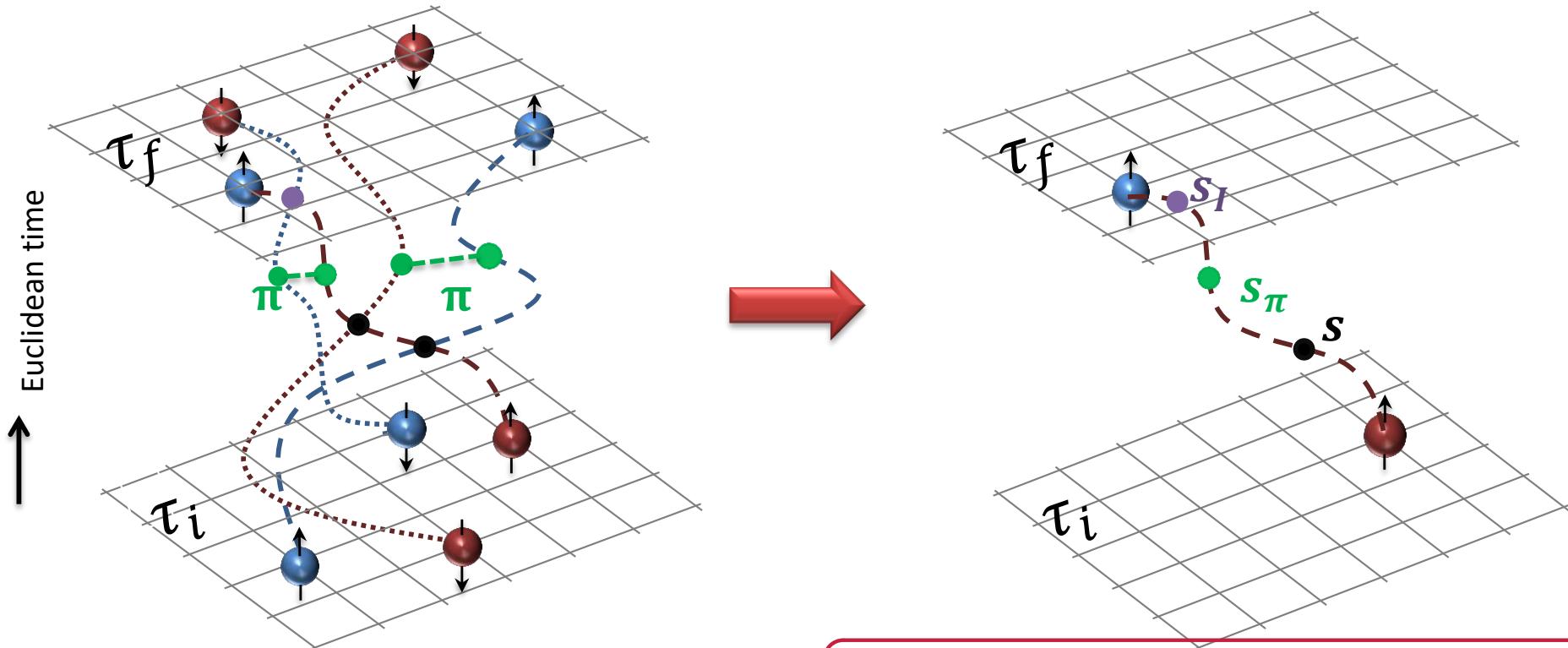
optimally suited for parallel computing!

Computational equipment

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

87 Pflops

– Ulf-G. Meißner, NLEFT: Status and Perspectives – talk, LENPIC meeting, RUB, Aug. 24, 2022 –

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

Accessible by Lattice QCD

Accessible by Lattice EFT

• similar methods:

   hybrid MC, parallel computing, . . .
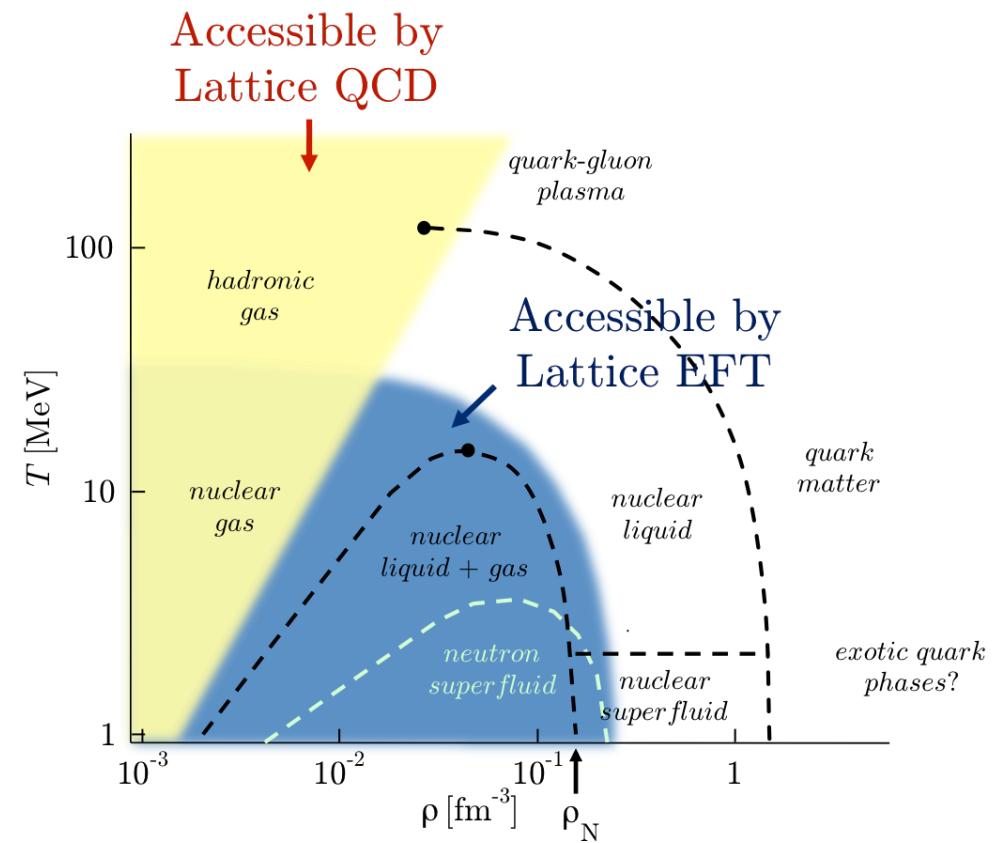
The hidden spin-isospin exchange symmetry

Nucleon-nucleon interaction in large-N_C

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

● General form of the non-relativistic NN potential:

$$V_{\mathrm{NN}} = V_C + V_S\,\vec{\sigma}_1\cdot\vec{\sigma}_2 + V_{LS}\,\vec{L}\cdot\vec{S} + V_T\,S_{12} + V_Q\,Q_{12}$$
$$+\left(W_C + W_S\,\vec{\sigma}_1\cdot\vec{\sigma}_2 + W_{LS}\,\vec{L}\cdot\vec{S} + W_T\,S_{12} + W_Q\,Q_{12}\right)\vec{\tau}_1\cdot\vec{\tau}_2$$

$$S_{12} = 3\vec{\sigma}_1\cdot\hat{r}\,\vec{\sigma}_2\cdot\hat{r} - \vec{\sigma}_1\cdot\vec{\sigma}_2$$

$$Q_{12} = \tfrac{1}{2}\left\{(\vec{\sigma}_1\cdot\vec{L}),(\vec{\sigma}_2\cdot\vec{L})\right\}$$

● Standard decomposition in central (V_C, W_C), spin (V_S, W_S), tensor (V_T, W_T), spin-orbit (V_{LS}, W_{LS}) and quadratic spin-orbit (V_Q, W_Q) interactions

● Large-N_C analysis: use one-quark operators of the quark model as basis

$$\hat{S}^i = q^\dagger\frac{\sigma^i}{2}q\,,\quad \hat{I}^i = q^\dagger\frac{\tau^a}{2}q\,,\quad \hat{G}^{ia} = q^\dagger\frac{\sigma^i\tau^a}{4}q\,,\quad q = (u,d)$$

Nucleon-nucleon interaction in large-N_C

- Putting pieces together:

Isospin	C	S	LS	T	Q
$V(r)\,1\cdot 1$	N_C	$1/N_C$	$1/N_C$	$1/N_C$	$1/N_C^3$
$W(r)\,\vec{\tau}_1\cdot\vec{\tau}_2$	$1/N_C$	N_C	$1/N_C$	N_C	$1/N_C$

$$V^{\mathrm{2N}}_{\mathrm{large}-N_c} = V_C + W_S\,\vec{\sigma}_1\cdot\vec{\sigma}_2\vec{\tau}_1\cdot\vec{\tau}_2 + W_T\,S_{12}\vec{\tau}_1\cdot\vec{\tau}_2 + \ldots$$

- 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

Short reminder of Wigner SU(4) symmetry

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

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

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

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

$\Rightarrow$ The exact symmetry limit corresponds to a scale invariant non-relativistic system

- $V^{\mathbf{2N}}_{\mathbf{large}-N_c}$ 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 $\checkmark$

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

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

Nucleon-nucleon phase shifts – lattice

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

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

$$\hookrightarrow \Lambda = \pi/a = 470 \,\text{MeV}$$

- 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.)
$^1\mathbf{S_0}, Q^0$	1.45(5)	$^3\mathbf{S_1}, Q^0$	1.56(3)
$^1\mathbf{S_0}, Q^2$	$-0.47(3)$	$^3\mathbf{S_1}, Q^2$	$-0.53(1)$
$^1\mathbf{S_0}, Q^4$	0.13(1)	$^3\mathbf{S_1}, Q^4$	0.12(1)
$^1\mathbf{D_2}, Q^4$	$-0.088(1)$	$^3\mathbf{D_{all}}, Q^4$	$-0.070(2)$

$\Rightarrow$ works pretty well
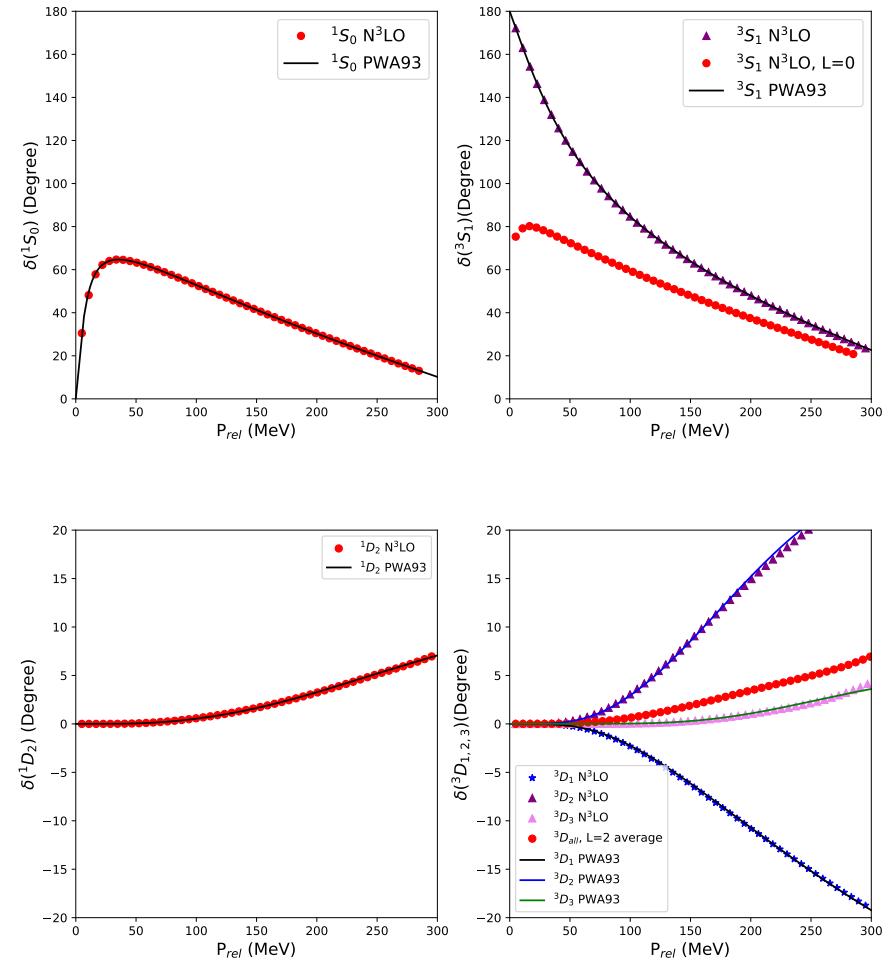
Nucleon-nucleon phase shifts – continuum

● Consider various (chiral) continuum potentials → also works √
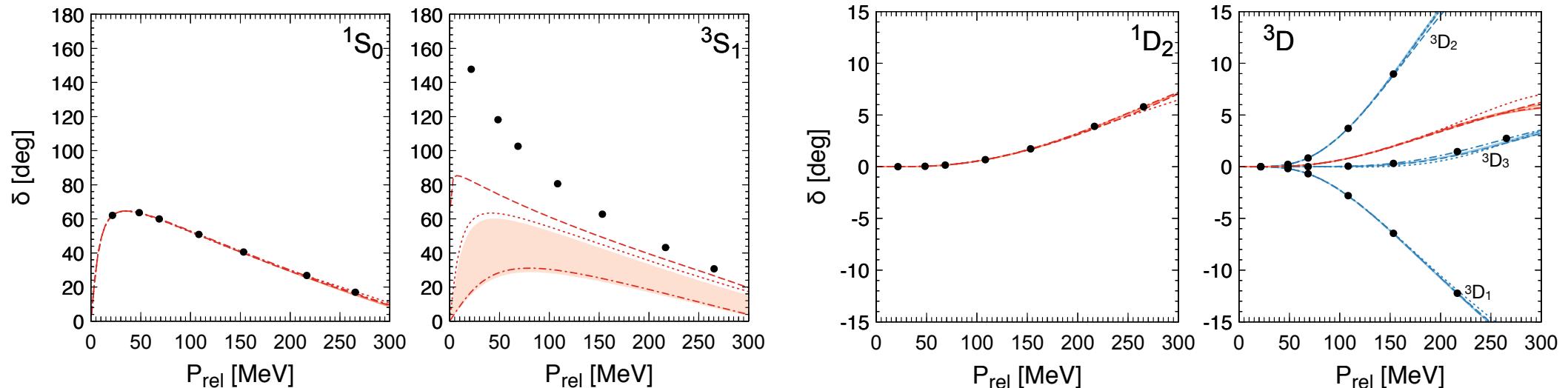
· · · · · ·   IDAHO N3LO   Entem, Machleidt, PRC **68** (2003) 041001

— — —   IDAHO N4LO ($\Lambda = 500\,\text{MeV}$)   Entem, Machleidt, Nosyk PRC **96** (2017) 024004

· — · —   CD-Bonn   Machleidt, PRC **63** (2001) 024001

▬▬▬   Bochum N4$^+$LO ($\Lambda = 400 - 550\,\text{MeV}$)

                                                           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)

$\rightarrow$ 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)

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

$\rightarrow$ 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 $\Lambda = 2.0, 2.5, 3.0, 3.5 \, \text{fm}^{-1}$

Two-nucleon matrix elements in the s-d shell

● Results for the AV18 and N3LO chiral potentials
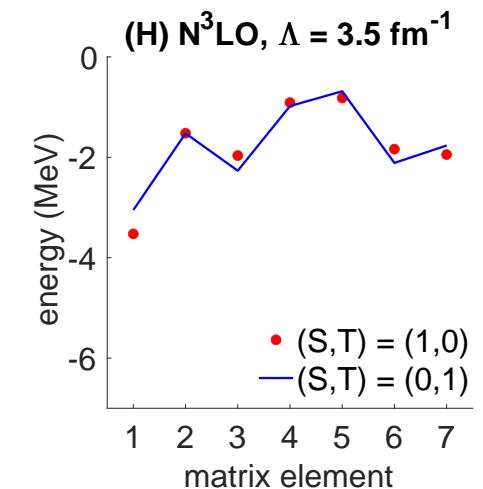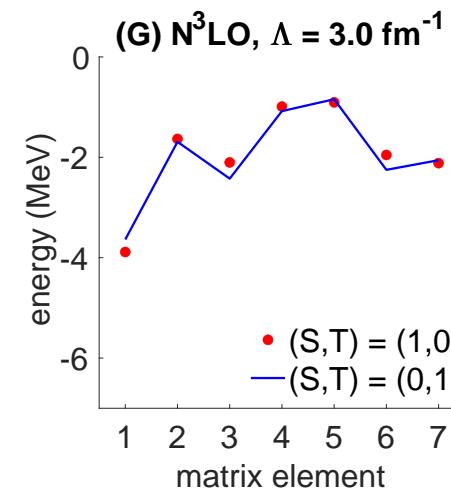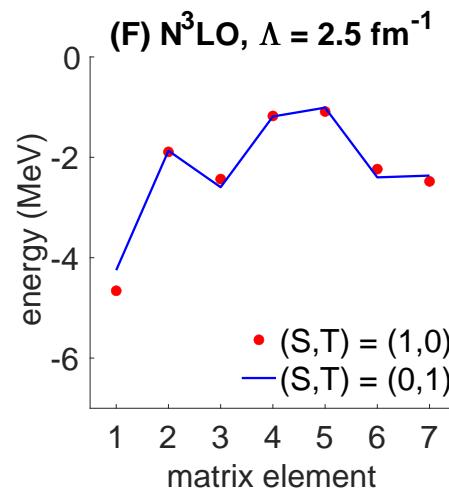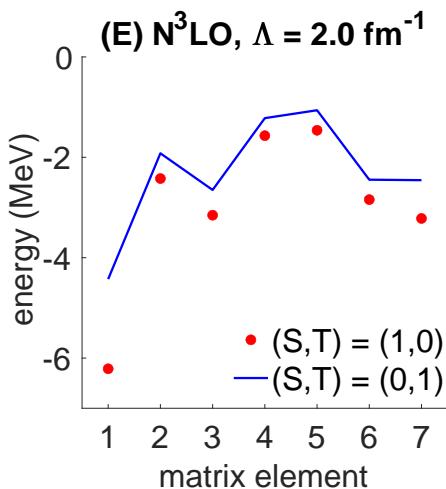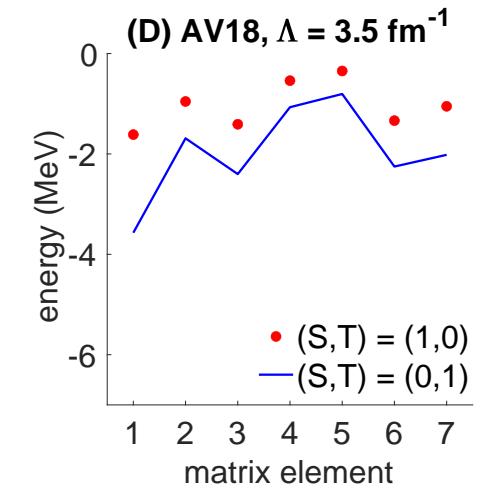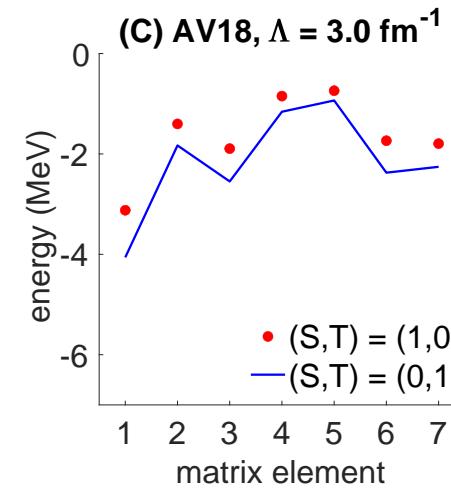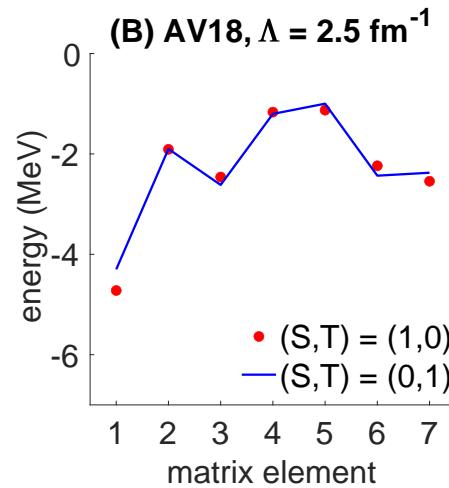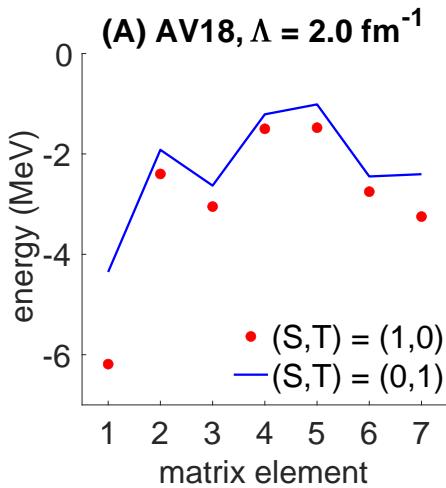
Two-nucleon matrix elements: Conclusions

• 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!** $\sqrt{}$

Three-nucleon forces

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

$$
\begin{aligned}
V_{\text{large}-N_c}^{\textbf{3N}} \;=\; & V_C^{\textbf{3N}} + [(\vec{\sigma}_1 \times \vec{\sigma}_2) \cdot \vec{\sigma}_3][(\vec{\tau}_1 \times \vec{\tau}_2) \cdot \vec{\tau}_3] W_{\textbf{123}}^{\textbf{3N}} \\
+ \;& \vec{\sigma}_1 \cdot \vec{\sigma}_2 \vec{\tau}_1 \cdot \vec{\tau}_2 W_{\textbf{12}}^{\textbf{3N}} + \vec{\sigma}_2 \cdot \vec{\sigma}_3 \vec{\tau}_2 \cdot \vec{\tau}_3 W_{\textbf{23}}^{\textbf{3N}} \\
+ \;& \vec{\sigma}_3 \cdot \vec{\sigma}_1 \vec{\tau}_3 \cdot \vec{\tau}_1 W_{\textbf{31}}^{\textbf{3N}} + \dots ,
\end{aligned}
$$

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

$$
\vec{\sigma}_1 \cdot \vec{\sigma}_2 [(\vec{\tau}_1 \times \vec{\tau}_2) \cdot \vec{\tau}_3] \,, \qquad [(\vec{\sigma}_1 \times \vec{\sigma}_2) \cdot \vec{\sigma}_3] \vec{\tau}_1 \cdot \vec{\tau}_2
$$

$\Rightarrow$ 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

$\Rightarrow$ relevant for calculations of the nuclear symmetry energy and its density dependence
    in dense nuclear matter

Wigner SU(4) symmetry in nuclear structure

Remarks on Wigner's SU(4) symmetry

• 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

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

• 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

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

  ↪ spin-orbit splittings are known to be weak

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

  ↪ start with cluster and shell-model configurations   → next slide

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

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

$$\rho_{\mathrm{NL}}(\mathbf{n}) = a^{\dagger}_{\mathrm{NL}}(\mathbf{n}) a_{\mathrm{NL}}(\mathbf{n})$$

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

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

  ↪ investigate the spectrum for $a = 1.64$ fm and $a = 1.97$ fm

Configurations

● Cluster and shell model configurations

S1
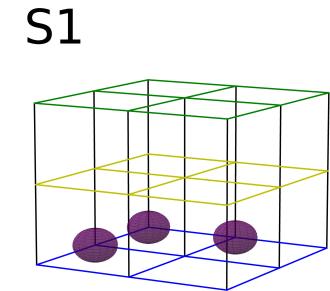
— isoscele right triangle

S2

— "bent-arm" shape

S3
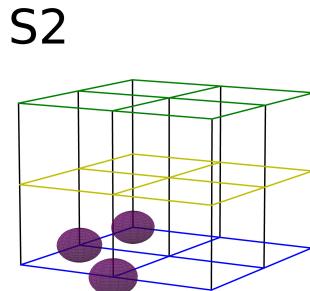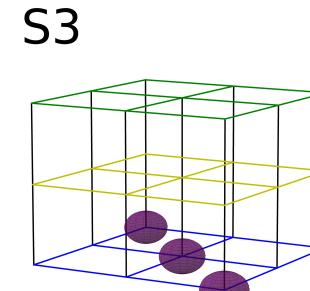
— linear diagonal chain

S4
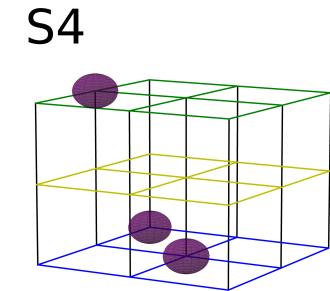
— acute isoscele triangle

Gaussian wave packets
$w = 1.7 - 2.1$ fm

20

1d$_{3/2}$
2s$_{1/2}$
1d$_{5/2}$

8

1p$_{1/2}$
1p$_{3/2}$

2

1s$_{1/2}$

— ground state $|0\rangle$

20

1d$_{3/2}$
2s$_{1/2}$
1d$_{5/2}$

8

1p$_{1/2}$
1p$_{3/2}$

2

1s$_{1/2}$

— $2p$-$2h$ state, $J_z = 0$

20

1d$_{3/2}$
2s$_{1/2}$
1d$_{5/2}$

8

1p$_{1/2}$
1p$_{3/2}$

2

1s$_{1/2}$
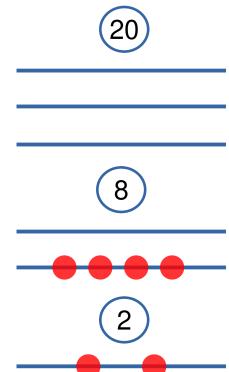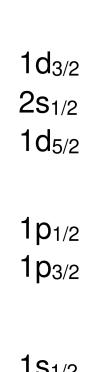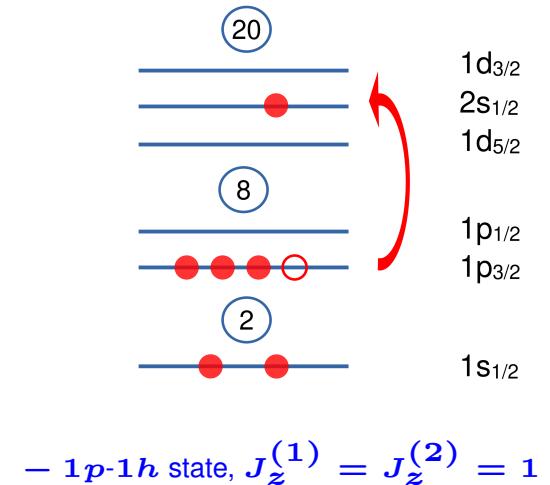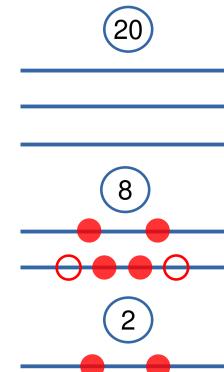
— $1p$-$1h$ state, $J_z^{(1)} = J_z^{(2)} = 1$

Transient energies

● Transient energies from cluster and shell-model configurations

Spectrum of ^{12}C

● Amazingly precise description → great starting point
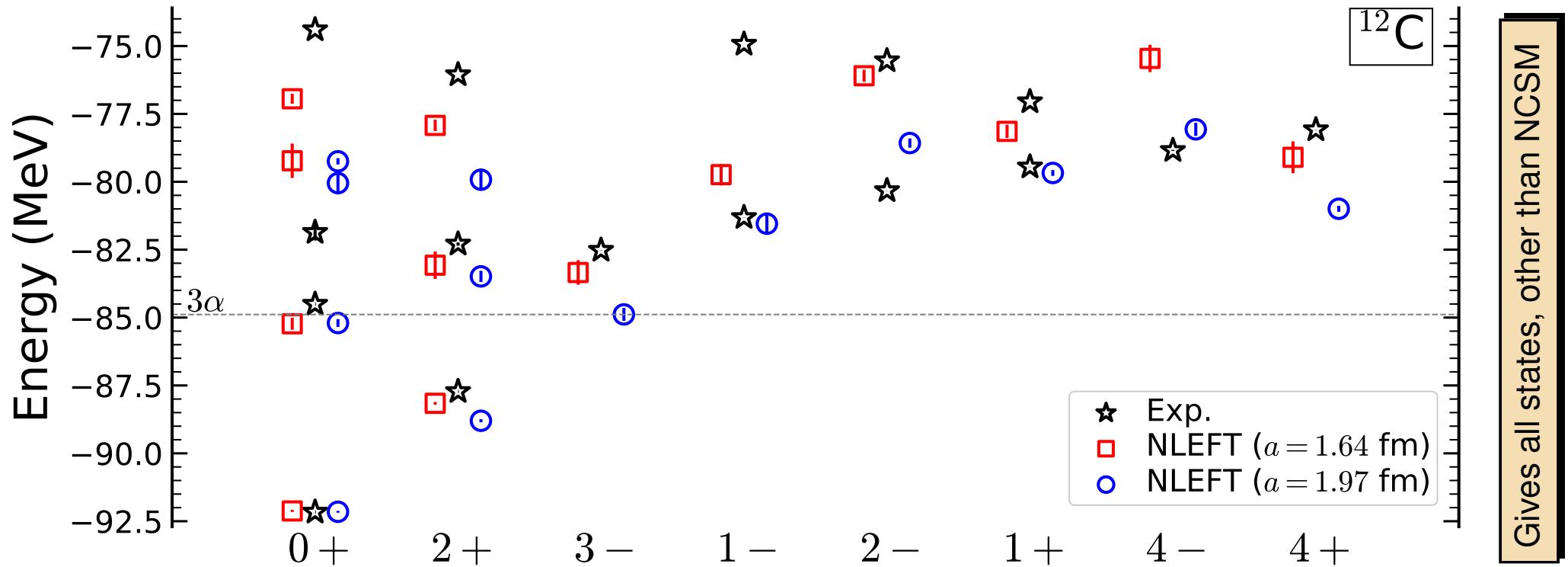
→ solidifies earlier NLEFT statements about the structure of the 0_2^+ and 2_2^+ states

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

Shen, Lähde, Lee, UGM, [arXiv:2202.13596 [nucl-th]]

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

- 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

S00-S00-S0D-S0D, A_1^+-E^+

$a = 1.97$ fm

-83.079 2_2^+
-85.039 0_2^+
-88.323 2_1^+
-92.038 0_1^+

E (MeV)

t (MeV^{-1})
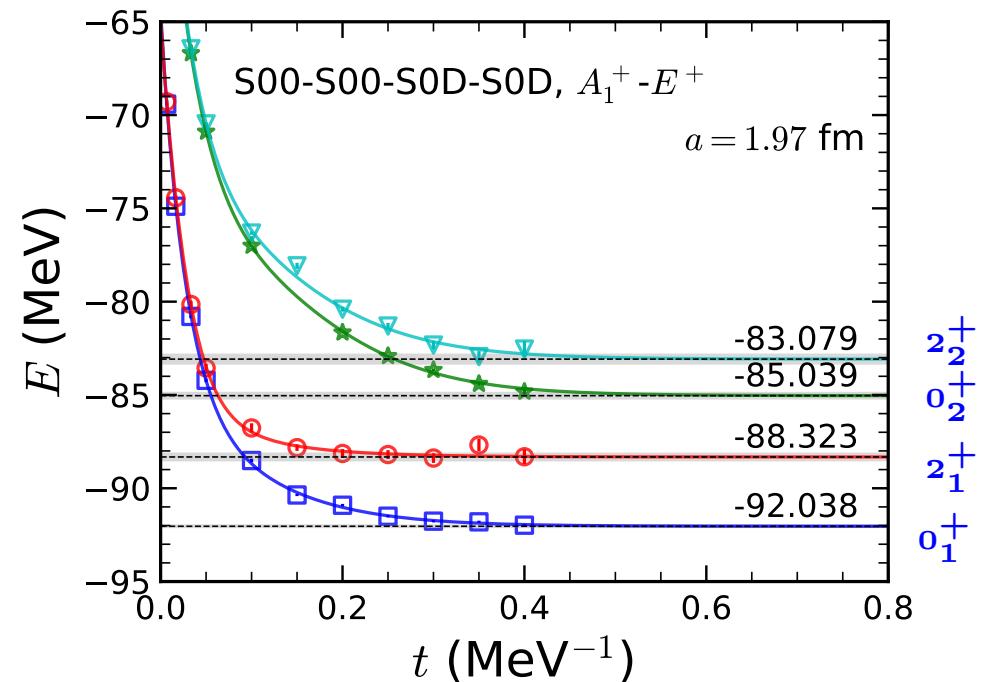
Spectrum of ^{12}C reloaded

Shen, Lähde, Lee, UGM, [arXiv:2202.13596 [nucl-th]]

- Improved description when 3NFs are included, amamzingly good
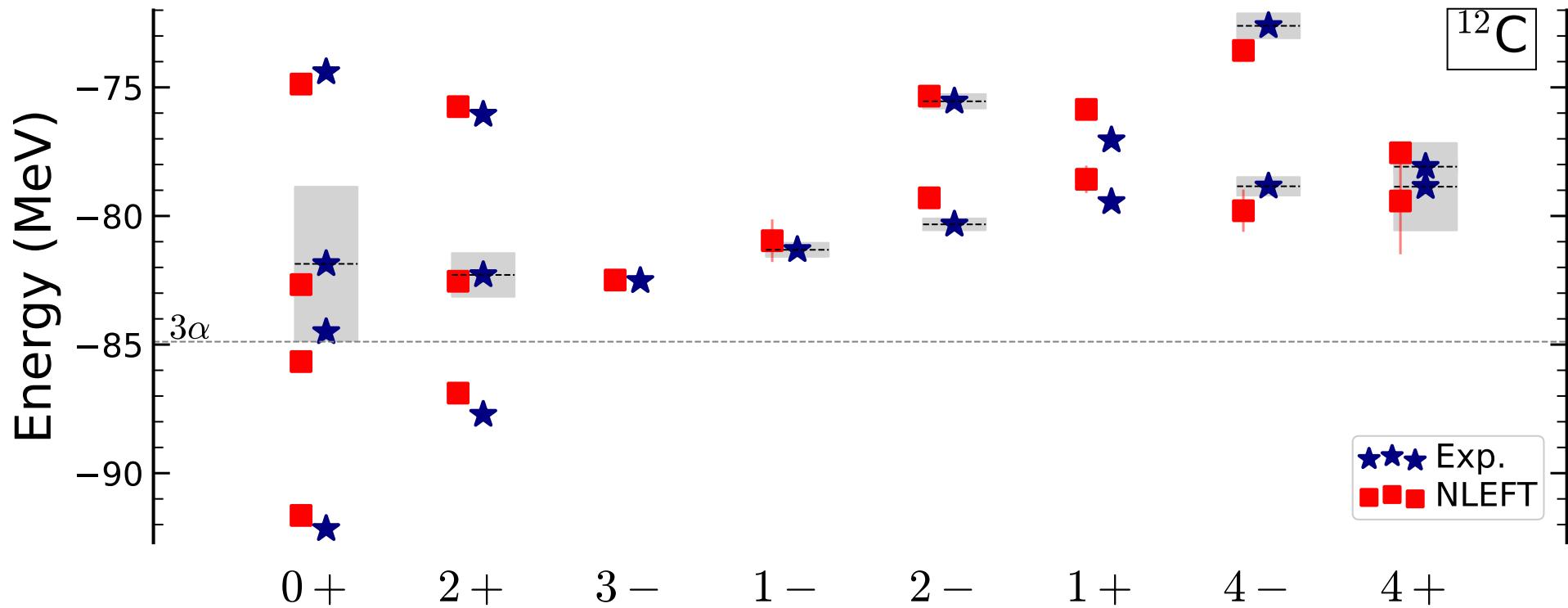
$\rightarrow$ solidifies earlier NLEFT statements about the structure of the 0_2^+ and 2_2^+ states

Electromagnetic properties

Shen, Lähde, Lee, UGM, [arXiv:2202.13596 [nucl-th]]

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

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

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

Electromagnetic properties

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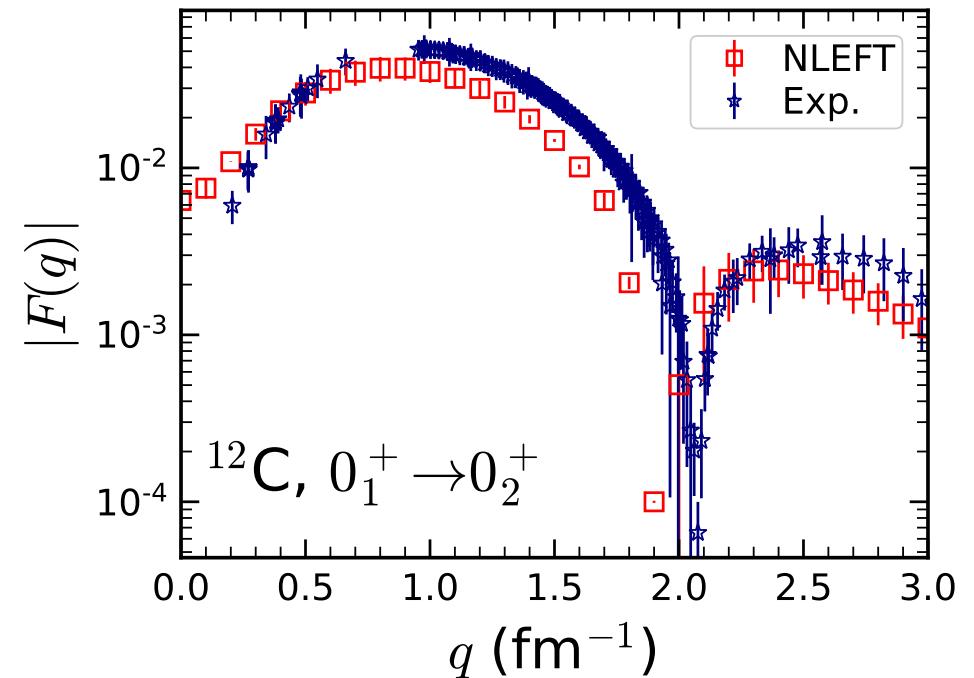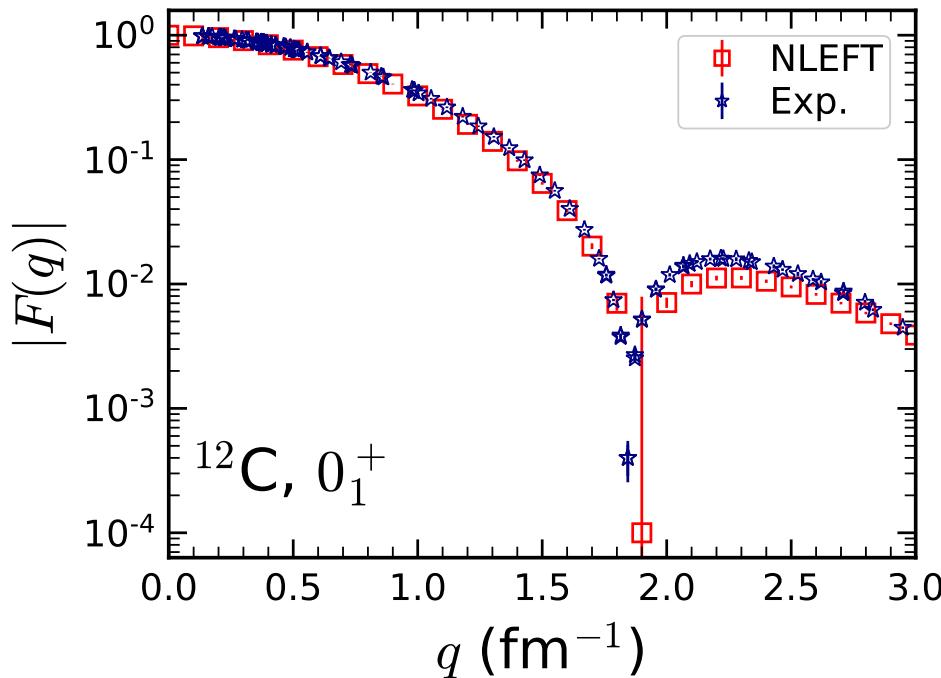

Sick, McCarthy, Nucl. Phys. A 150 (1970) 631
Strehl, Z. Phys. 234 (1970) 416
Crannell et al., Nucl. Phys. A 758 (2005) 399

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

Emergence of geometry

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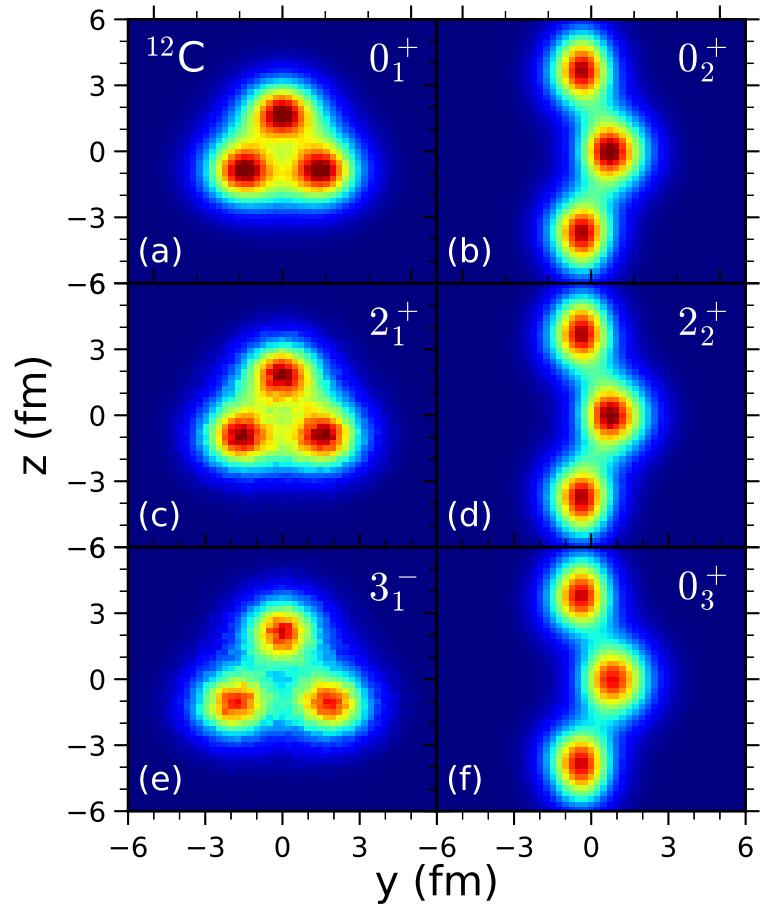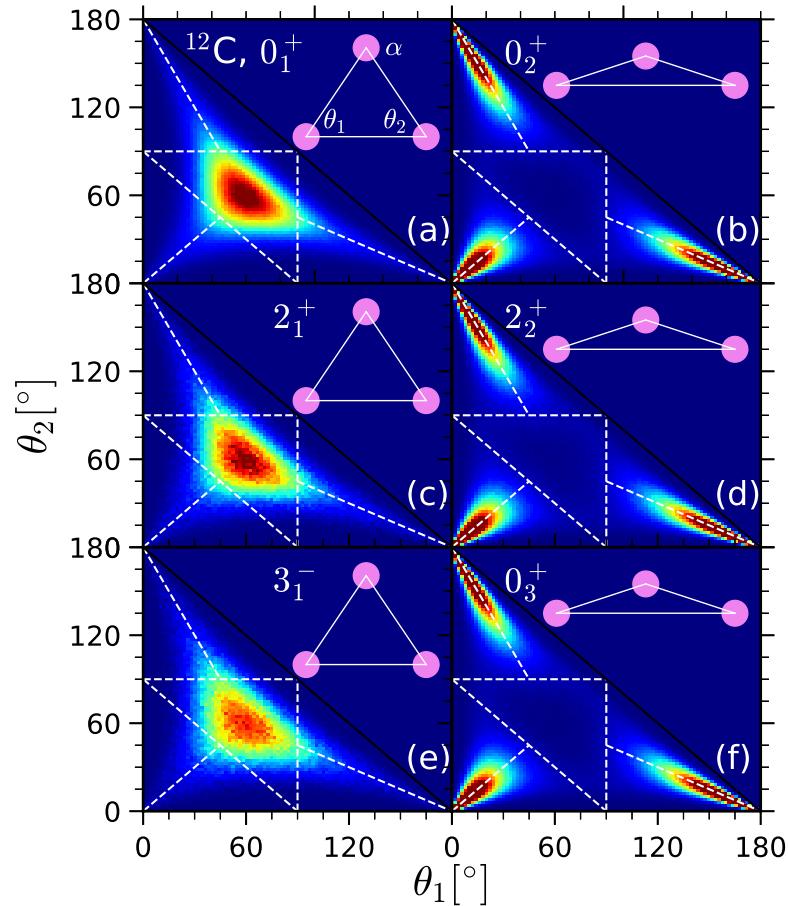

● equilateral & obstuse triangles $\rightarrow$ 2^+ states are excitations of the 0^+ states

Emergence of duality

Shen, Lähde, Lee, UGM, [arXiv:2202.13596 [nucl-th]]

- ^{12}C spectrum shows a cluster/shell-model duality
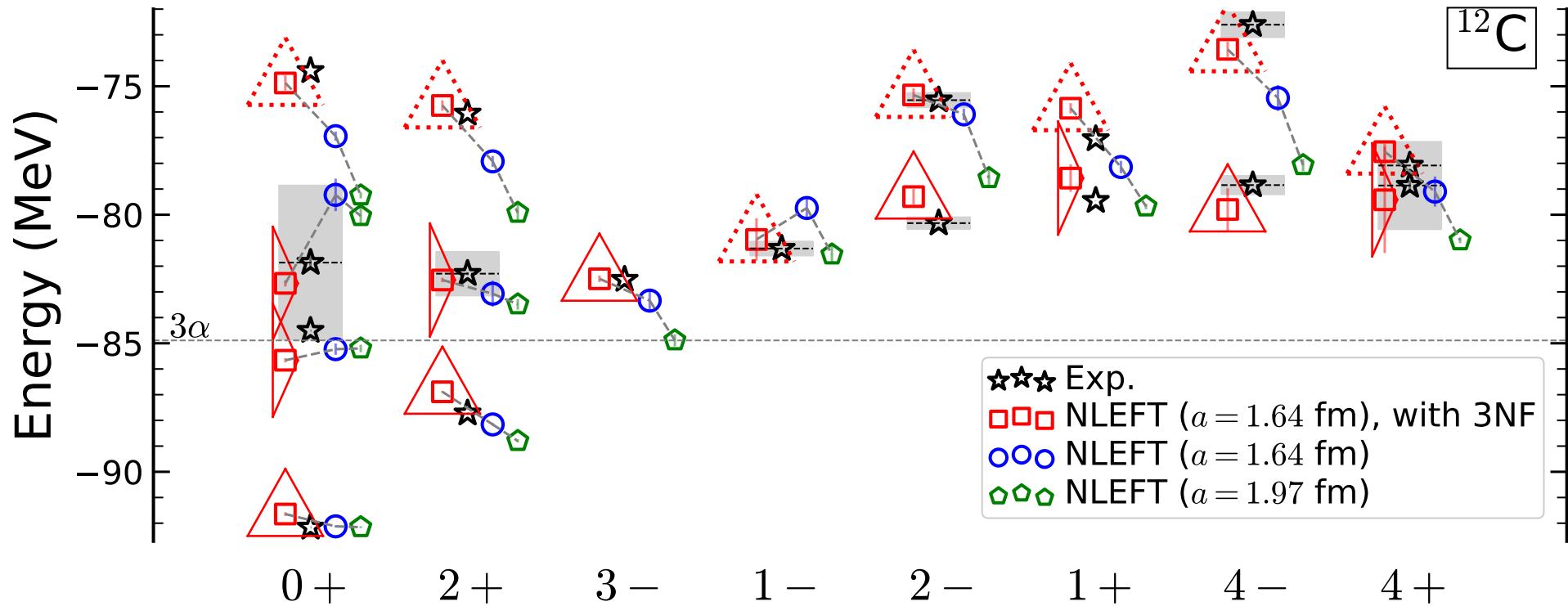
- dashed triangles: strong 1p-1h admixture in the wave function

Towards heavy nuclei 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 $\checkmark$

2) Work out the corrections to N3LO

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

$\hookrightarrow$ second for the spectra of nuclei

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

Going to higher orders

- **Step 2**: Work out NN phase shifts to N3LO

    $\hookrightarrow$ calculate nuclear properties based on NN forces only $\checkmark$

    $\hookrightarrow$ add three-nucleon forces (chiral plus special SU(4) symm. config's)

- Starting Hamiltonian:

$$H_{2N} = H_{\text{free}} + H_{\text{SU(4)}}(C_3 = 0) + H_{\text{OPE}}$$

    $\hookrightarrow$ consistent with the power counting (3NFs appear at N2LO)

    $\hookrightarrow$ OPE induces some sign problem (but manageable)

- NN forces to N3LO worked out for 4 latt. spacings $a = 0, 99, 1.32, 1.64, 1.98$ fm
 with local and non-local smearing and restoration of Galilean invariance breaking

    $\hookrightarrow$ used as input for nuclear structure calculations

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

NN interaction at N3LO

• np phase shifts including uncertainties for $a = 1.64$ fm (cf. Nijmegen PWA)

NLO
N2LO
N3LO
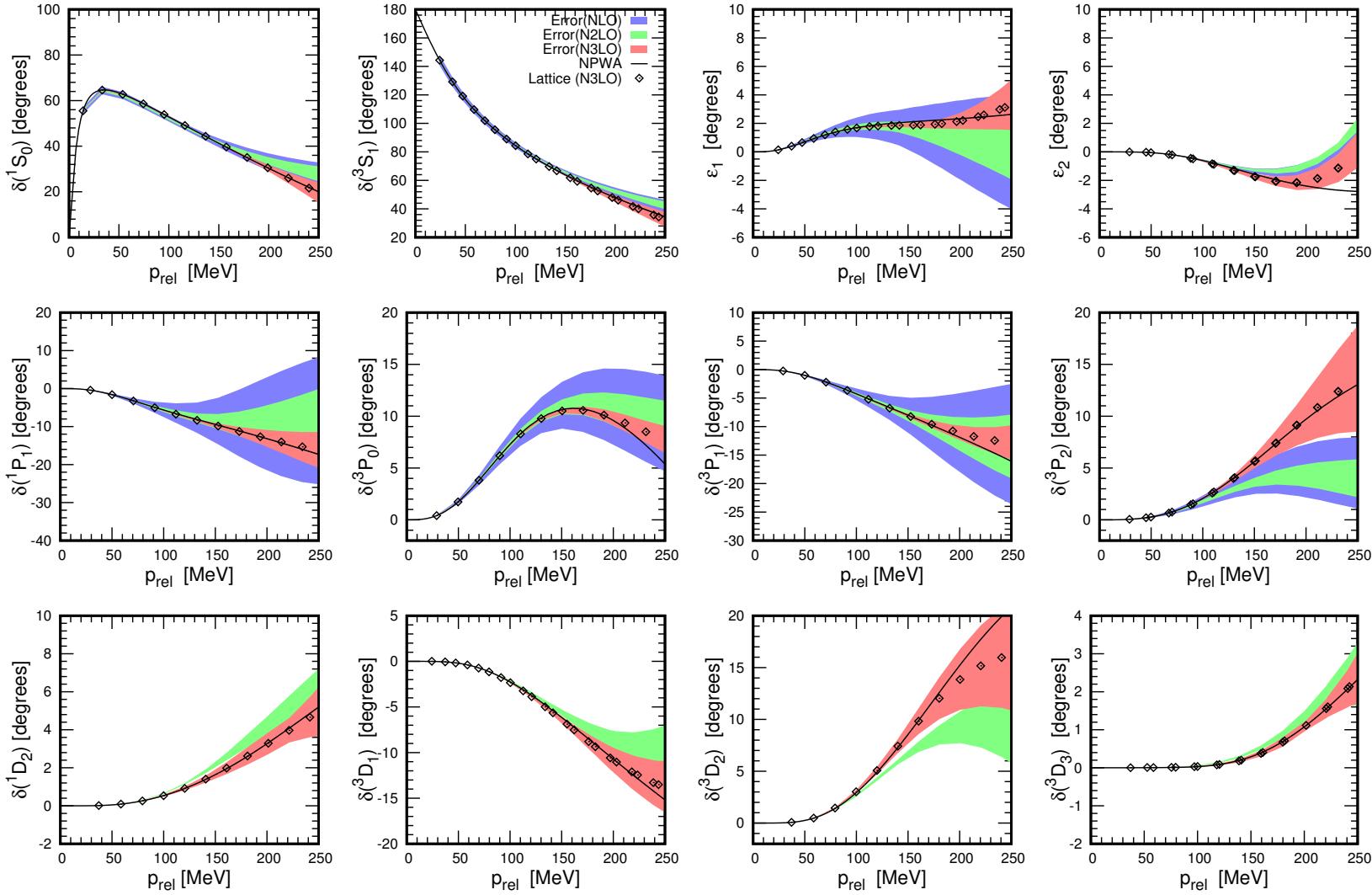
Nuclei at N3LO

- A bit of work: Binding energies of nuclei for $a = 1.64\,\mathrm{fm}$

Elhatisari et al., in preparation
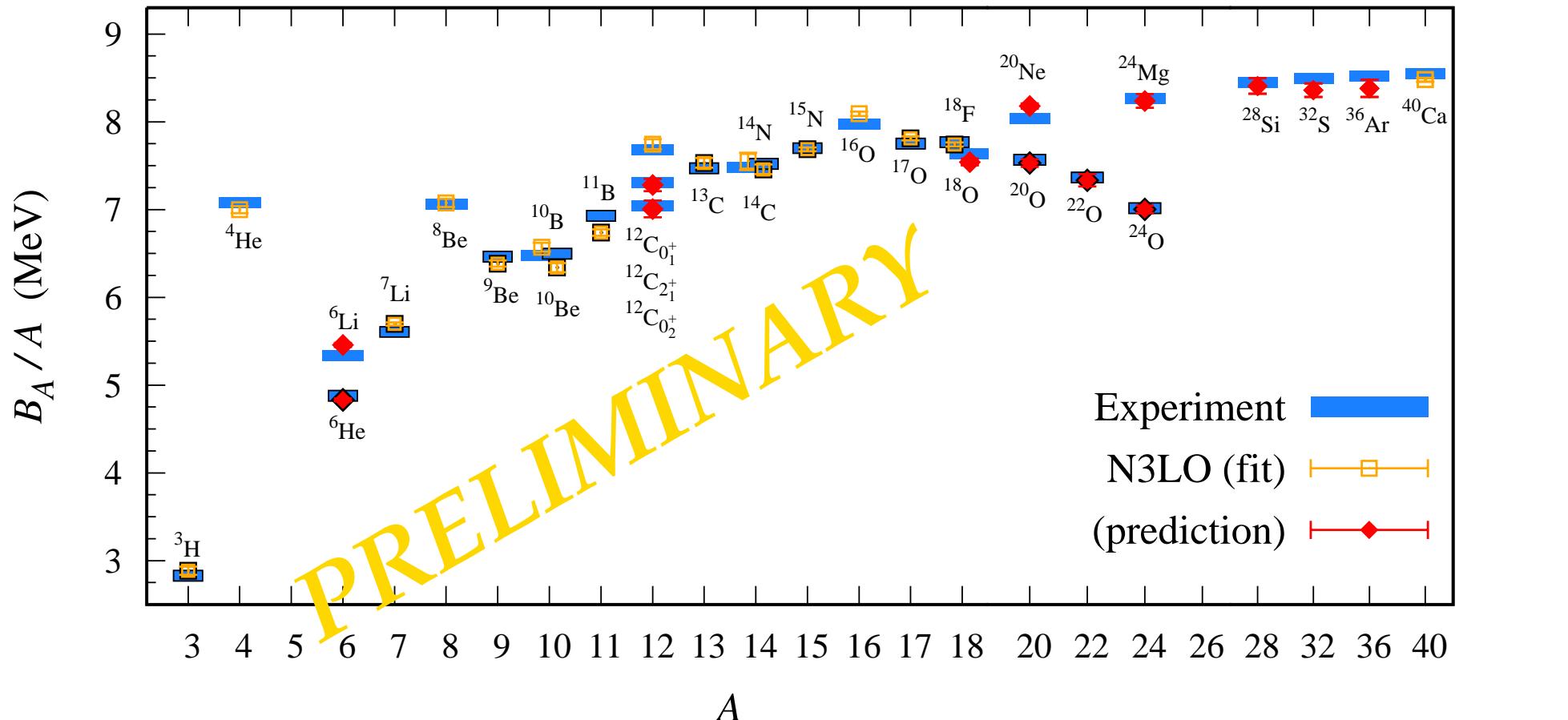

$\rightarrow$ excellent starting point for precision studies

Charge densities at N3LO

● Charge densities from the pinhole algorithm: Elhatisari et al., in preparation
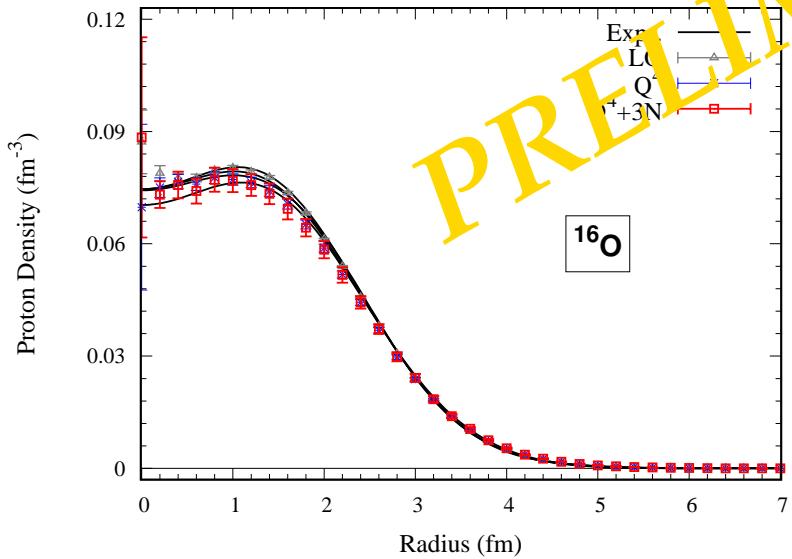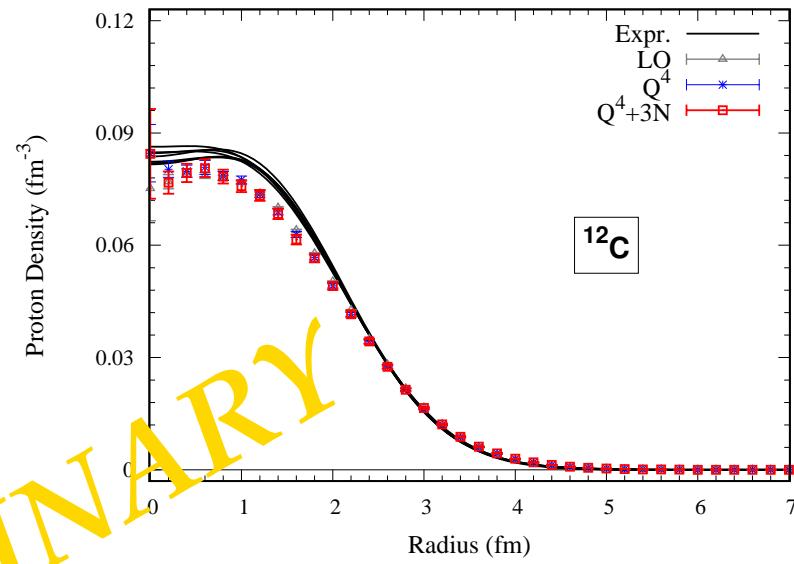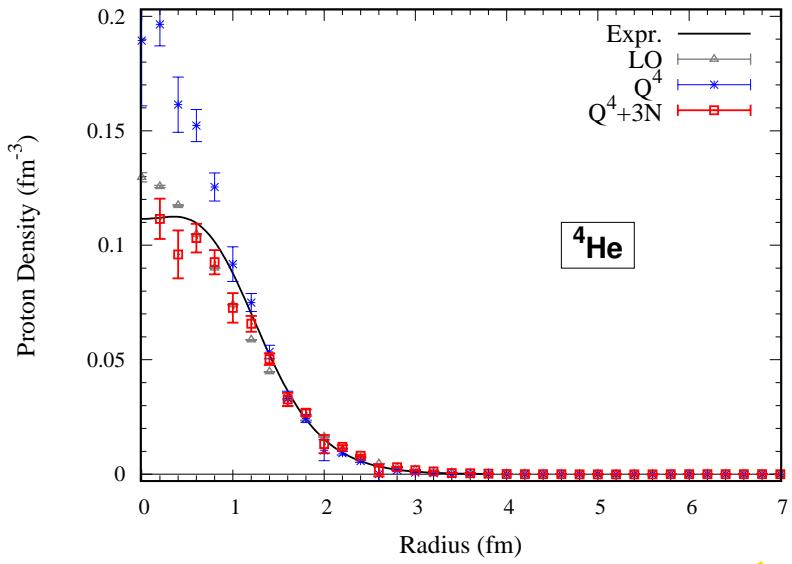
→ more to come ...

Charge radii at N3LO

● Presently determined charge radii

Elhatisari et al., in preparation
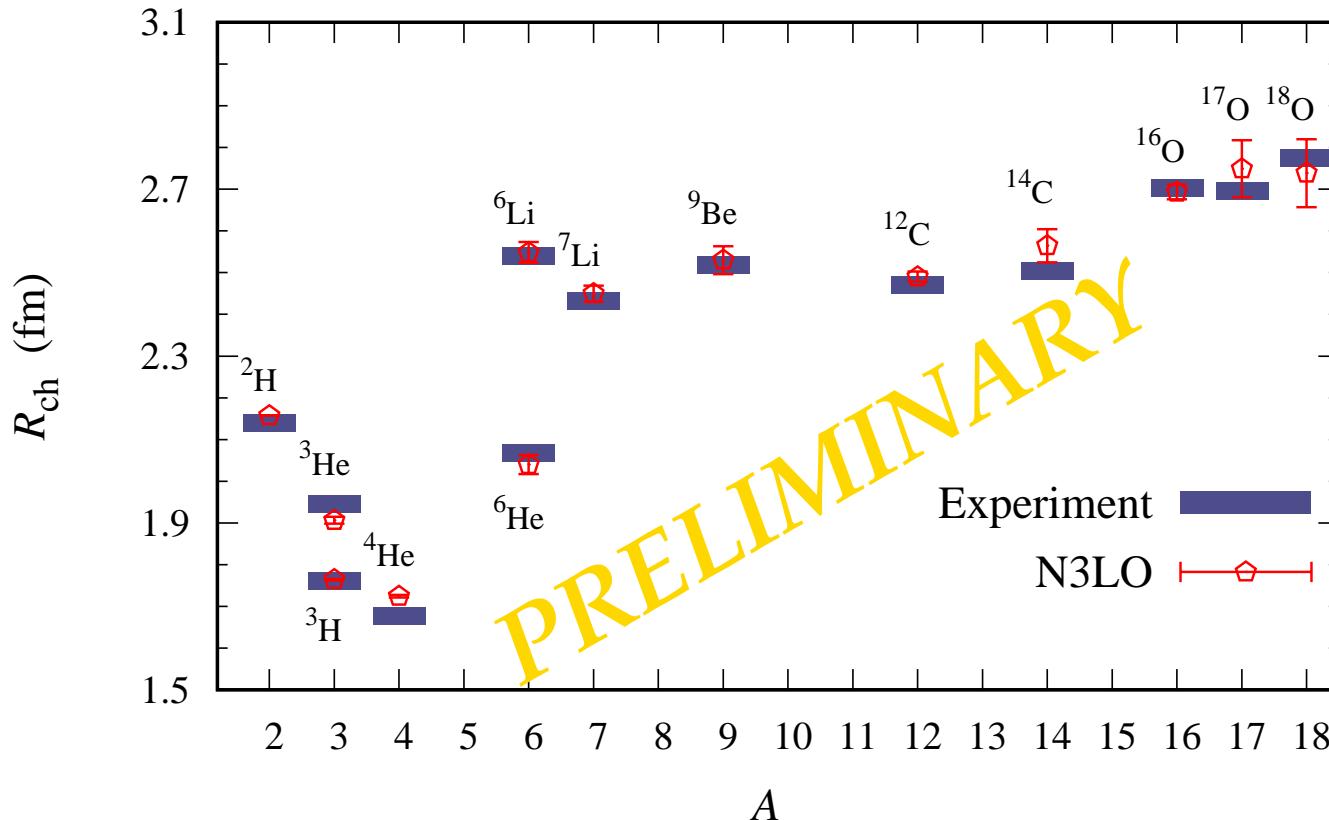
Nucleus	R_c [fm]	Exp. [fm]
^{2}H	2.157	2.140
^{3}H	1.764(2)	1.759
^{3}He	1.906(8)	1.945
^{4}He	1.724(3)	1.676
^{6}He	2.040(2)	2.068(11)
^{6}Li	2.569(3)	2.589(39)
^{7}Li	2.450(2)	2.444(42)
^{9}Be	2.530(4)	2.518
^{12}C	2.490(12)	2.470
^{14}C	2.565(40)	2.504
^{16}O	2.693(18)	2.701
^{17}O	2.749(69)	2.695
^{18}O	2.739(81)	2.775

↪ on the right track ...

Ab Initio Nuclear Thermodynamics

- Sketch of the phase diagram of strongly interacting matter
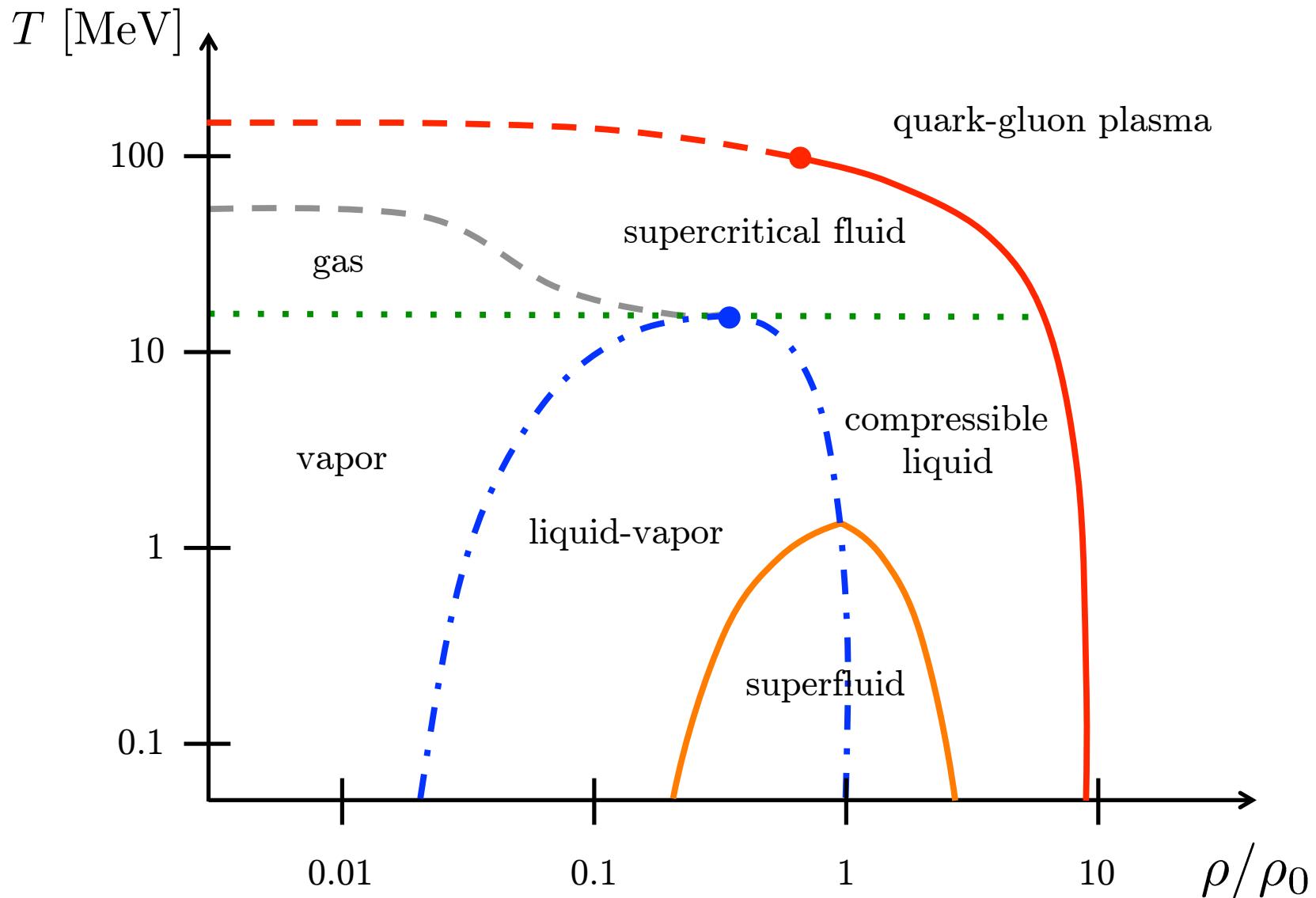
Pinhole trace algorithm (PTA)

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

- The canonical partition function can be expressed using pinholes:

Metropolis updates of pinholes

hybrid Monte Carlo
updates of auxiliary/pion fields

Take trace using periodic
boundary condition in
time dimension

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

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

- allows to study: liquid-gas phase transition $\rightarrow$ this talk

  thermodynamics of finite nuclei

  thermal dissociation of hot nuclei

 cluster yields of dissociating nuclei
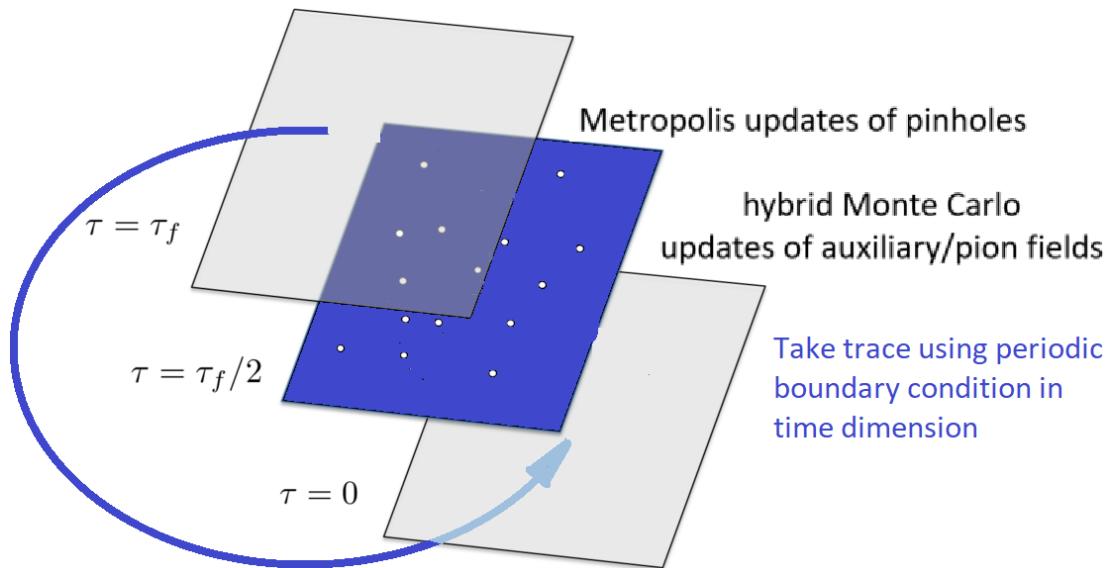
New paradigm for nuclear thermodynamics

• 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 ($t_{\mathrm{CPU}} \sim V N^2$ vs. $t_{\mathrm{CPU}} \sim V^3 N^2$)

• 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: $\boxed{\Delta t \sim N^2 L^3}$

Chemical potential

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

— Ulf-G. Meißner, NLEFT: Status and Perspectives – talk, LENPIC meeting, RUB, Aug. 24, 2022 –
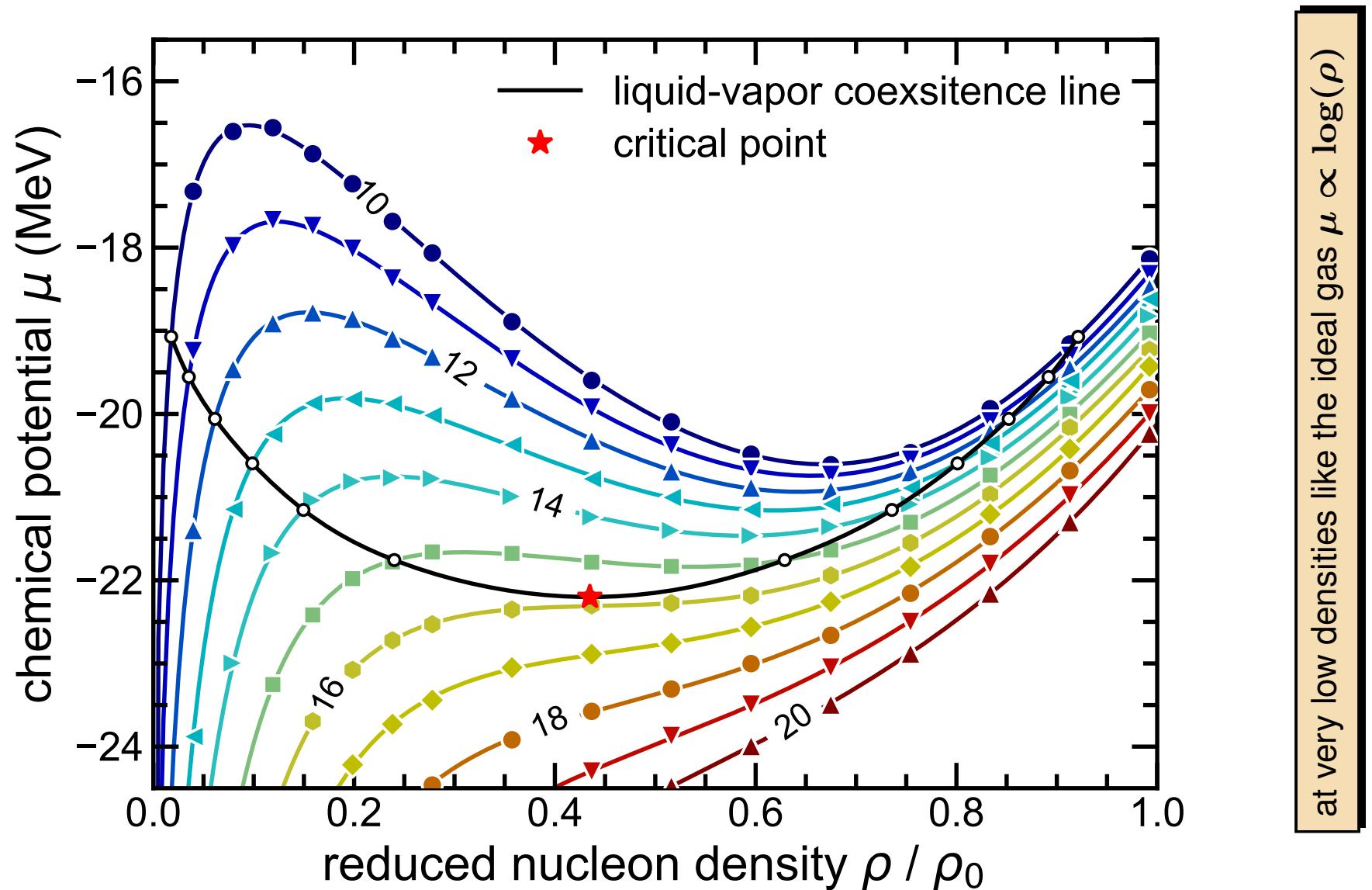
Equation of state

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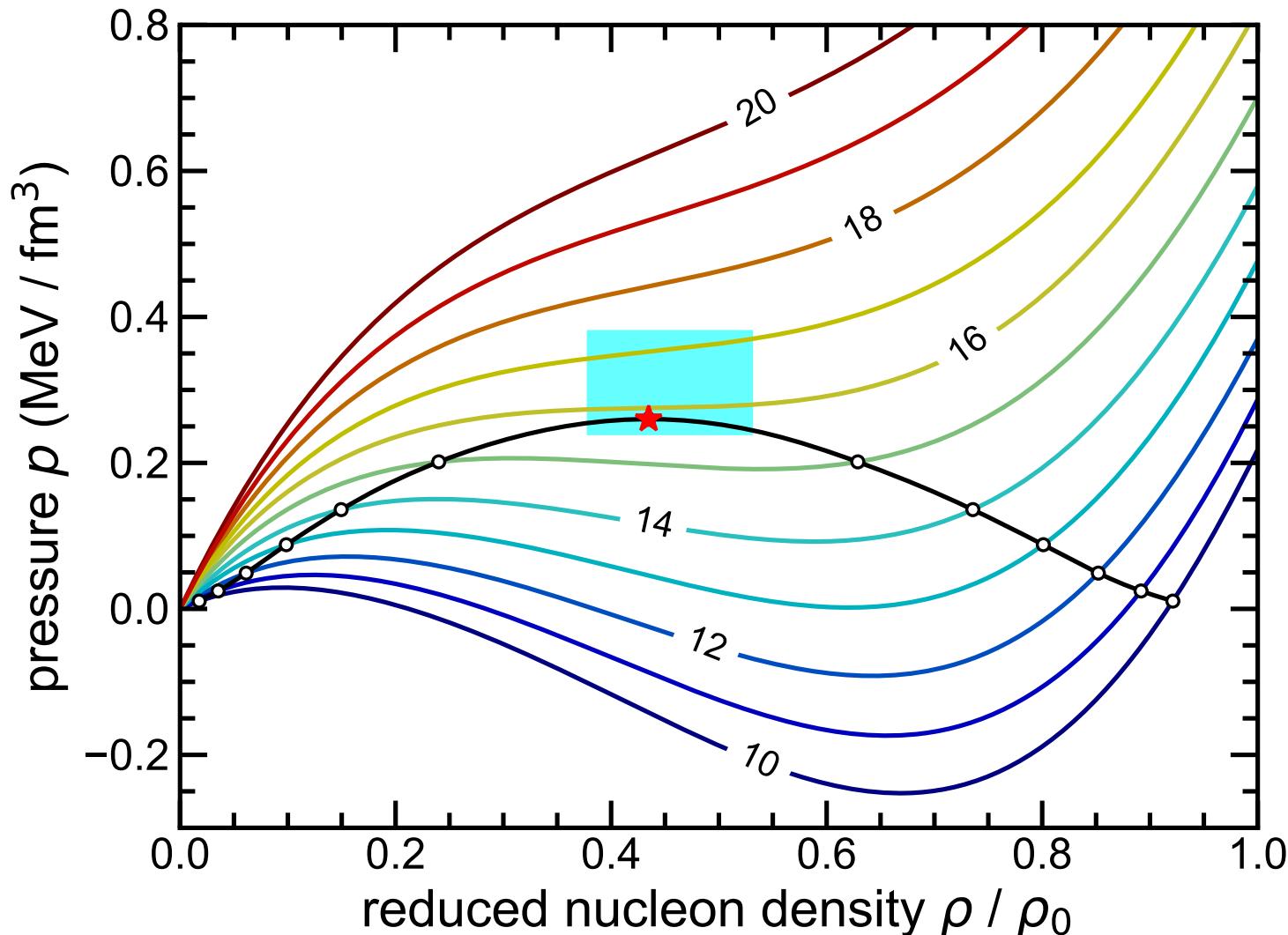
Experiment: $T_c = 15.0(3)$ MeV, $P_c = 0.31(7)$ MeV/fm^3, $\rho_c = 0.06(2)$ fm^{-3}

– Ulf-G. Meißner, NLEFT: Status and Perspectives – talk, LENPIC meeting, RUB, Aug. 24, 2022 –

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 $\mu = \partial F / \partial A$
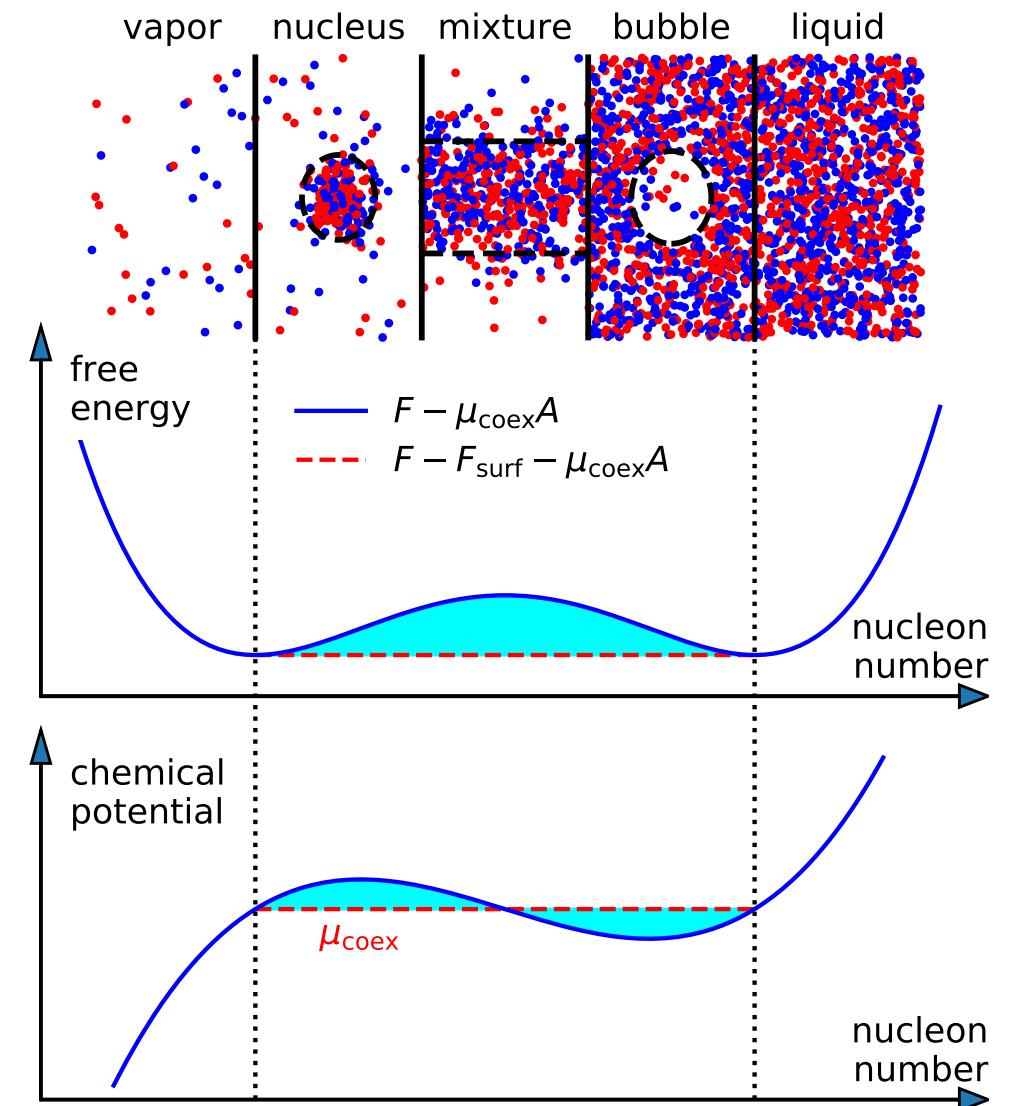
Summary & outlook

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

- Recent developments
    - → hidden spin-isospin exchange symmetry
        - ↪ optimal cut-off $\Lambda \simeq 500$ MeV, validates Weinberg counting
    - → Wigner SU(4) symmetry in nuclear structure
        - ↪ emergence of geometry and duality in the ^{12}C spectrum

- Towards heavier nuclei & higher precision
    - → highly improved LO action based on SU(4)
    - → NN interaction at N3LO, first results for nuclei at N3LO
        - ↪ promising results up to ^{40}Ca, oxygen neutron dripline

- Ab initio nuclear thermodynamics
    - → partition function via the pinhole trace algorithm
        - ↪ first promising results for the phase diagram of nuclear matter at finite temperature
        - ↪ prediction of the vapor-liquid phase transition within reasonable accuracy

Summary & outlook

- Strangeness nuclear physics
  - $\rightarrow$ treat hyperons as impurities, ILMC algorithm
    - $\hookrightarrow$ first exploratory study, $t_{\mathbf{CPU}} \sim A$ Frame et al., Eur. Phys. J. A **56** (2020) 248
    - $\hookrightarrow$ hypernuclear landscape up to $A = 20$ within one year

- Studies of the oxygen and calcium isotopic chains
  - $\rightarrow$ first results for oxygen from $A = 16$ to $A = 26$ $\checkmark$
    - $\hookrightarrow$ 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

# Algorithmic developments

shuttle algorithm: Lu et al., Phys. Lett. B**797** (2019) 134863

pinhole algorithm: Elhatisari et al., Phys. Rev. Lett. **19** (2017) 222505

pinhole trace algorithm: Lu et al., arXiv:1912.05105, subm. for publication

THE SHUTTLE ALGORITHM

- Auxiliary fields $s(n_t, \vec{n})$ are updated on one time slice only

- Proceed to the next time slice, update, ... , turn around at the end of the time series

$\rightarrow$ very efficient for small temporal lattice spacings, $a_t = 0.001$ MeV^{-1}

$\rightarrow$ high acceptance rate, typically $\sim 50\%$

$\rightarrow$ more efficient than HMC

$\rightarrow$ about 10 times more configurations per hour generated

$\rightarrow$ further acceleration by GPUs

– Ulf-G. Meißner, NLEFT: Status and Perspectives – talk, LENPIC meeting, RUB, Aug. 24, 2022 –
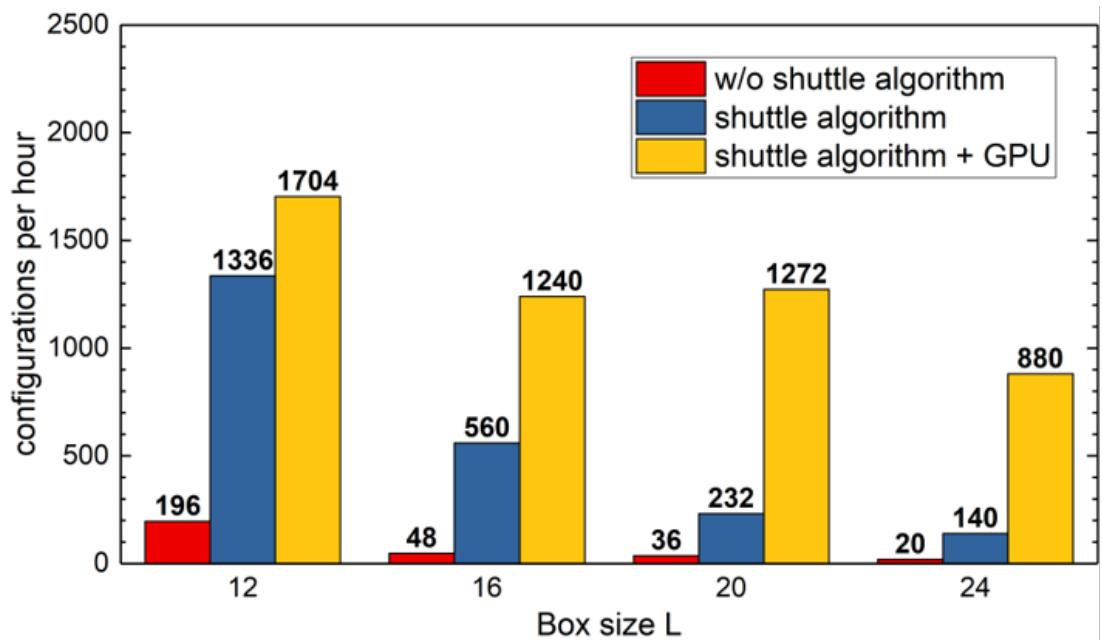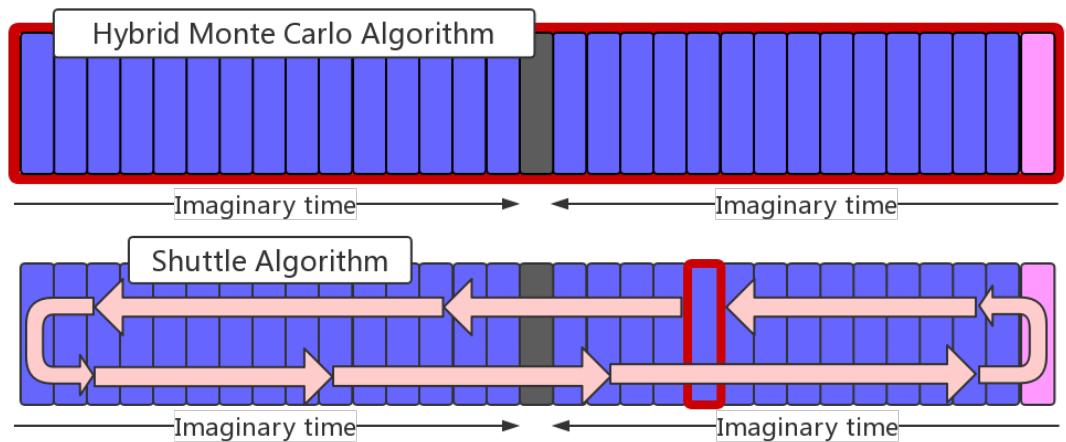
CENTER-of-MASS PROBLEM

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

$$Z_A(\tau) = \langle \Psi_A(\tau) | \Psi_A(\tau) \rangle$$

$$|\Psi_A(\tau)\rangle = \exp(-H\tau/2)|\Psi_A\rangle$$
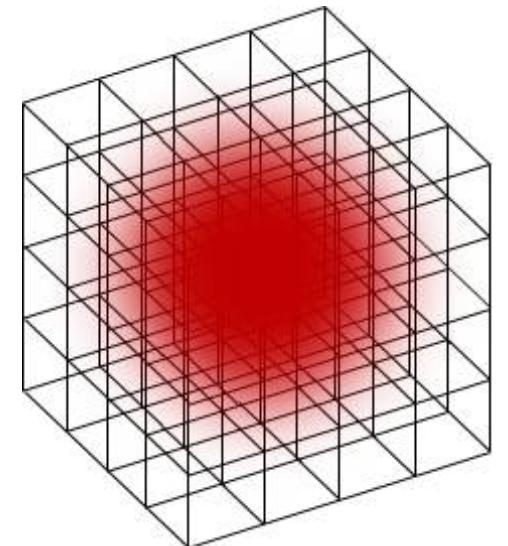
• but: translational invariance requires summation over all transitions

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

i_{com} (j_{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 $\mathbf{r}_{\mathbf{cm}}$ is an integer $\mathbf{n}_{\mathbf{cm}}$ times a/A

HMC updates for aux./pion fields

$\tau_i = \tau$

i_5,j_5 i_3,j_3 i_7,j_7

i_2,j_2

i_4,j_4 i_6,j_6

i_8,j_8

i_1,j_1

Euclidean time

$\tau/2$

Metropolis updates for pinholes

$\tau_i = 0$
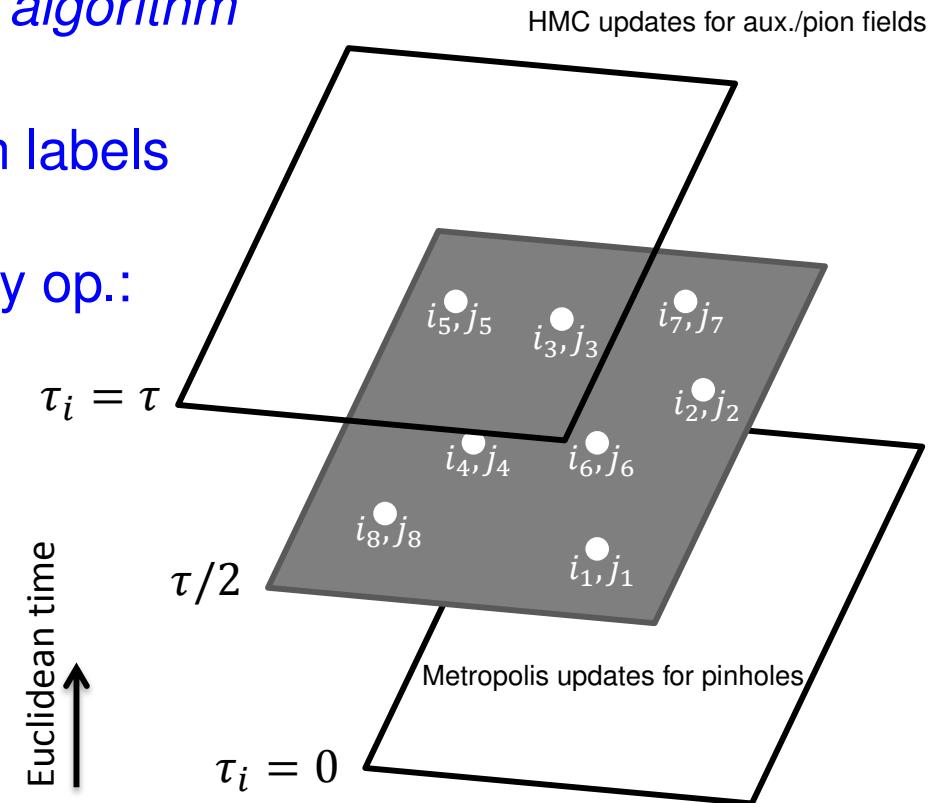
PROTON and NEUTRON DENSITIES in CARBON

- first NLEFT calculation of the charge density in ^{12}C [proton size accounted for]

- asymptotic properties of the distributions from the volume
  dependence of N-body bound states

  König, Lee, Phys. Lett. B779 (2018) 9

- open symbols: neutron / closed symbols: proton
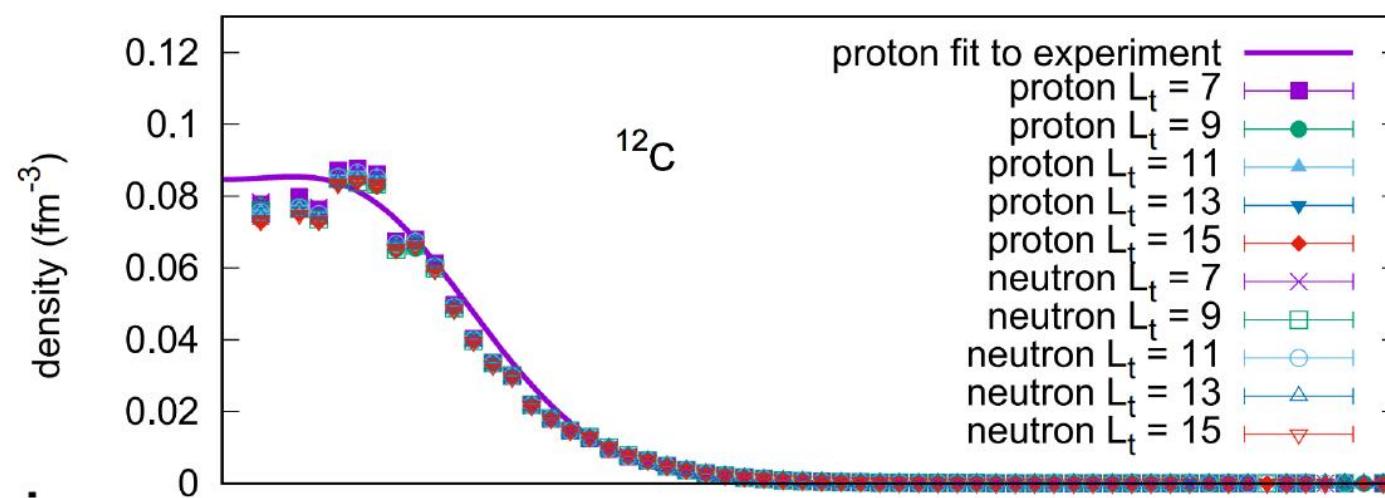
$\Rightarrow$ independent of projection time $\rightarrow$ ground state

$\Rightarrow$ small error bars $\rightarrow$ sign problem under control

FORM FACTORS

- Fit charge distributions by a Wood-Saxon shape
  - ↪ get the form factor from the Fourier-transform (FT)
  - ↪ uncertainties from a direct FT of the lattice data
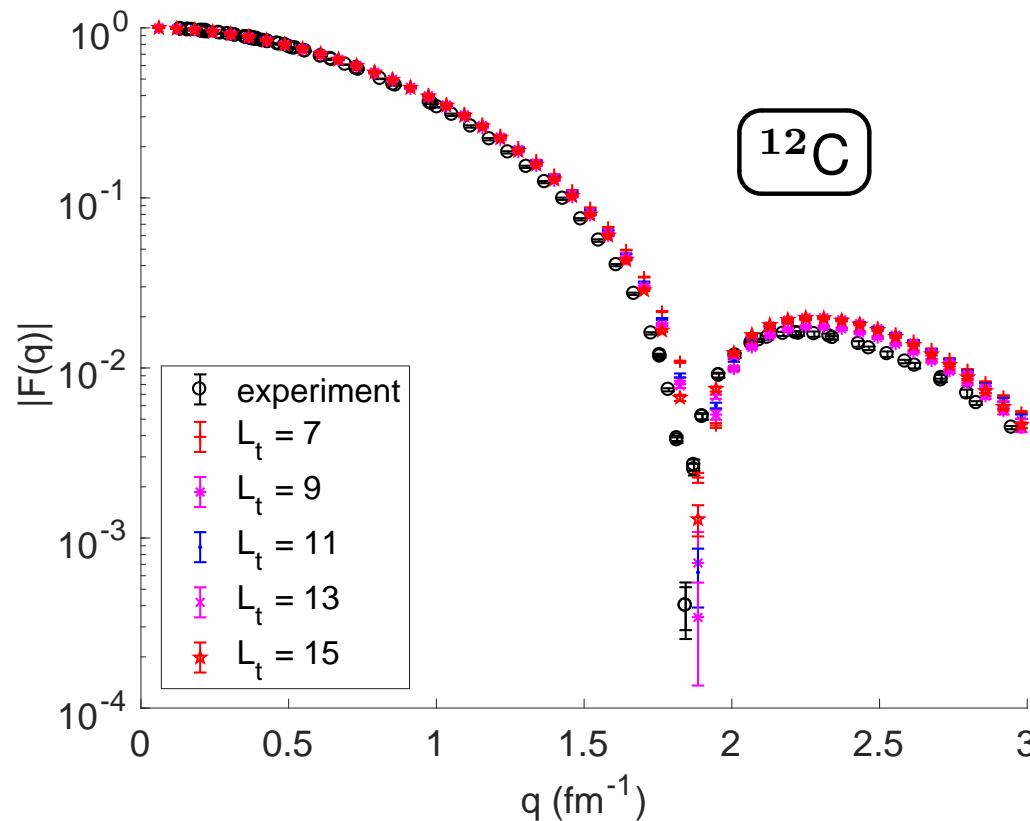
$\Rightarrow$ detailed structure studies become possible

PINHOLE TRACE ALGORITHM (PTA)

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

- The canonical partition function can be expressed using pinholes:

Metropolis updates of pinholes

hybrid Monte Carlo
updates of auxiliary/pion fields

$\tau = \tau_f$

$\tau = \tau_f/2$

$\tau = 0$

Take trace using periodic
boundary condition in
time dimension

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

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

- allows to study: liquid-gas phase transition $\rightarrow$ this talk

    thermodynamics of finite nuclei

    thermal dissociation of hot nuclei

    cluster yields of dissociating nuclei
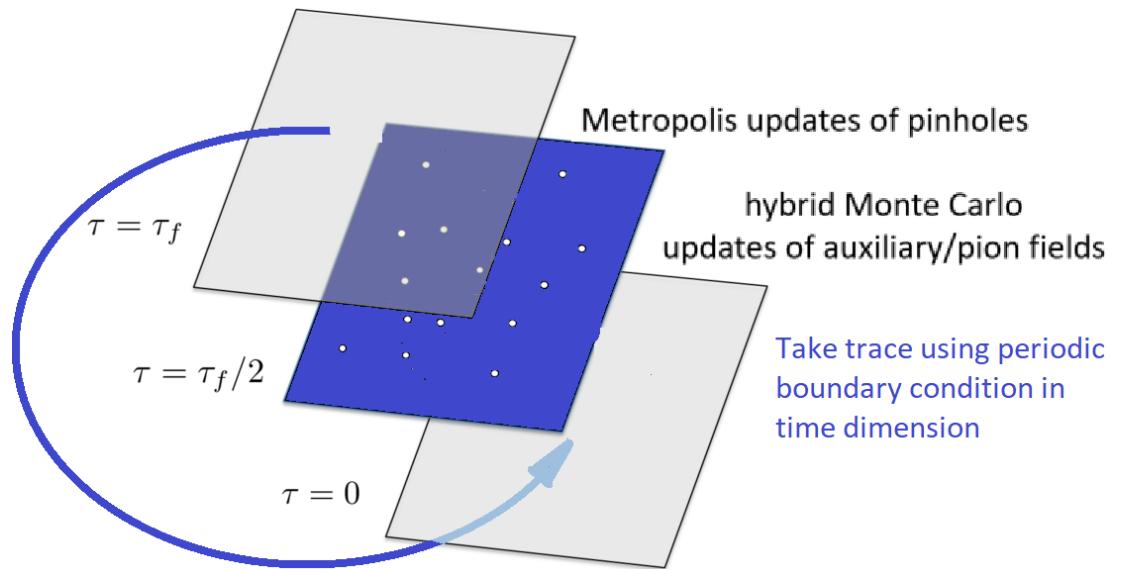
Similarity renormalization group studies

● Investigation of Wigner SU(4) symmetry using the SRG, use AV18:
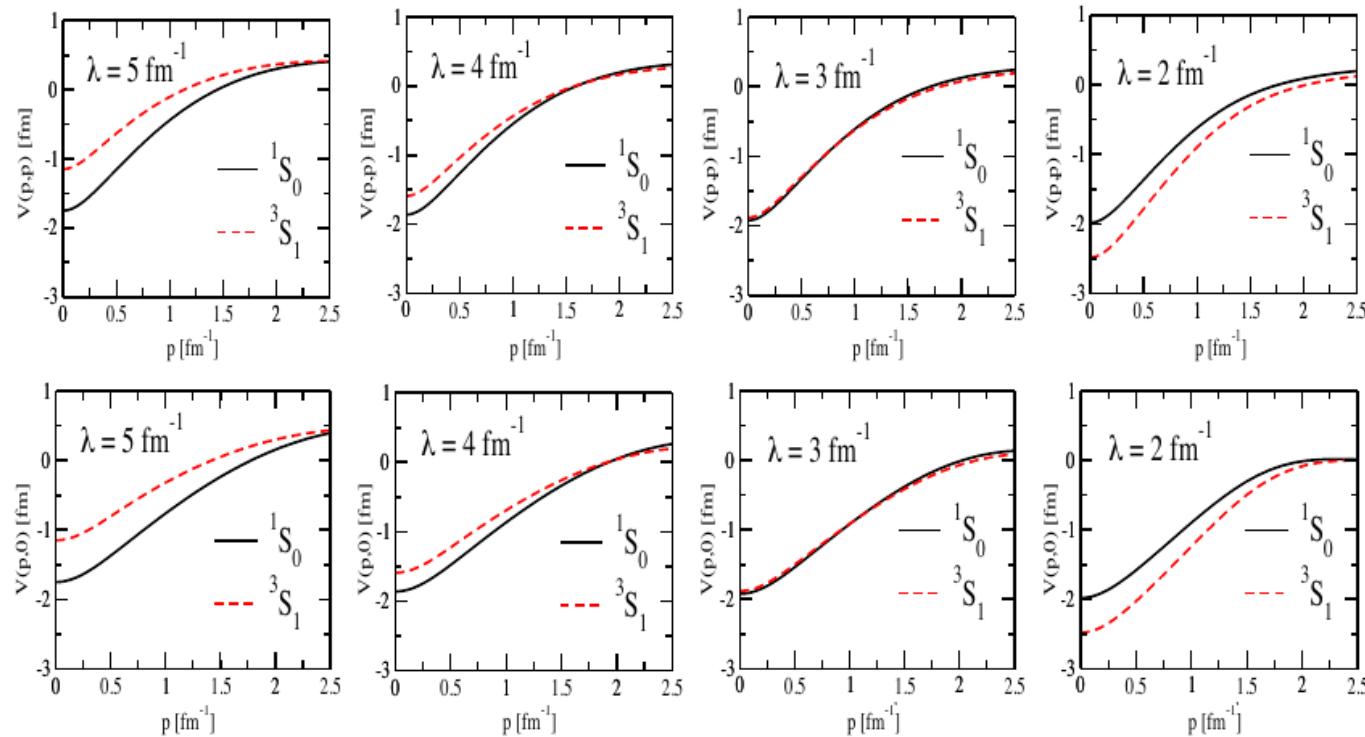
● At the scale $\lambda_{\mathbf{Wigner}} \simeq 3\,\mathbf{fm}^{-1}$ one has $V_{{}^1S_0,\mathbf{Wigner}}(p',p) \approx V_{{}^3S_1,\mathbf{Wigner}}(p',p)$

Two-nucleon matrix elements

- Calculate two-body MEs for the np pair in the $1s_{1/2}$ orbitals

- Start with AV18 and use renormalization group flow to construct a
  $V_{\mathrm{low-k}}$ at momentum scale $\Lambda = 2.5$ fm^{-1} = 490 MeV

$$\Rightarrow M(1^+) = -2.54 \text{ MeV and } M(0^-) = -2.37 \text{ MeV}$$

$\Rightarrow$ relative error consistent with the expected $1/N_C^2$ suppression

- Repeat the same exercise with chiral N3LO interaction

$$\Rightarrow M(1^+) = -2.48 \text{ MeV and } M(0^-) = -2.36 \text{ MeV } \sqrt{}$$

- Now use again AV18 at $\Lambda = 6.0$ fm^{-1} = 1.18 GeV

$$\Rightarrow M(1^+) = -1.58 \text{ MeV and } M(0^-) = 0.19 \text{ MeV } \updownarrow$$

$\Rightarrow$ spin-isospin symmetry largely violated and $\Lambda_{\mathrm{large-}N_c} \simeq 500\,\mathrm{MeV}$