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CENTER FOR SCIENCE & THOUGHT

JÜLICH Forschungszentrum

# Recent Developments in Nuclear Lattice EFT

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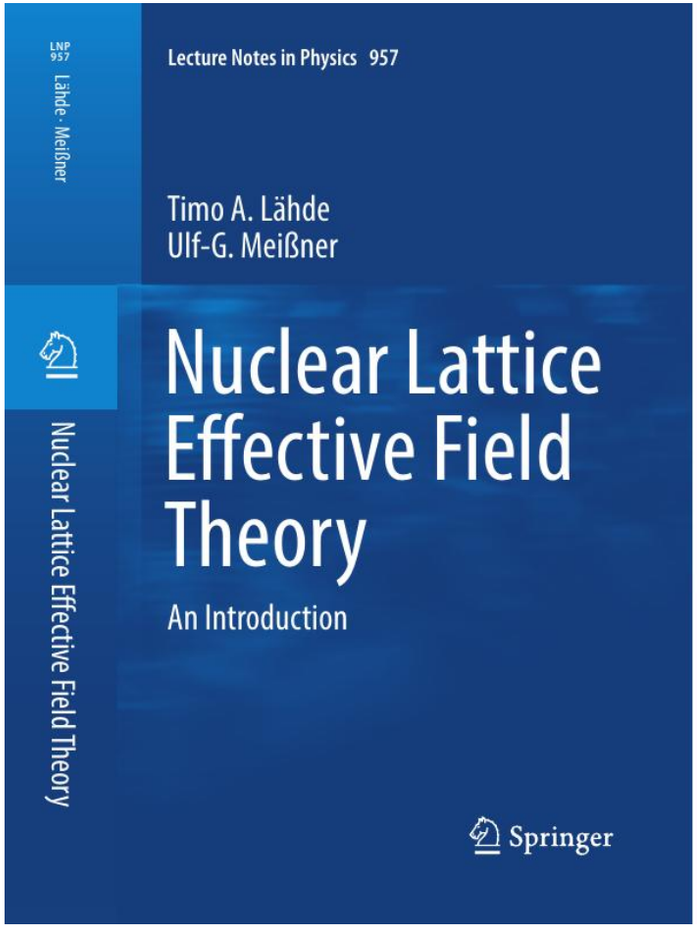
# Chiral EFT on a lattice




T. Lähde & UGM

*Nuclear Lattice Effective Field Theory - An Introduction*

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

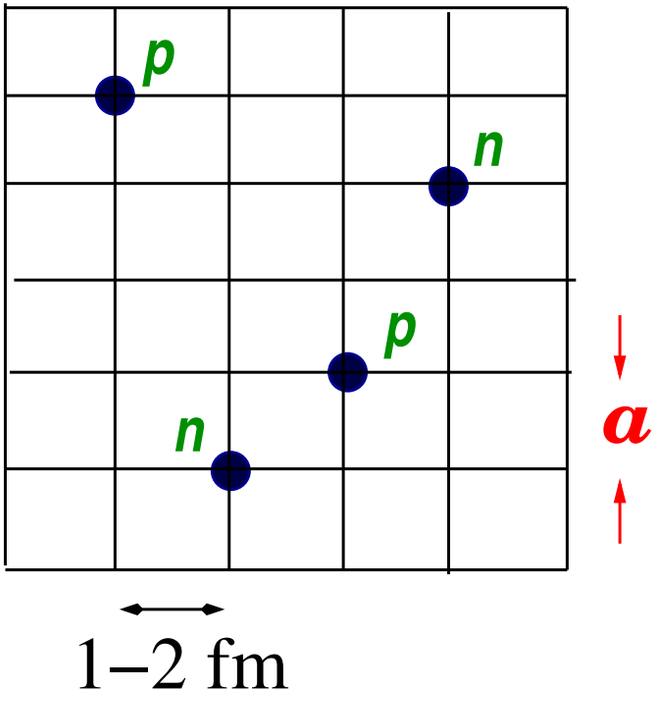
# Nuclear lattice effective field theory



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 $\Psi_A$ a Slater determinant for A free nucleons

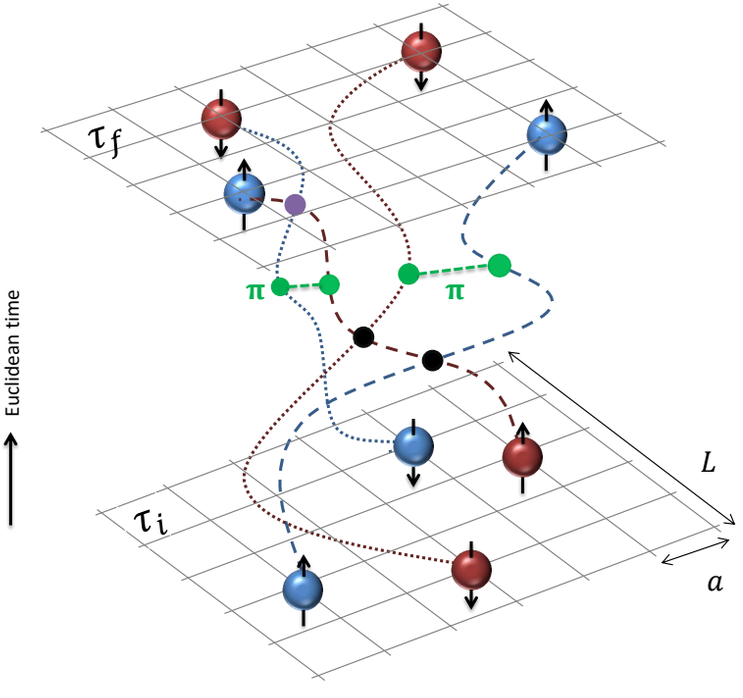
  [or a more sophisticated (correlated) initial/final state]

Euclidean time

- Transient energy

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

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



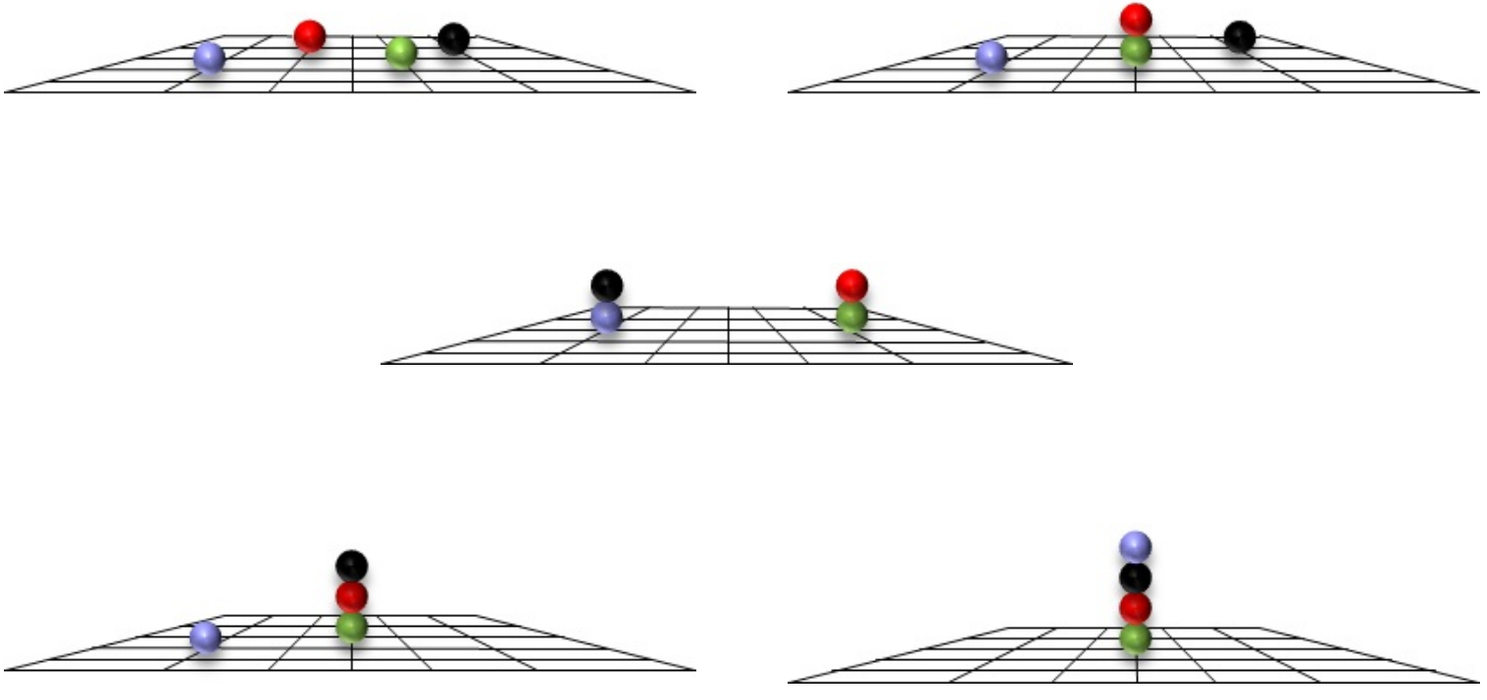

- Exp. value of any normal–ordered operator $\mathcal{O}$

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

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

# Configurations





$\Rightarrow$ all *possible* configurations are sampled

$\Rightarrow$ preparation of *all possible* initial/final states

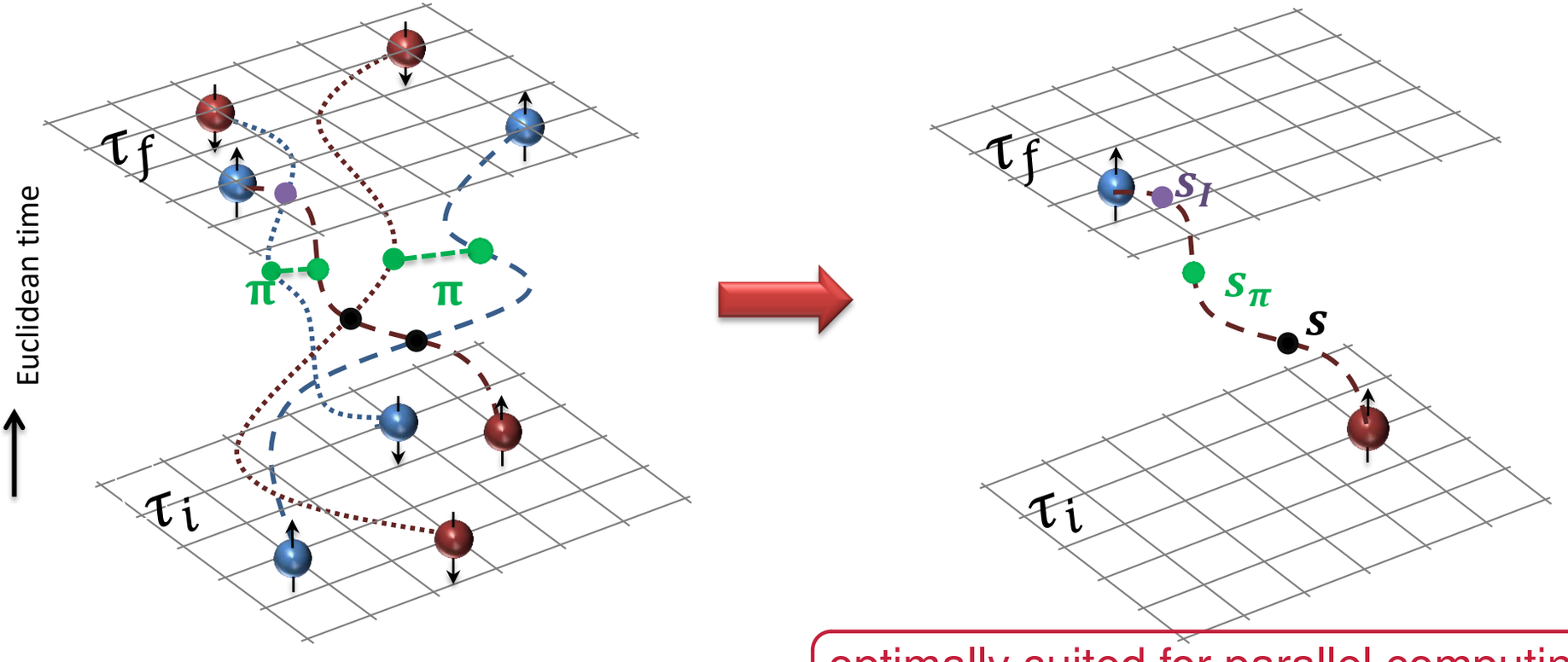
$\Rightarrow$ *clustering* emerges *naturally*

# Auxiliary field method



- Represent interactions by auxiliary fields:

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




optimally suited for parallel computing!

# Computational equipment

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

# 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:

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

- 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]]

- $V^{\mathrm{2N}}_{\mathrm{large}-N_c}$ 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 $\Delta$less 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 $\Lambda$ $\surd$

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

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

# 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]]

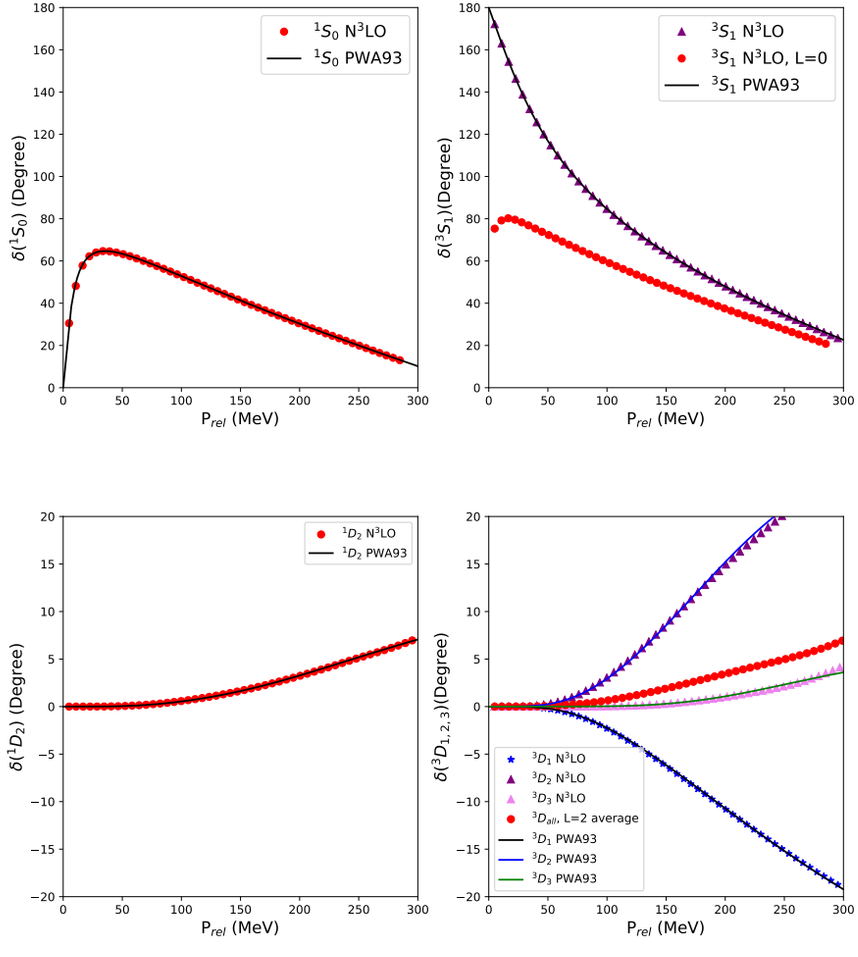
- Use N3LO action (w/ TPE absorbed in contact interactions) at $a = 1.32$ fm

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

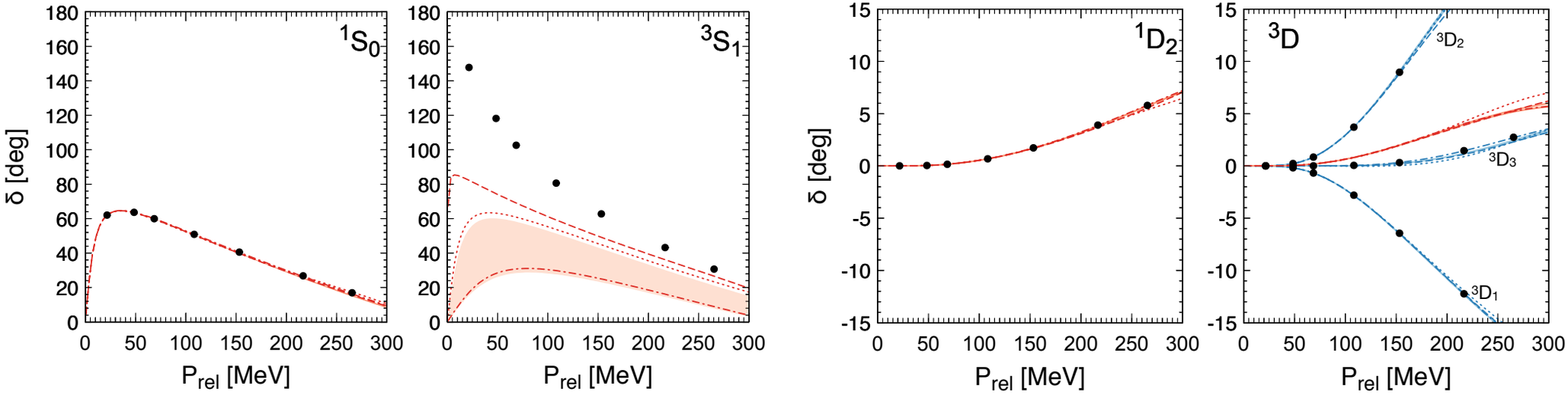
| ch., order | LEC (l.u.) | ch., order | LEC (l.u.) |
|---|---|---|---|
| ${}^1\mathrm{S}_0, Q^0$ | 1.45(5) | ${}^3\mathrm{S}_1, Q^0$ | 1.56(3) |
| ${}^1\mathrm{S}_0, Q^2$ | −0.47(3) | ${}^3\mathrm{S}_1, Q^2$ | −0.53(1) |
| ${}^1\mathrm{S}_0, Q^4$ | 0.13(1) | ${}^3\mathrm{S}_1, Q^4$ | 0.12(1) |
| ${}^1\mathrm{D}_2,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




| | | |
|---|---|---|
| · · · · · · | 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 |
| ▭ | 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)

$\rightarrow$ 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 $A$

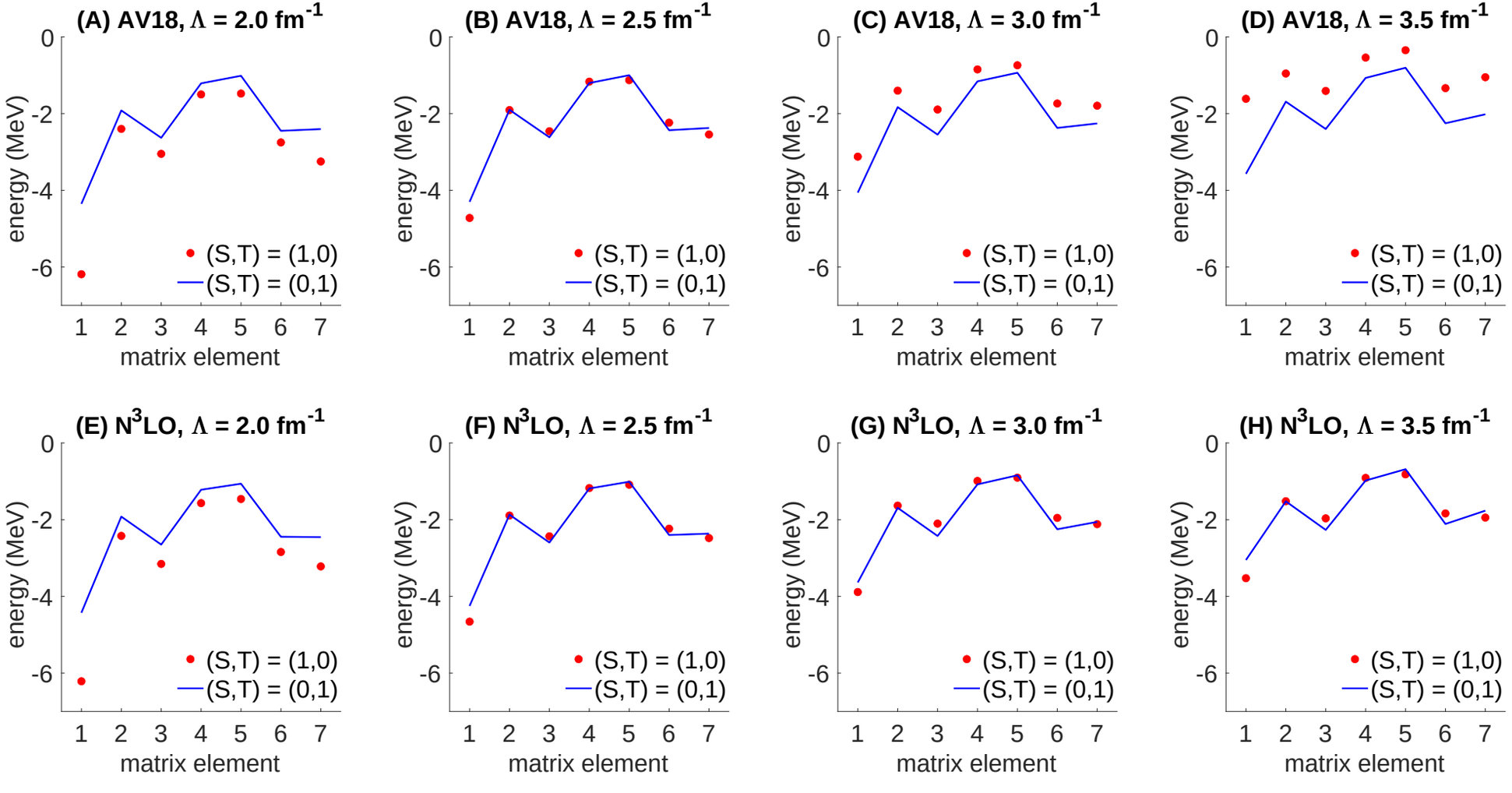
ME 7 corresponds to the $1s_{1/2}$ orbitals discussed before

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

$\rightarrow$ Work out $M(S,T)$ for various forces at $\Lambda = 2.0, 2.5, 3.0, 3.5$ 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 $\Lambda \sim 500\,\text{MeV}$
  - 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:

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

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

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

$\Rightarrow$ 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

  $\hookrightarrow$ 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 $\alpha$-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

  ↪ 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:

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

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

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

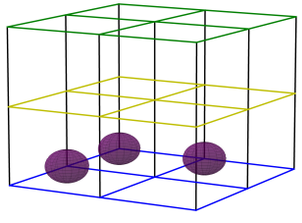
↪ only two adjustable parameters ($C_2, s_L$) fitted to $E_{^4\rm He}$ & $E_{^{12}\rm C}$

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

# Configurations

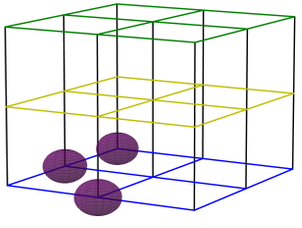
- Cluster and shell model configurations

S1



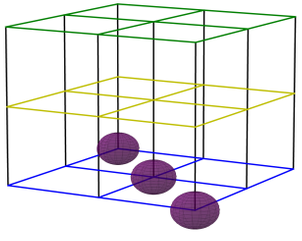
— isoscele right triangle

S2



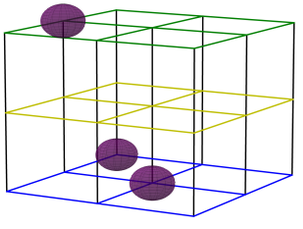
— “bent-arm” shape

S3



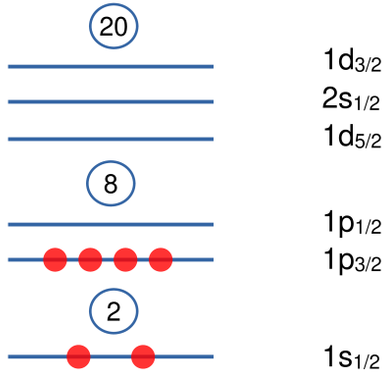
— linear diagonal chain

S4

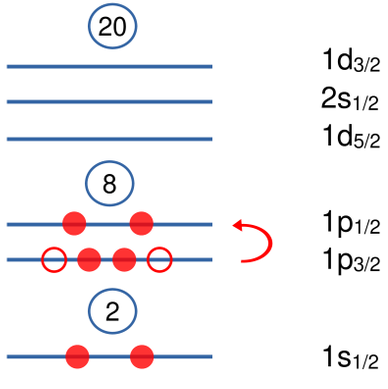


— acute isoscele triangle

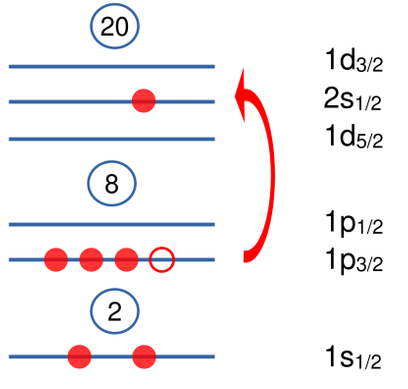
Gaussian wave packets
$w = 1.7 - 2.1$ fm




— ground state $|0\rangle$




— $2p$-$2h$ state, $J_z = 0$

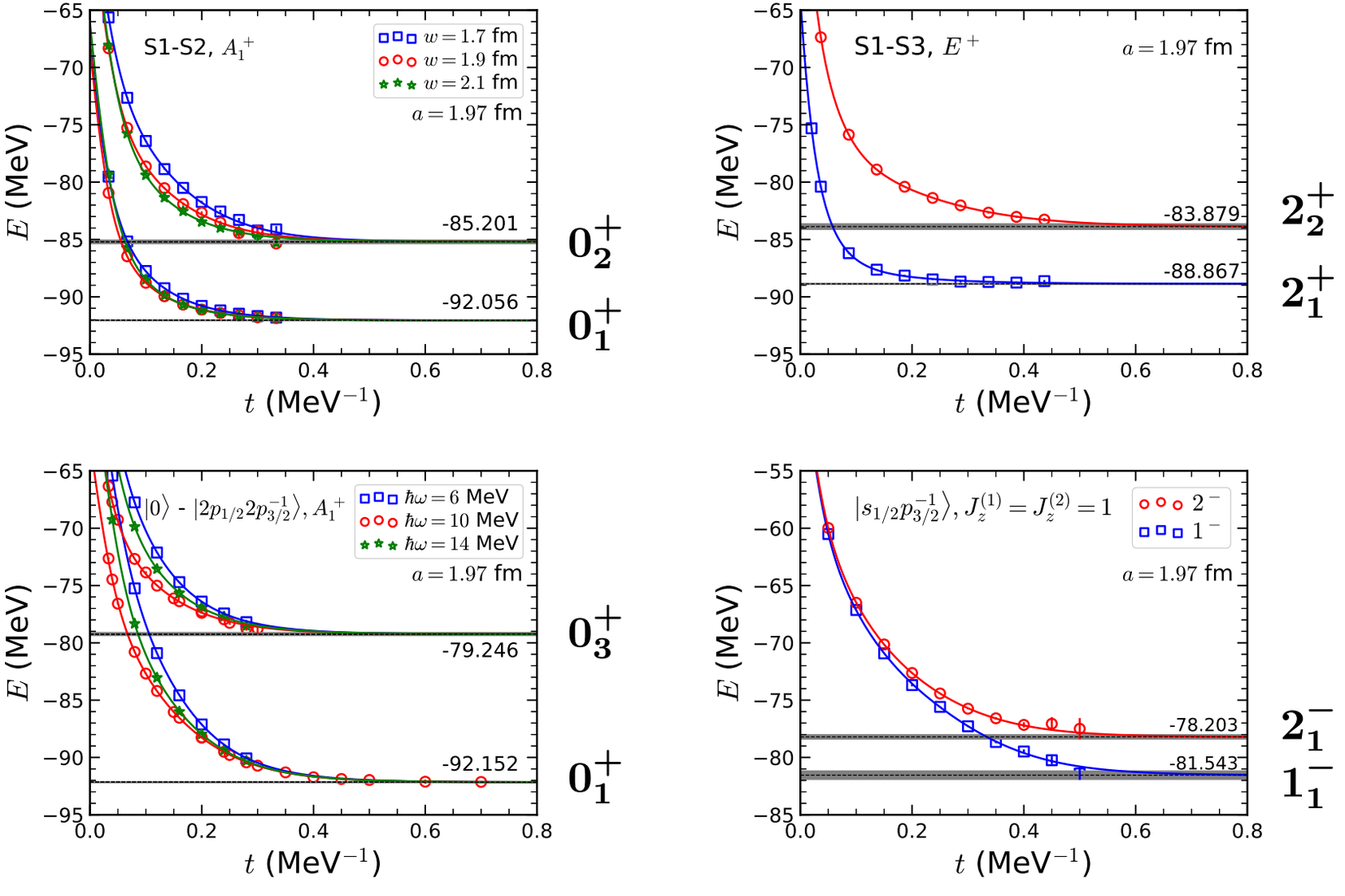



— $1p$-$1h$ state, $J_z^{(1)} = J_z^{(2)} = 1$

# Transient energies



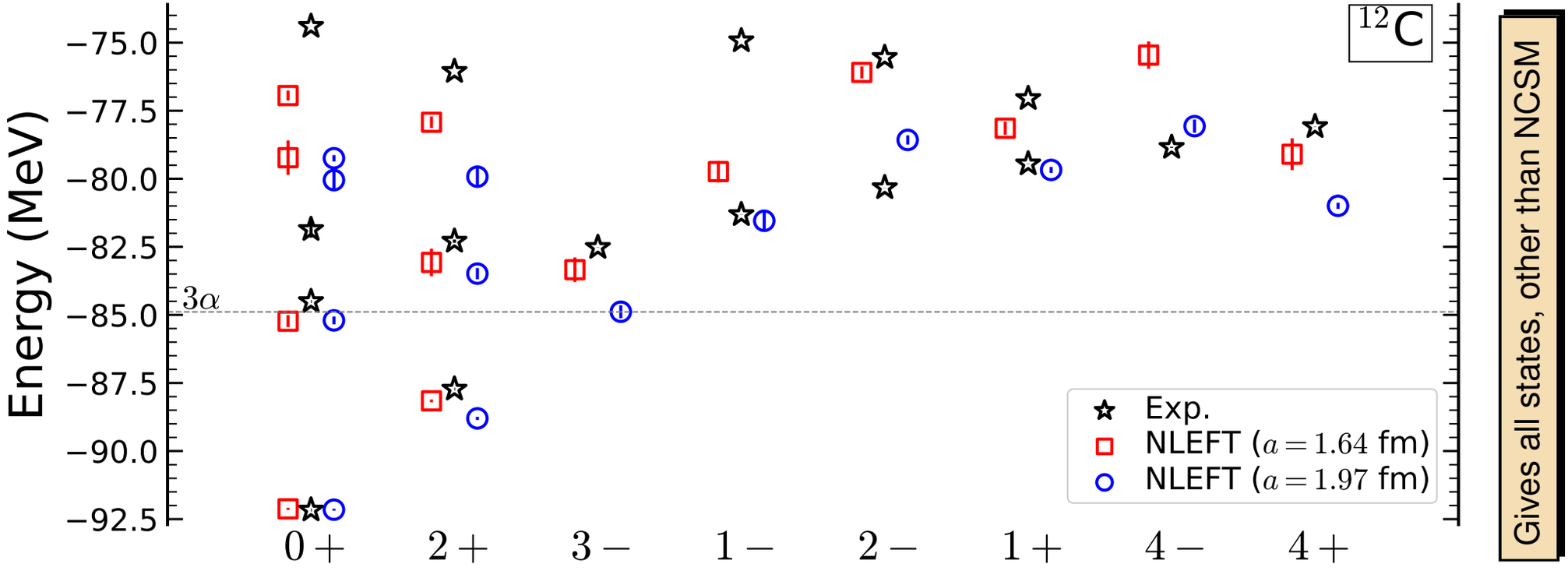
- Transient energies from cluster and shell-model configurations



# Spectrum of $^{12}$C

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

- Amazingly precise description → great starting point




→ 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, [arXiv:2202.13596 [nucl-th]]

- 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

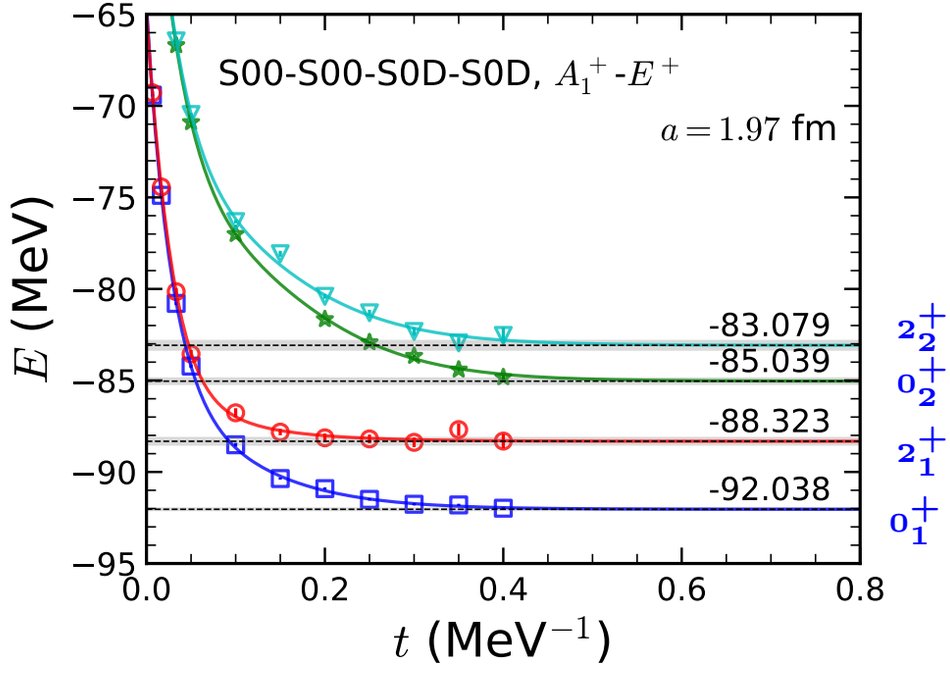
  $s_{\mathrm{L}}$ – radius of $^{12}$C around 2.4 fm

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

- Calculation of em transitions

  requires coupled-channel approach

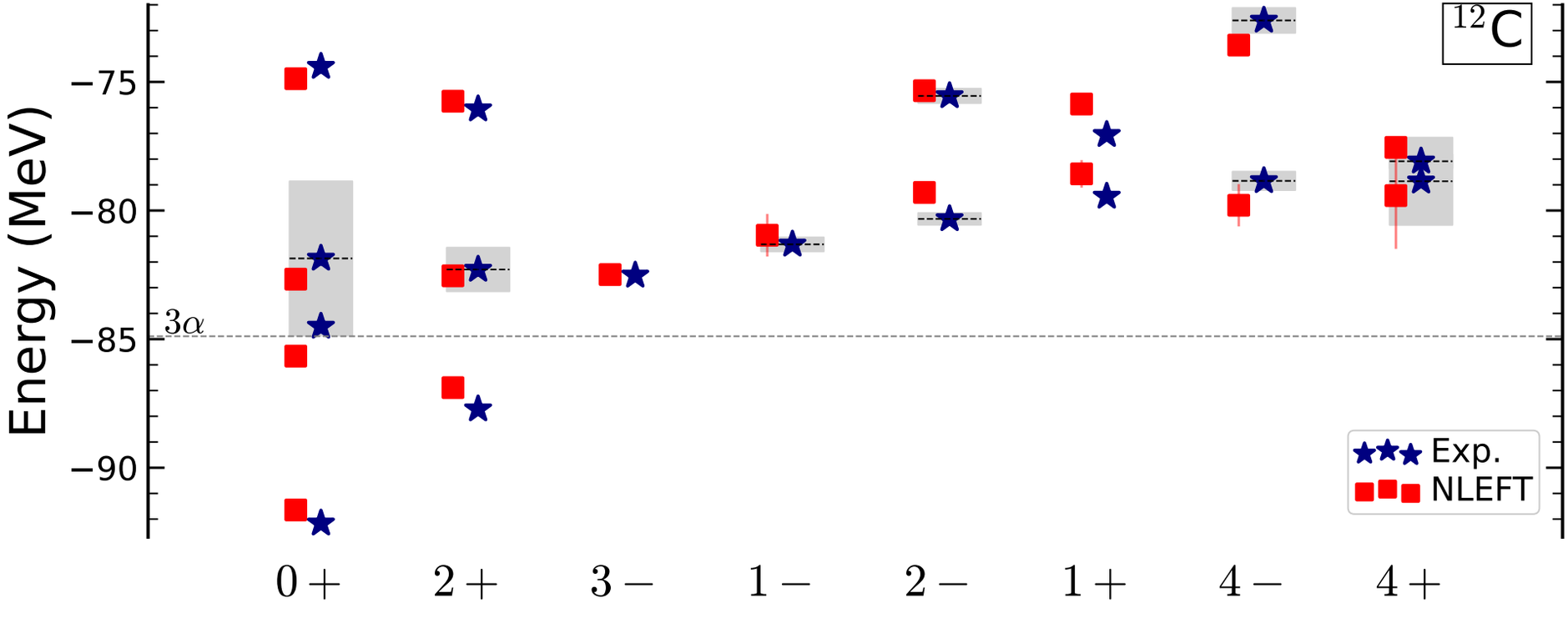
  e.g. $0^+$ and $2^+$ states



# Spectrum of $^{12}$C reloaded

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

- 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, [arXiv:2202.13596 [nucl-th]]

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

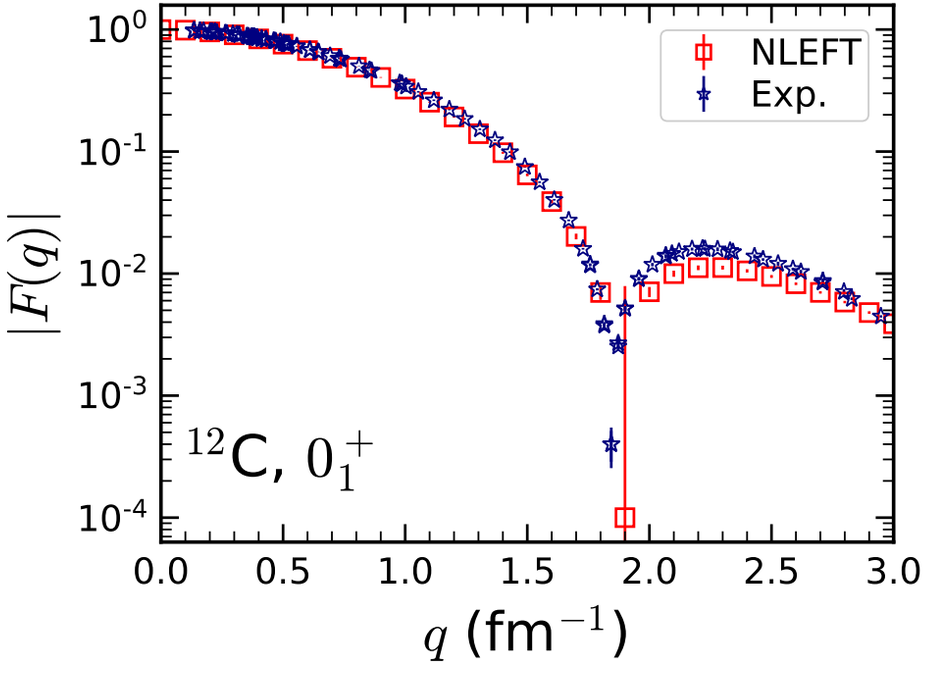
| | NLEFT | FMD | $\alpha$ cluster | BEC | RXMC | Exp. |
|---|---|---|---|---|---|---|
| $r_c(0_1^+)$ [fm] | $\mathbf{2.53(1)}$ | 2.53 | 2.54 | 2.53 | 2.65 | $\mathbf{2.47(2)}$ |
| $r(0_2^+)$ [fm] | $\mathbf{3.45(2)}$ | 3.38 | 3.71 | 3.83 | 4.00 | – |
| $r(0_3^+)$ [fm] | $\mathbf{3.47(1)}$ | 4.62 | 4.75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

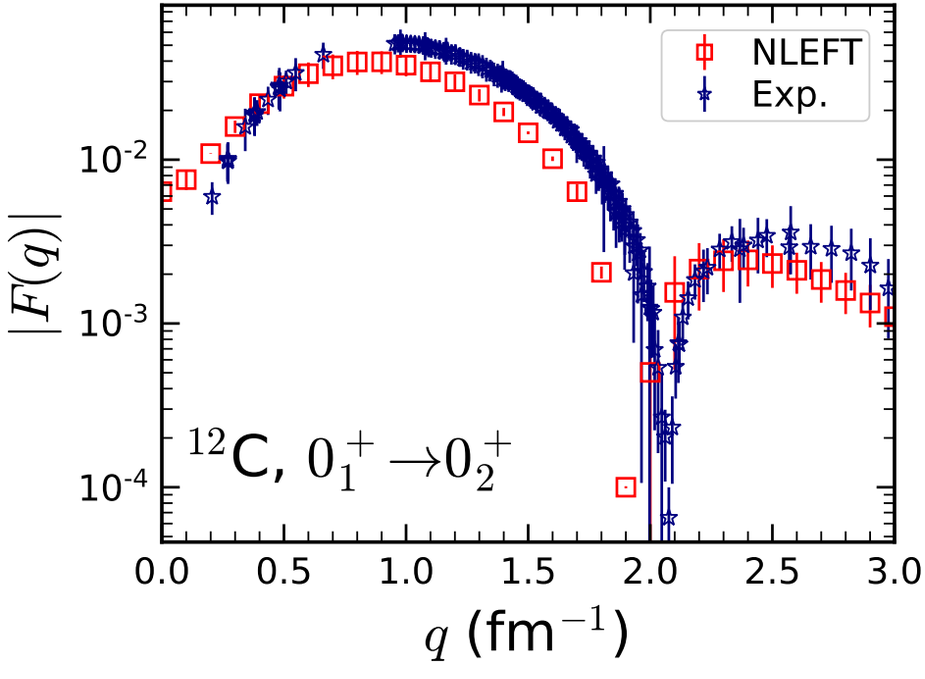
| | NLEFT | FMD | $\alpha$ cluster | NCSM | Exp. |
|---|---|---|---|---|---|
| $Q(2_1^+)$ [$e$ fm$^2$] | $\mathbf{6.8(3)}$ | – | – | 6.3(3) | $\mathbf{8.1(2.3)}$ |
| $Q(2_2^+)$ [$e$ fm$^2$] | $\mathbf{-35(1)}$ | – | – | – | – |
| $M(E0, 0_1^+ \to 0_2^+)$ [$e$ fm$^2$] | $\mathbf{4.8(3)}$ | 6.5 | 6.5 | – | $\mathbf{5.4(2)}$ |
| $M(E0, 0_1^+ \to 0_3^+)$ [$e$ 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, [arXiv:2202.13596 [nucl-th]]

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



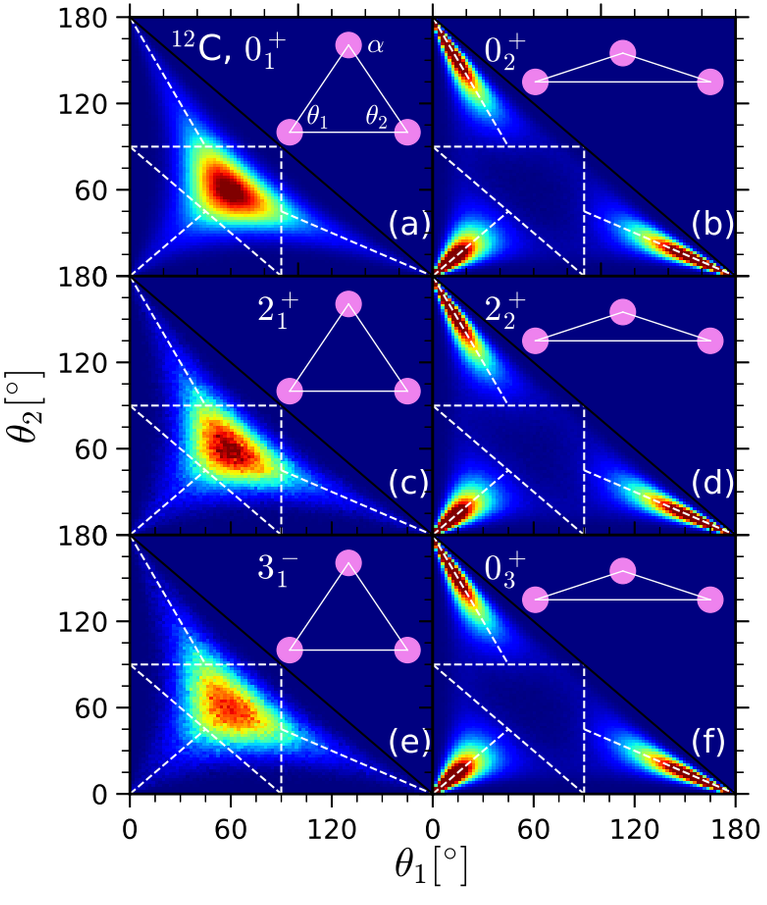

Sick, McCarthy, Nucl. Phys. A 150 (1970) 631
Strehl, Z. Phys. 234 (1970) 416
Crannell et al., Nucl. Phys. A 758 (2005) 399

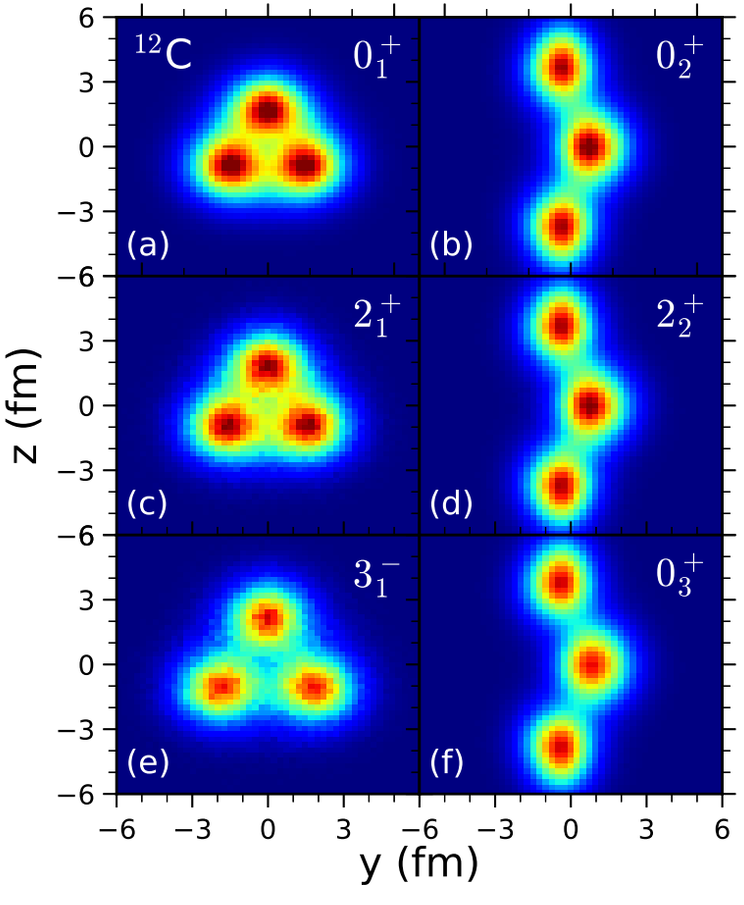
Chernykh et al., Phys. Rev. Lett. 105 (2010) 022501

# Emergence of geometry



- Use the pinhole algorithm to measure the distribution of $\alpha$-clusters/matter:



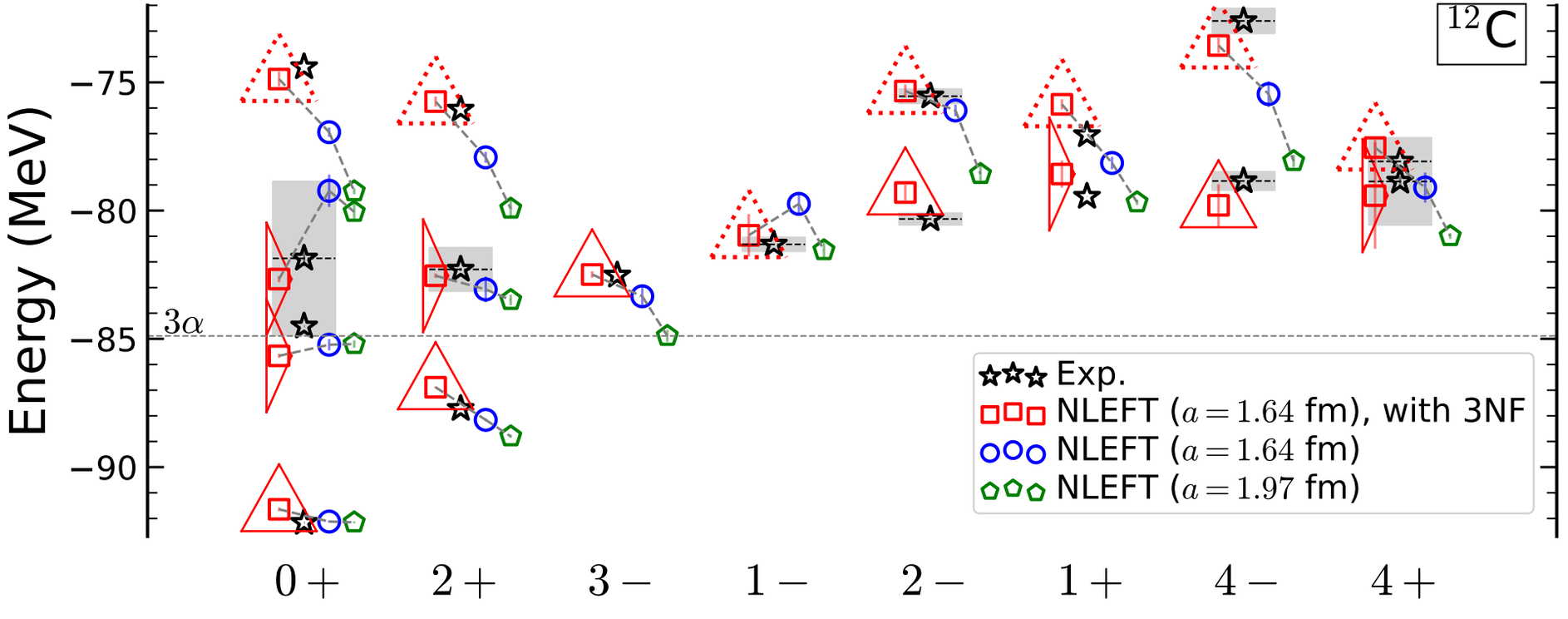




- equilateral & obstuse triangles $\longrightarrow 2^+$ states are excitations of the $0^+$ states

# 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

  ↪ minimize the sign oscillations

  ↪ minimize the higher-body forces

  ↪ gain an understanding of the essentials of nuclear binding

  ↪ essentially done $\surd$

  **2)** Work out the corrections to N3LO

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

  ↪ new important technique: **wave function matching** → Dean's talk

  ↪ second for the spectra/radii/... of nuclei (first results)

  ↪ third for nuclear reactions (nuclear astrophysics)

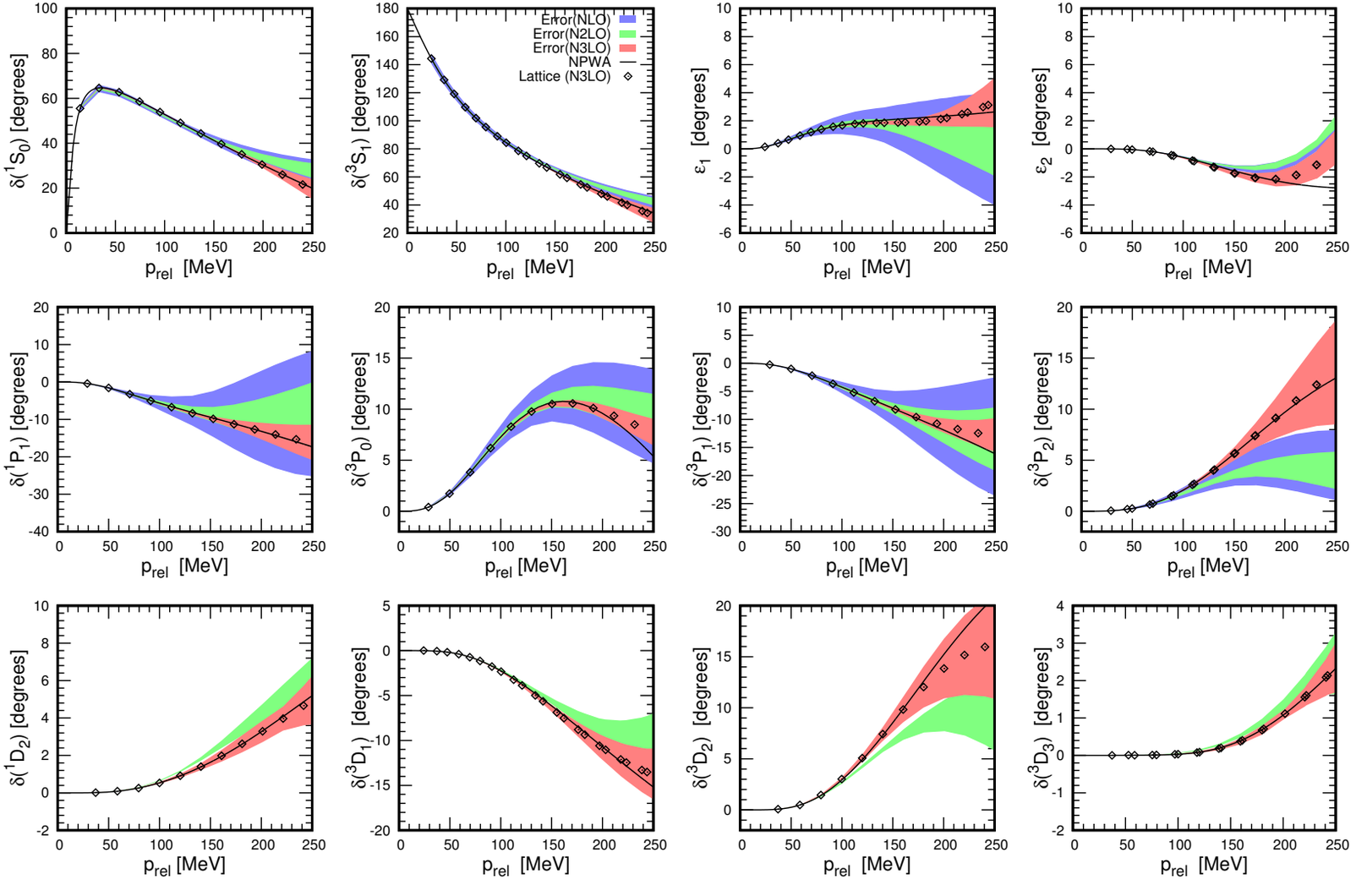
# NN interaction at N3LO



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



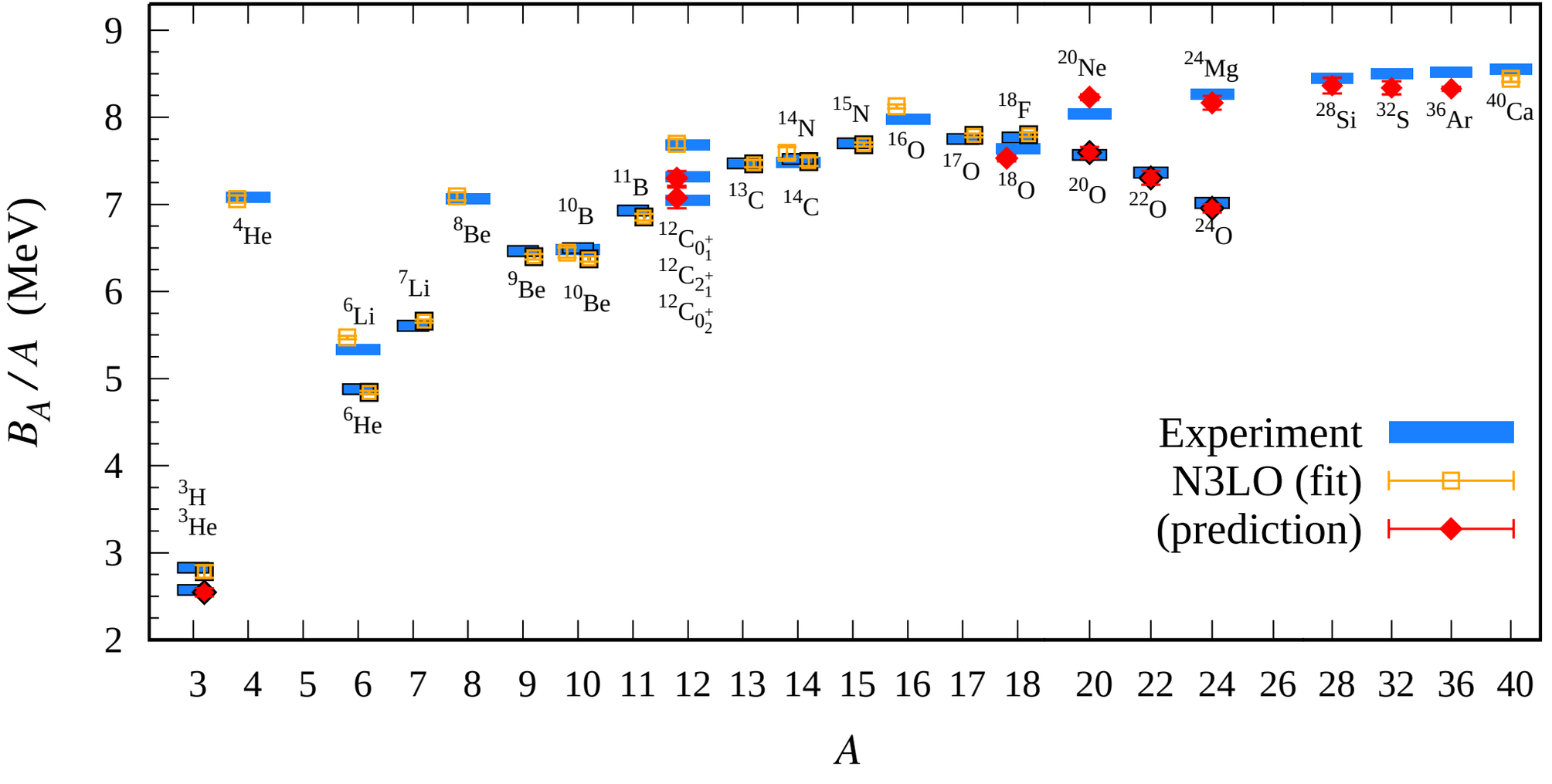

uncertainty estimates á la Epelbaum, Krebs, UGM, Eur. Phys. J. A **51** (2015) 53

# Nuclei at N3LO



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

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

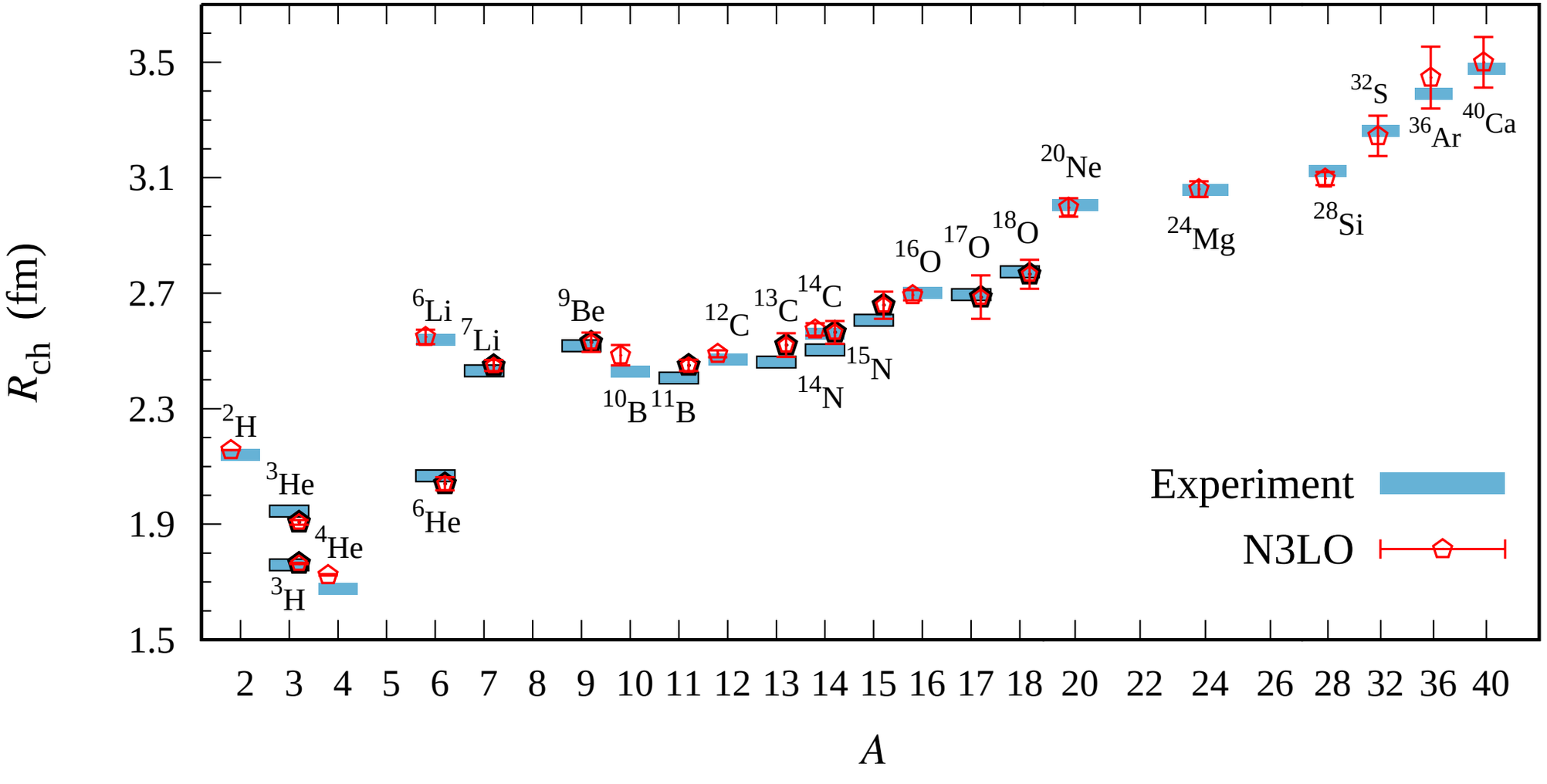


# Charge radii at N3LO



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

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

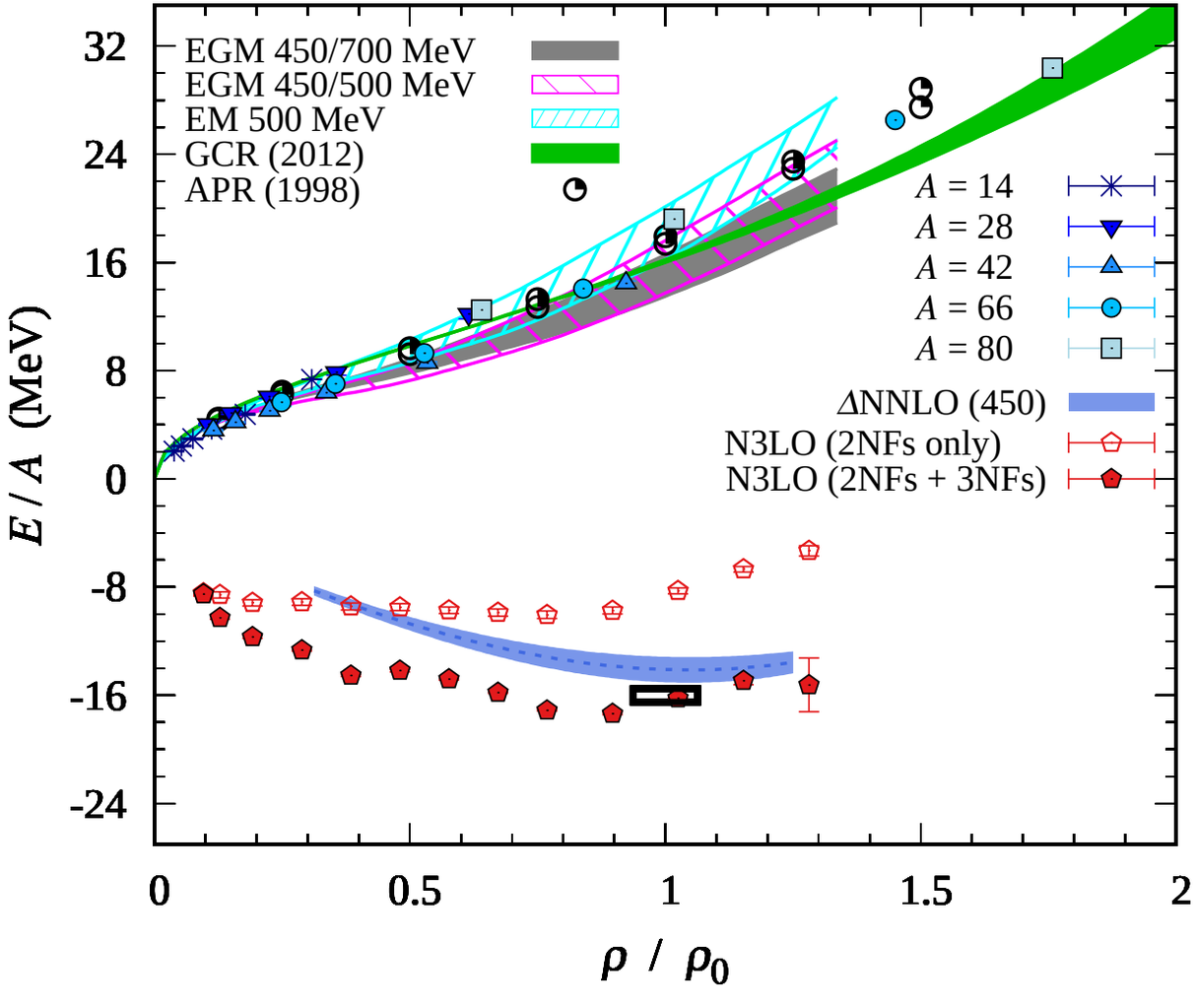


# Neutron & nuclear matter at N3LO



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

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



# *Ab Initio* Nuclear Thermodynamics

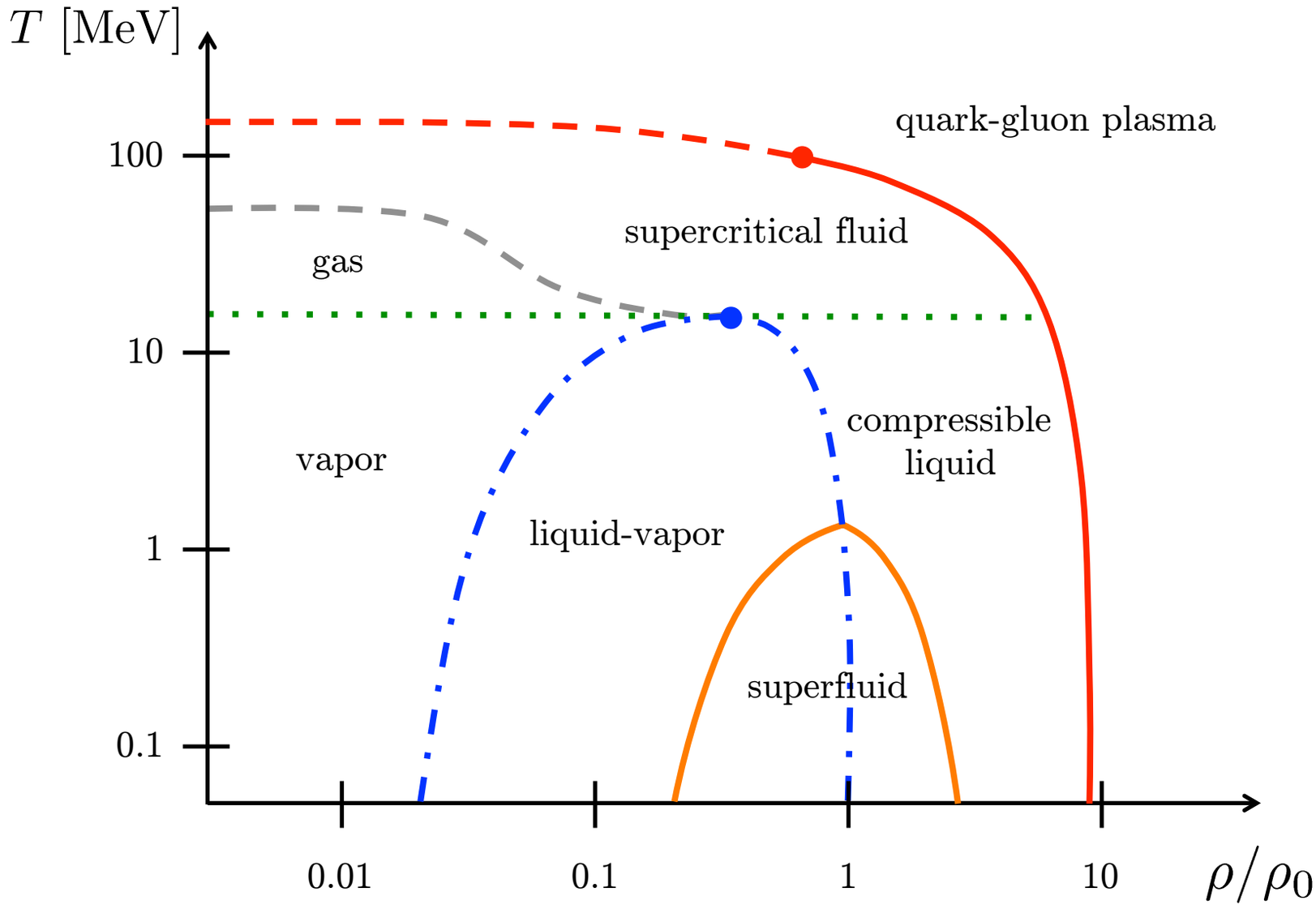
B. N. Lu, N. Li, S. Elhatisari, D. Lee, J. Drut, T. Lähde, E. Epelbaum, UGM,
Phys. Rev. Lett. **125** (2020) 192502 [arXiv:1912.05105]

# Phase diagram of strongly interacting matter



- Sketch of the phase diagram of strongly interacting matter

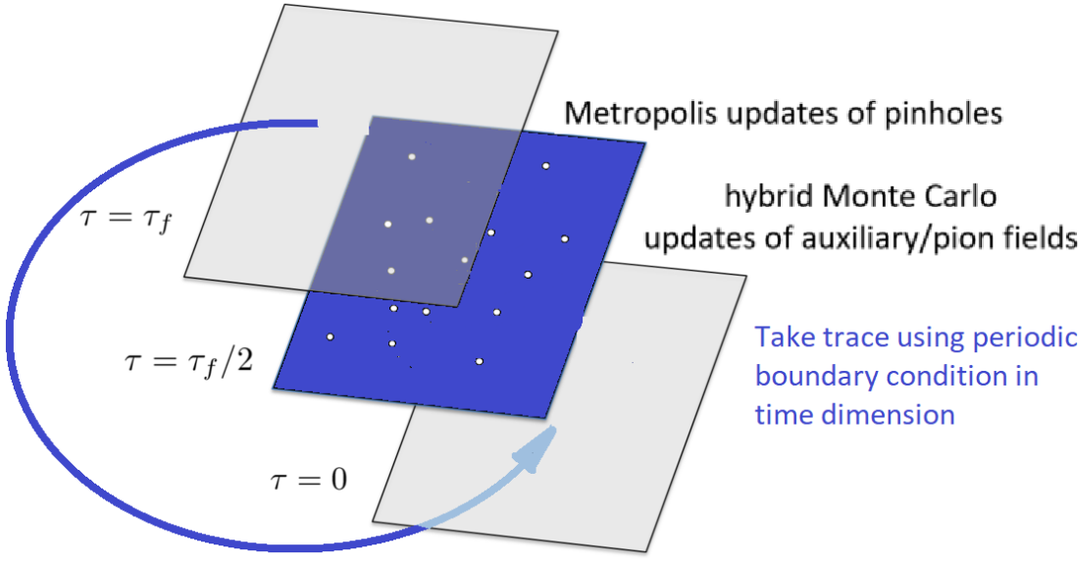
Fig. courtesy B.-N. Lu



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

- 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

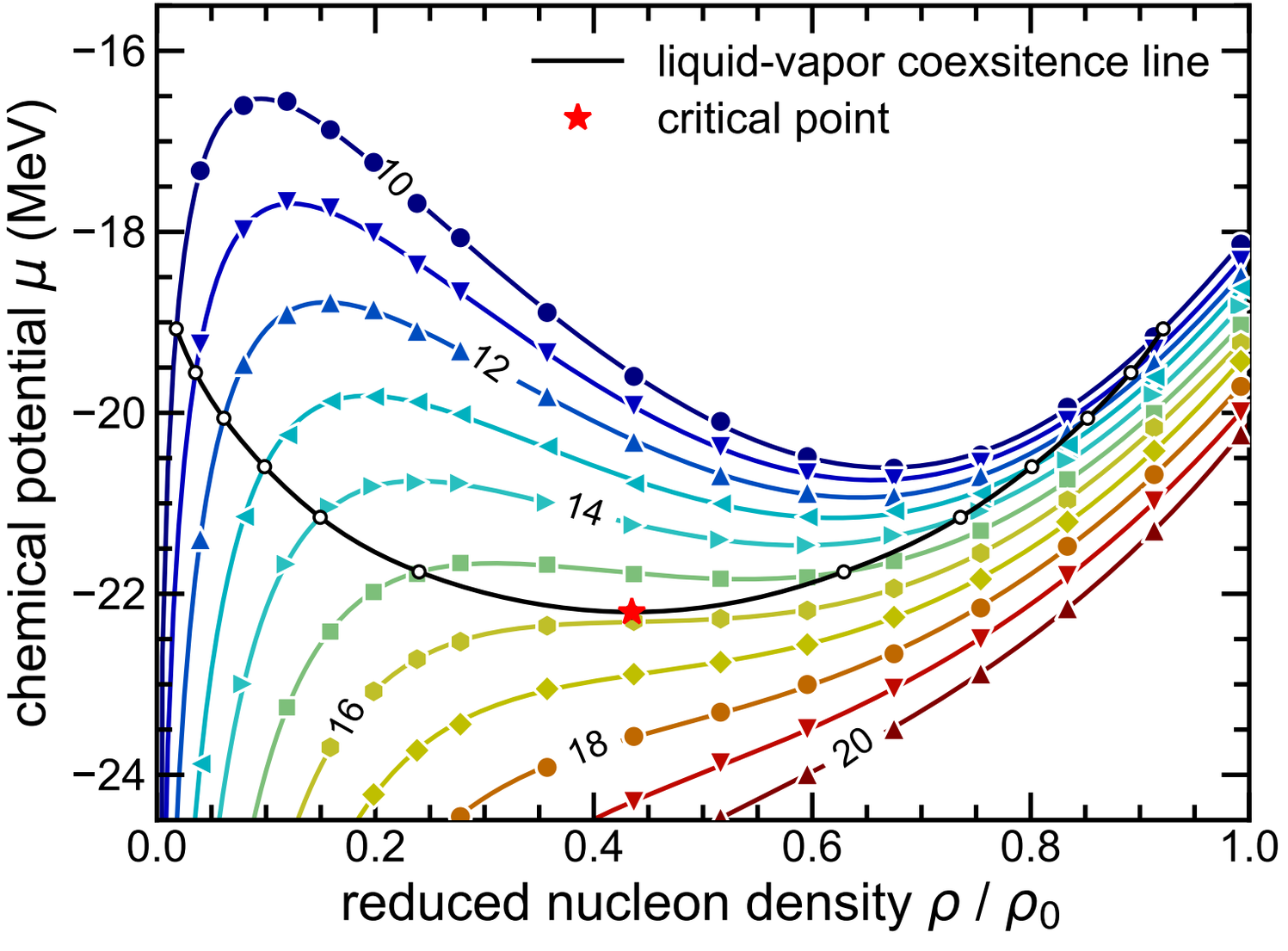
consider $T = 10 \ldots 20$ MeV

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

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

# Chemical potential

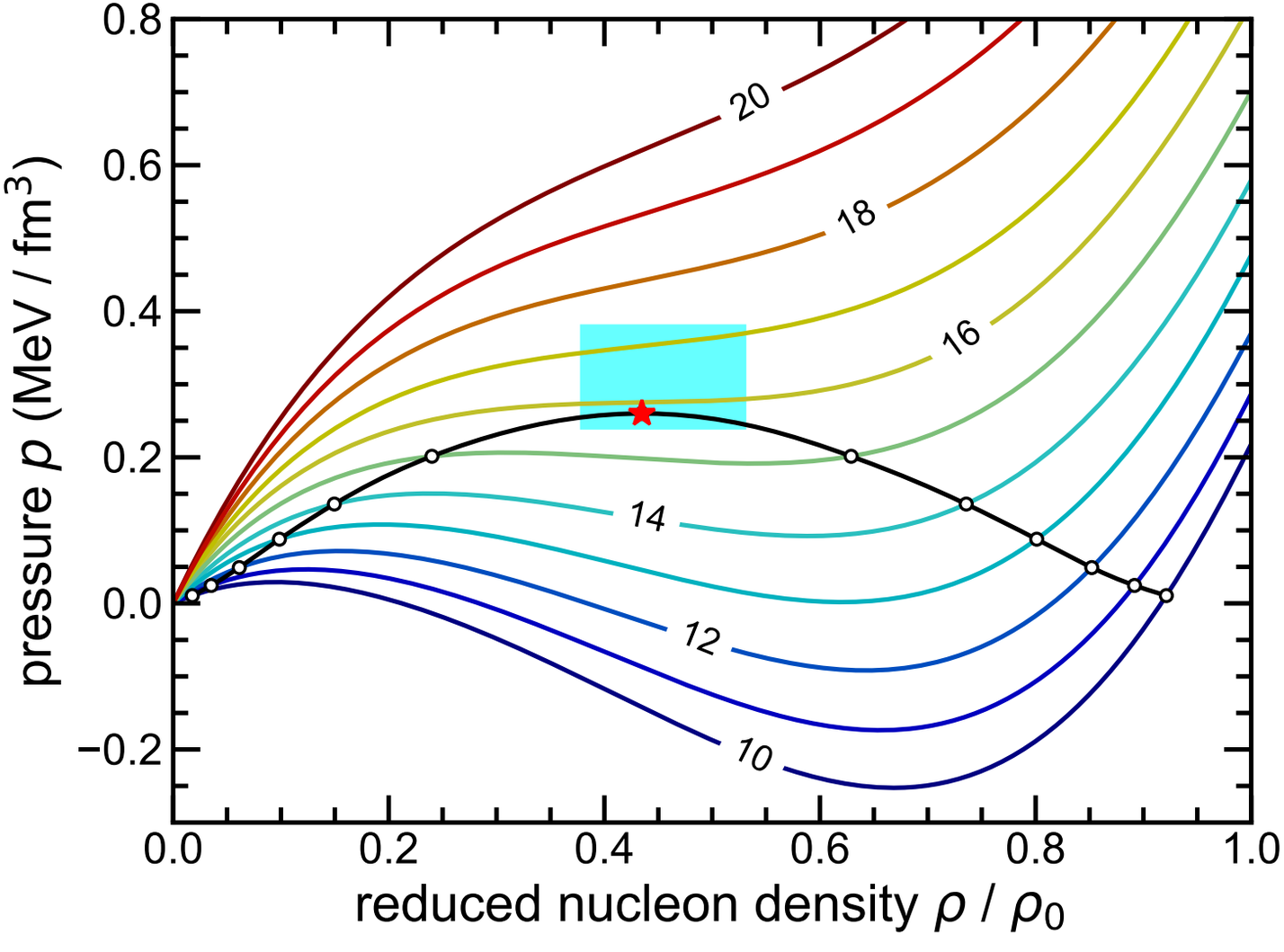
- Calculated from the free energy: $\mu = (F(N+1) - F(N-1))/2$




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$^{-3}$

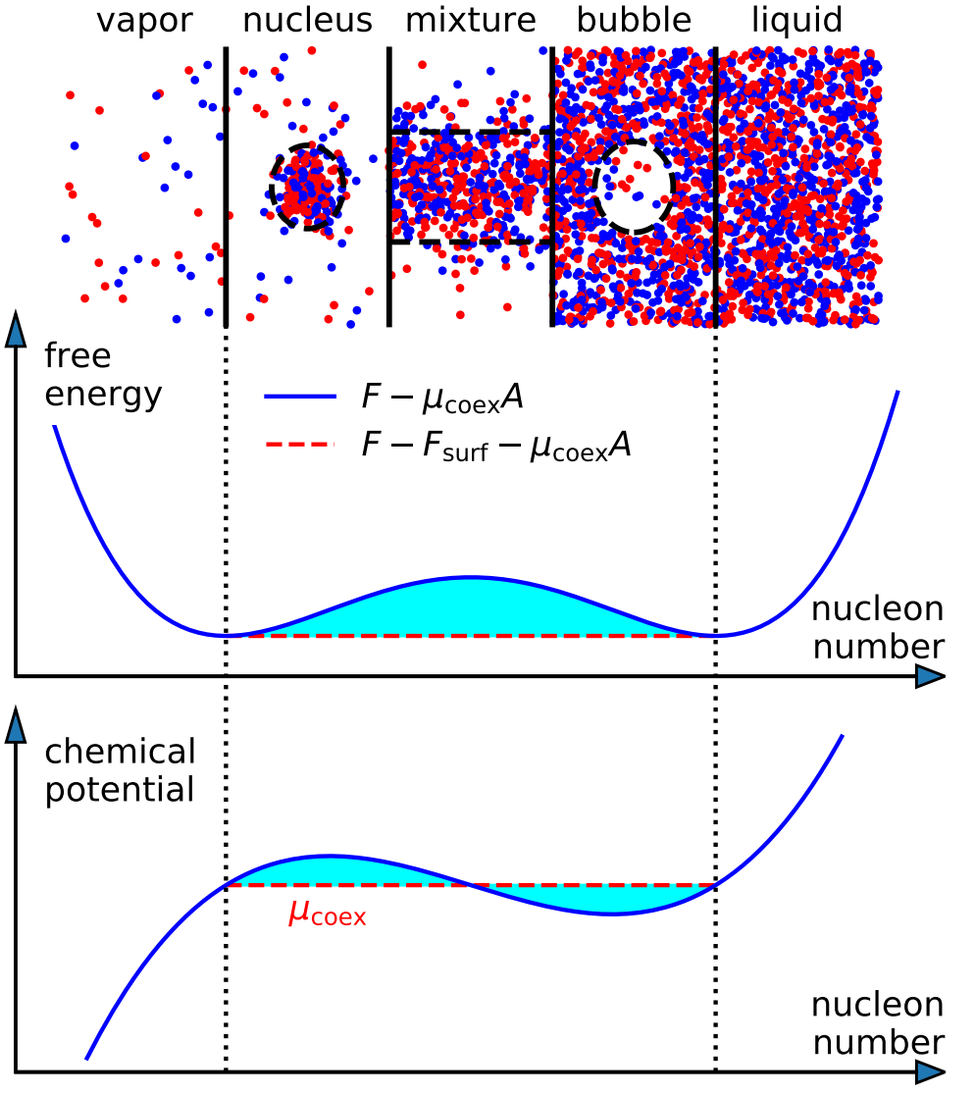



Experiment: $T_c = 15.0(3)$ MeV, $P_c = 0.31(7)$ MeV/fm$^3$, $\rho_c = 0.06(2)$ fm$^{-3}$

# 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 $\mu = \partial F / \partial A$



# 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 promosing results for nuclei at N3LO
    - ↪ requires the new wave function matching technique → Dean's talk

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

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

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

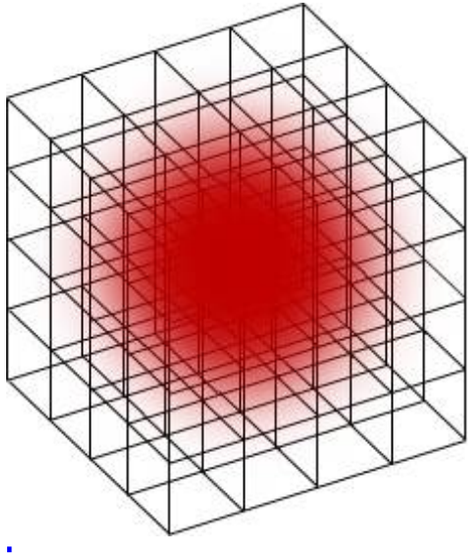
- and . . .

# SPARES

# 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

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

$i_{\rm com}$ $(j_{\rm com})$ = 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

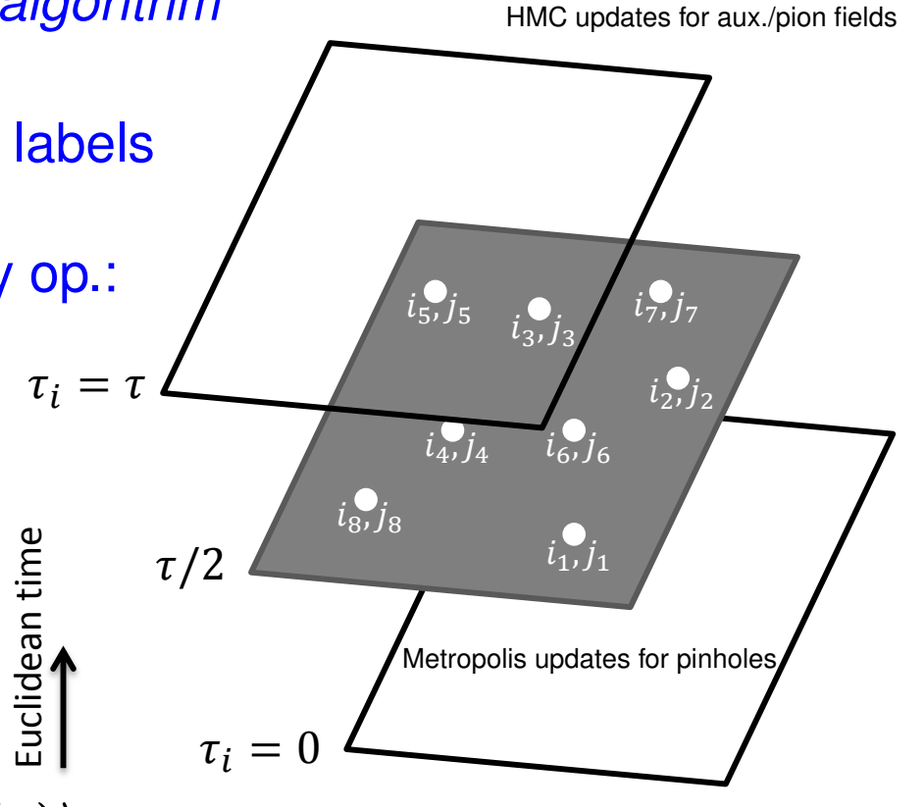


- Solution to the CM-problem:

  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:

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

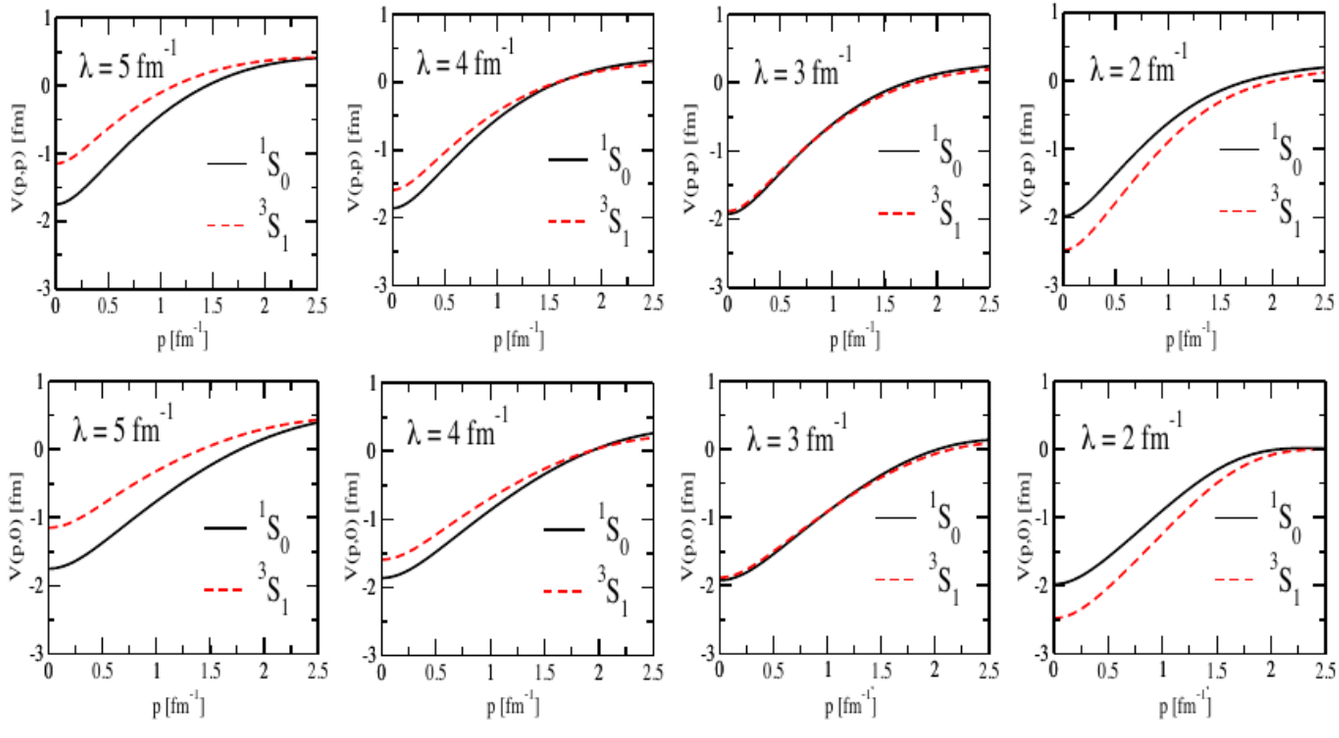
- Allows to measure proton and neutron distributions

- Resolution scale $\sim a/A$ as cm position $\mathbf{r}_{\mathbf{cm}}$ is an integer $\mathbf{n}_{\mathbf{cm}}$ 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 $V_{^1S_0,{\rm Wigner}}(p',p) \approx V_{^3S_1,{\rm Wigner}}(p',p)$