EMERGENT GEOMETRY AND DUALITY IN THE CARBON NUCLEUS

ESNT Workshop “Espace de Structure et de Réactions Nucléaires Théorique”, CEA Paris-Saclay

04/12 2024 I TIMO A. LÄHDE (FORSCHUNGSZENTRUM JÜLICH)

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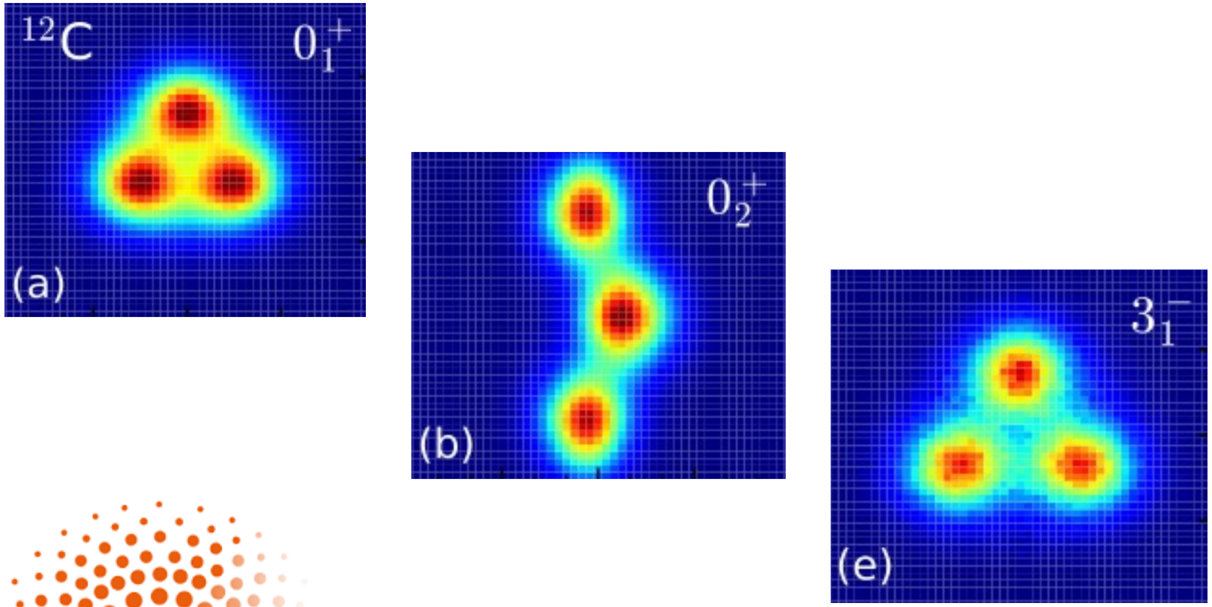
Emergent geometry and duality in the carbon nucleus

Collaborators: Shihang Shen, Dean Lee, Bing-Nan Lu, Ulf-G. Meißner



Light
Nuclei
Workshop
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2024

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CONTENTS

- Methods of Nuclear Lattice Effective Field Theory (NLEFT) — see also talk (Friday) by Lukas Bovermann
- Calculating the spectrum of ^{12}C — Wigner SU(4) symmetry
- Accessing the cluster structure — Pinhole Algorithm
- Emergence of alpha clustering in ^{12}C — Tomography
- Summary & Outlook

AB INITIO STUDIES (A SAMPLE) OF ^{12}C

- Green's function Monte Carlo —> see Gandolfi, Lonardoni, Lovato, Piarulli, Front. Phys. **8** (2020) 117
- Monte Carlo Shell Model —> see Otsuka, Abe, Yoshida, Tsunoda et al., Nature Commun. **13** (2022) 2234
- No-core shell model —> see Choudhary, Srivastava, Gennari, Navrátil, PRC **107** (2023) 014309

- Our method — Auxiliary Field Quantum Monte Carlo (AFQMC)
  - First NLEFT work on ground and Hoyle states of ^{12}C

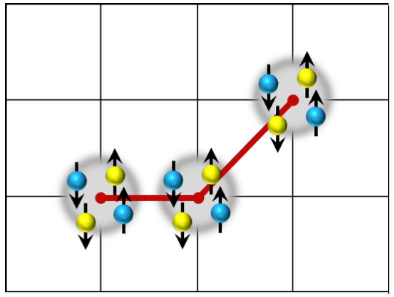
    Epelbaum, Krebs, Lee, Meißner, PRL **106** (2011) 192501

    Epelbaum, Krebs, Lähde, Lee, Meißner, PRL **109** (2012) 252501

  - Structure of the Hoyle state?

    Freer, Fynbo, Prog. Part. Nucl. Phys. **78** (2014) 1

- Methods have progressed since 2012 — full AFQMC calculation of the ^{12}C spectrum now possible



24 rotational orientations

NUCLEAR LATTICE EFT

Frank, Brockmann (1992); Koonin, Müller, Seki, van Kolck (2000); Lee, Schäfer (2004) ...

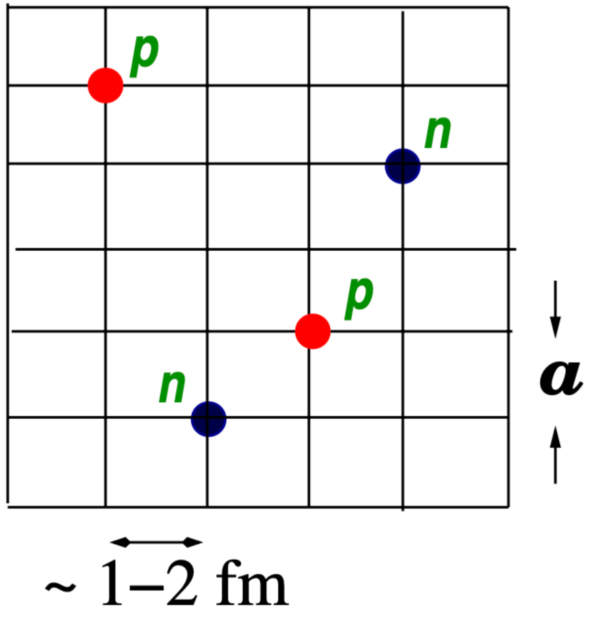
Borasoy, Krebs, Lee, Meißner, NPA **768** (2006) 179; Borasoy, Epelbaum, Krebs, Lee, Meißner, EPJA **31** (2007) 105

- A new method for the nuclear many-body problem
- Discrete space and Euclidean time, theory of fermions (nucleons) with spin and isospin

$$V = L_s^3 \times L_t$$

- Chiral EFT potential with (smeared) contact interactions, pion exchanges + Coulomb

—> see Epelbaum, Hammer, Meißner, Rev. Mod. Phys. **81** (2009) 1773



- Physics independent of lattice spacing

$$a = 1 \ldots 2 \text{ fm} \longrightarrow p_{\max} = \pi/a = 315 \ldots 630 \text{ MeV}$$

Alarcòn et al., EPJA **53** (2017) 83; Klein et al., EPJA **54** (2018) 121

- Strong suppression of sign oscillations due to (approximate) Wigner SU(4) spin-isospin symmetry — very important for Monte Carlo methods

Wigner, Phys. Rev. **51** (1937) 106; Mehen et al., PRL **83** (1999) 931

Chen, Lee, Schäfer, PRL **93** (2004) 242302

EUCLIDEAN TIME PROJECTION

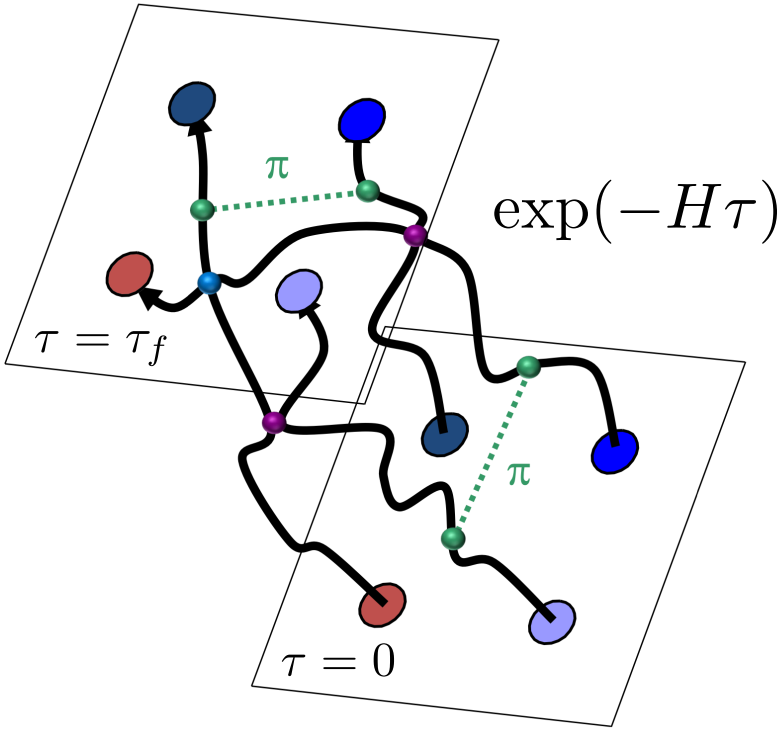
Lee, Prog. Part. Nucl. Phys. **63** (2009) 117

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

- Euclidean time projection amplitude (for many-body Hamiltonian *H*)

$$Z(\tau) = \langle \Psi | \exp(-H\tau) | \Psi \rangle$$

Slater determinant for A nucleons
(more sophisticated trial states also possible)



- Transient energy

$$E(\tau) = -\frac{d}{d\tau} \ln Z(\tau), \quad E_0 = \lim_{\tau\to\infty} E(\tau)$$

Ground state obtained for large times
(usually reached by extrapolation)

- Expectation values of operators

$$Z^{\mathcal{O}}(\tau) = \langle \Psi | \exp(-H\tau/2) \mathcal{O} \exp(-H\tau/2) | \Psi \rangle$$

$$\langle \Psi_0 | \mathcal{O} | \Psi_0 \rangle = \lim_{\tau\to\infty} \frac{Z^{\mathcal{O}}(\tau)}{Z(\tau)}$$

Normal-ordered operators

TRANSFER MATRIX METHOD

Lee, Prog. Part. Nucl. Phys. **63** (2009) 117

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

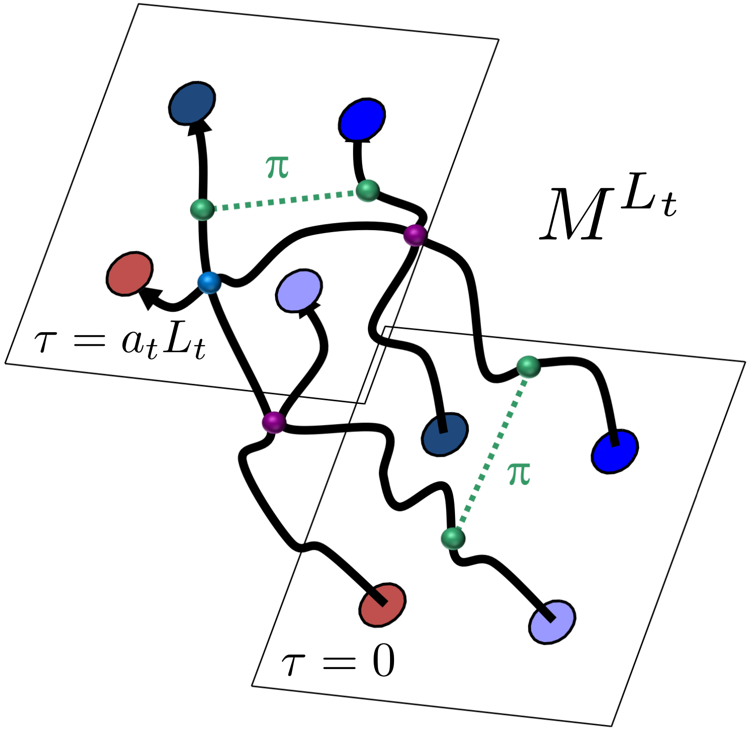
- Hamiltonian evolution divided into (small) transfer matrix steps

$$Z(L_t) = \langle \Psi | M^{L_t} | \Psi \rangle$$

$$M = :\exp(-\alpha_t H):, \quad H = H_{\rm kin} + V$$

$$\alpha_t = a_t/a, \quad \tau = a_t L_t$$

Suzuki-Trotter discretization of the Euclidean time evolution



- Transient energy and expectation values

$$E_i(L_t) = -\frac{1}{\alpha_t} \ln \frac{Z(L_t+1)}{Z(L_t)}$$

$$Z^{\mathcal{O}}(L_t) = \langle \Psi | M^{L_t/2} \mathcal{O} M^{L_t/2} | \Psi \rangle$$

Practical simulations close to Hamiltonian limit, requires special MC algorithm –> see next pages

AUXILIARY FIELD METHOD

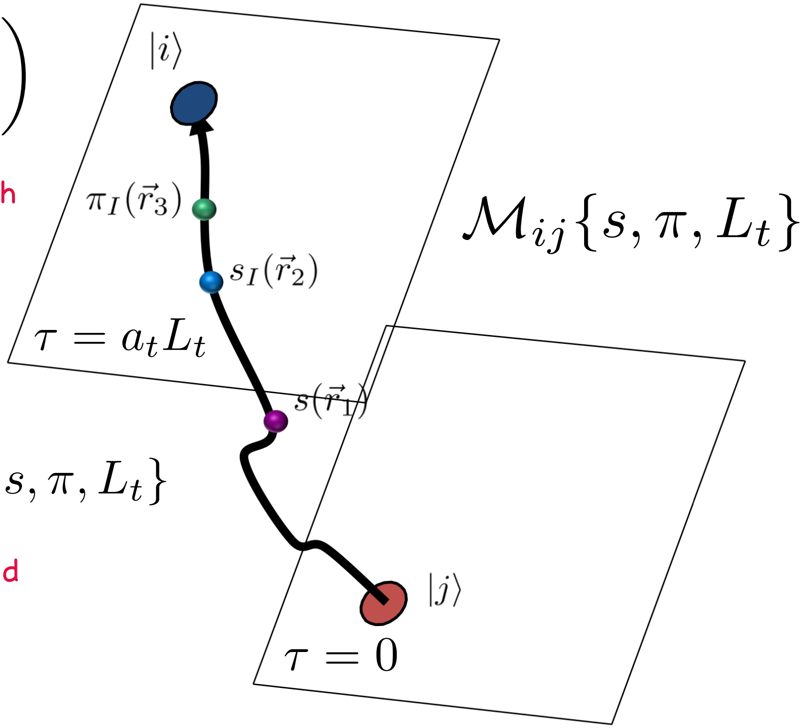
Lee, Prog. Part. Nucl. Phys. **63** (2009) 117

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

- Interactions between nucleons are represented by a path integral over auxiliary and pion fields

$$\exp\left(-\frac{C}{2}\rho(\boldsymbol{n})^2\right) = \frac{1}{\sqrt{2\pi}}\int ds\,\exp\left(-\frac{s^2}{2}+\sqrt{C}\rho(\boldsymbol{n})s\right)$$

Applied on every lattice site (many types of Hubbard-Stratonovich transformations possible)



- Auxiliary Field Quantum Monte Carlo (AFQMC)

$$Z(L_t) = \int \mathcal{D}s\mathcal{D}\pi\,\langle\Psi|M^{L_t}\{s,\pi\}|\Psi\rangle = \int \mathcal{D}s\mathcal{D}\pi\,\det\mathcal{M}\{s,\pi,L_t\}$$

Each nucleon is evolved independently in a fluctuating background

- Fermion correlation matrix

$$\mathcal{M}_{kl}\{s,\pi,L_t\} = \langle\phi_k|M^{L_t}\{s,\pi\}|\phi_l\rangle$$

The trial state is defined in terms of the single-nucleon components of the Slater determinant
—> Great simplification (at the price of introducing a path integral)

MONTE CARLO ALGORITHMS

Lu, Li, Elhatisari, Lee, Epelbaum, Meißner, PLB **797** (2019) 134863

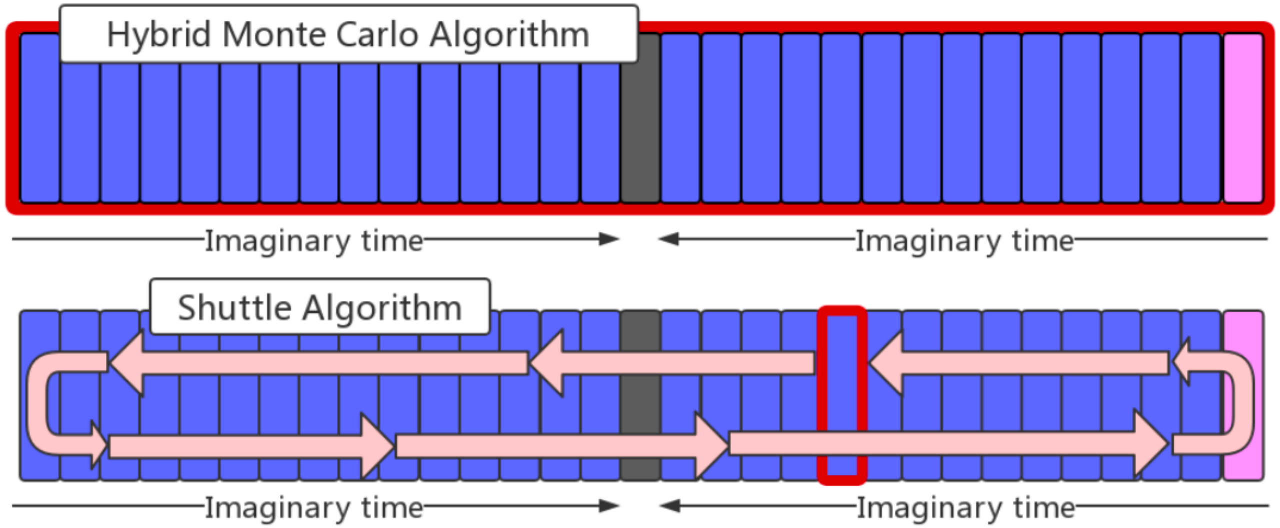
Lähde, Meißner, Springer Lecture Notes in Physics **957** (2019) 1-396

- Hybrid Monte Carlo (HMC) algorithm — *à la* Lattice QCD

Global Molecular Dynamics updates, slow for large number of time slices

- "Shuttle algorithm" — designed specifically for NLEFT (also further acceleration with GPU computing)

Heat bath updates one time slice at a time, efficient for larger number of time slices



First time step: projection onto cubic irreps (A1+, E+, T2+, etc.)

- Very favorable computational scaling $\propto A^{2\ldots3}$

SPECTRUM OF ^{12}C

Shen, Lähde, Lee, Meißner, EPJA **57** (2021) 276 [arXiv:2106.04834[nucl-th]]

- To compute excited states and transition rates, use Euclidean time projection with coupled channels

Rokash, Pine, Elhatisari, Epelbaum et al., PRC **92** (2015), 054612
Elhatisari, Lee, Rupak, Epelbaum et al., Nature **528** (2015) 111

$$Z_{a,b}(L_t) = \langle \Psi_a | M^{L_t} | \Psi_b \rangle$$

- “Adiabatic transfer matrix” — introduced in the cluster Hamiltonian treatment of alpha-alpha scattering)

$$M^{(a)}_{qq'}(L_t) = \sum_{q''} Z^{-1}_{qq''}(L_t) Z_{q''q'}(L_t+1)$$

Typically 2-4 channels per calculation,
with different choices of trial states –> next page

$$\lambda_i(L_t) = \exp(-\alpha_t E_i(L_t))$$

$$E_i(L_t) = -\ln(\lambda_i(L_t))/\alpha_t$$

Eigenvalues of adiabatic transfer matrix
give transient energies

- Angular momentum/parity projection (cubic irreps)
- Extrapolation to infinite Euclidean time (multi-exponential fit)

Lähde, Epelbaum, Krebs, Lee, Meißner, J. Phys. G **42** (2015) 034012

SPECTRUM OF ^{12}C

Shen, Lähde, Lee, Lu, Meißner, Nature Commun. **14** (2023) 2777 [arXiv:2202.13596[nucl-th]]

- Wigner SU(4) symmetric interaction, with three-nucleon force (3NF)

Lu, Li, Elhatisari, Lee et al.,. PLB **797** (2019) 134863

$$H = H_{\text{kin}} + \frac{C_2}{2!}\sum_{\boldsymbol{n}} :\tilde{\rho}(\boldsymbol{n})^2: + \frac{C_3}{3!}\sum_{\boldsymbol{n}} :\tilde{\rho}(\boldsymbol{n})^3:$$

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

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

Sign problem largely suppressed
Neutron matter well described
Ground state properties of light and medium-mass nuclei well described

- 4 parameters to determine:
  - C_2, C_3 — ground states energies of ^{4}He and ^{12}C
  - s_L — radius of ^{12}C around 2.4 fm
  - s_{NL} — optimal E0 and E2 transition rates

In the sense of Chiral EFT
→ smearings are regulators of EFT

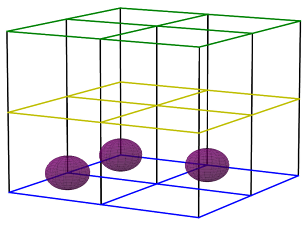
- Basis for high-fidelity NLEFT calculations (currently up to N3LO in the chiral EFT expansion) Elhatisari, Bovermann, Ma, Epelbaum et al., Nature **630** (2024) 59

SPECTRUM OF ^{12}C

Shen, Lähde, Lee, Meißner, EPJA **57** (2021) 276 [arXiv:2106.04834[nucl-th]]

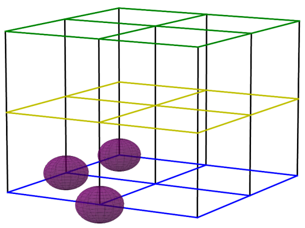
- Alpha cluster configurations of Gaussian wave packets

S1



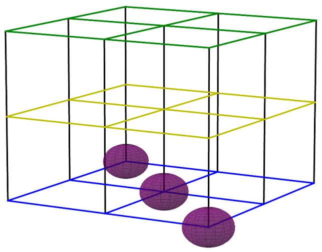
isosceles right triangle

S2



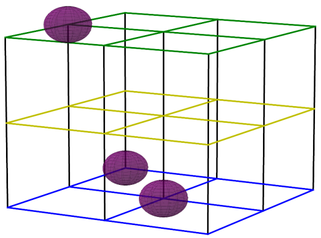
“bent-arm” shape

S3



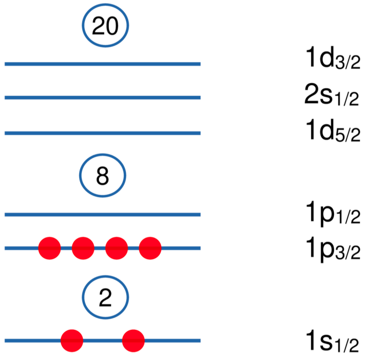
linear chain (diagonal)

S4

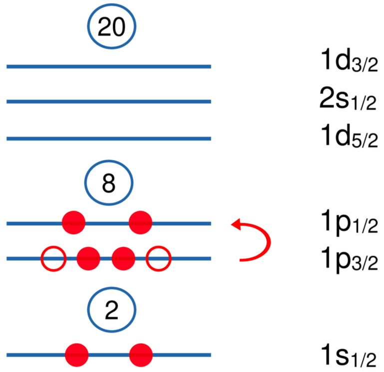


isosceles acute triangle

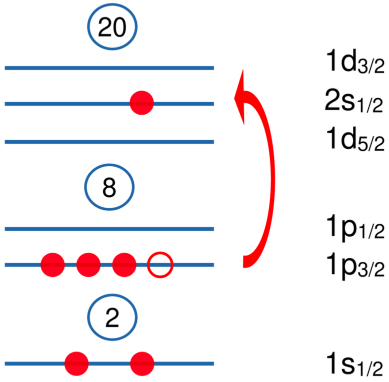
- Shell model (proton) particle-hole harmonic oscillator wave functions



ground state



2p-2h excitation

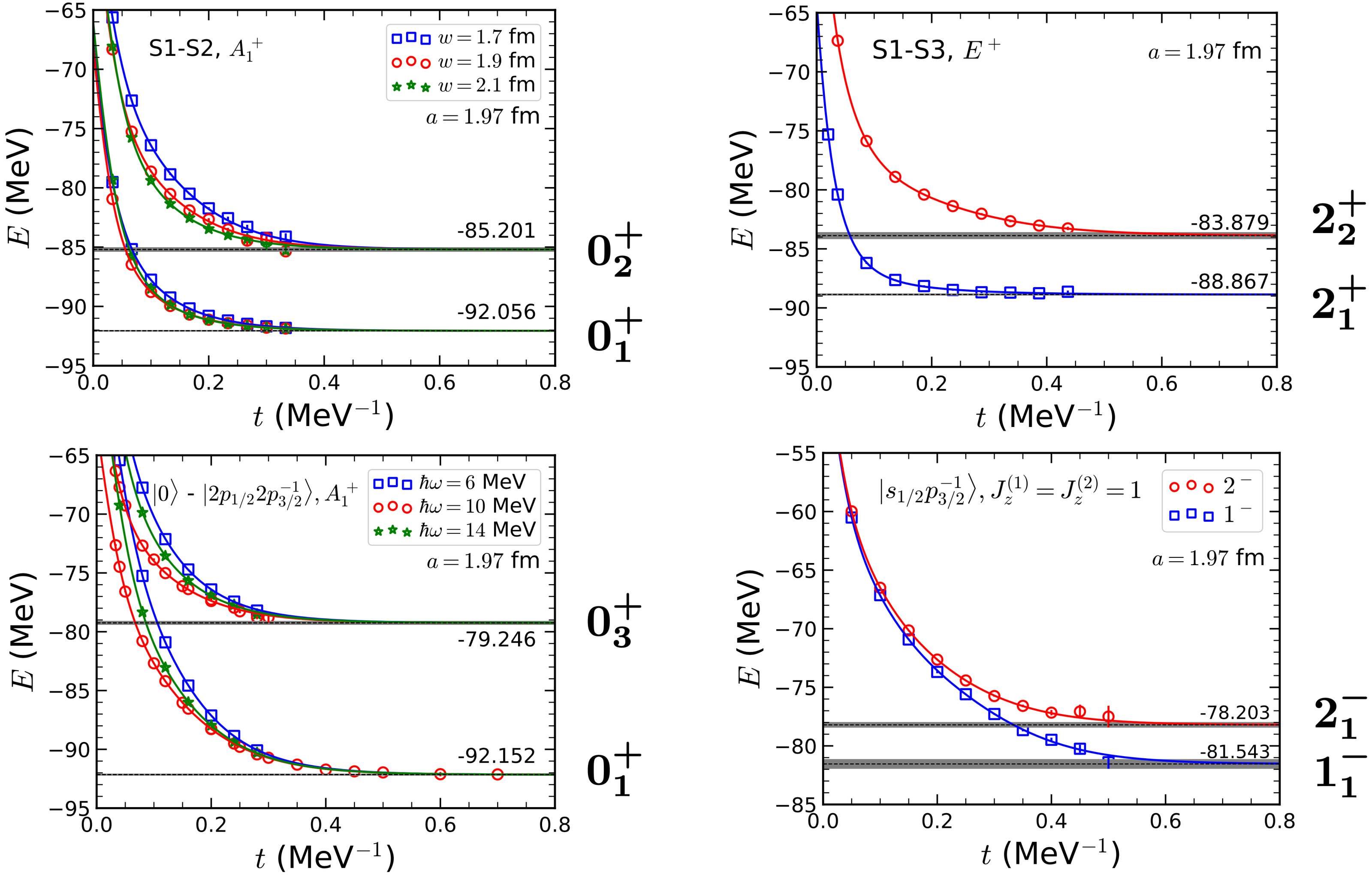


1p-1h excitation

SPECTRUM OF ^{12}C

Shen, Lähde, Lee, Meißner, EPJA **57** (2021) 276 [arXiv:2106.04834[nucl-th]]

- Transient energies (examples) with extrapolation to large projection time

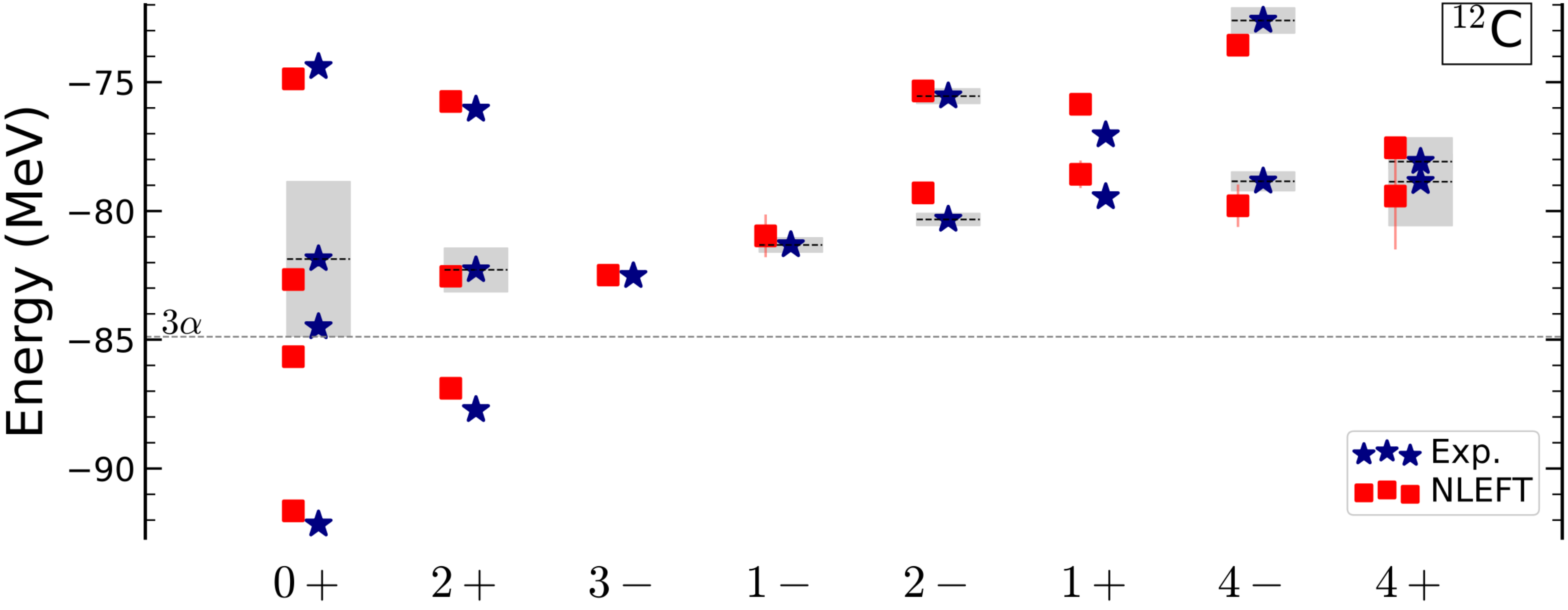


SPECTRUM OF ^{12}C

Shen, Lähde, Lee, Lu, Meißner, Nature Commun. **14** (2023) 2777 [arXiv:2202.13596[nucl-th]]

- All low-lying states amazingly good — resonances above the 3α threshold: need analysis of finite-volume spectrum

Bernard, Lage, Meißner, Rusetsky, JHEP **08** (2008) 024



- Next question — what is the structure of each state?

TOMOGRAPHY OF ^{12}C STATES

Shen, Lähde, Lee, Lu, Meißner, Nature Commun. **14** (2023) 2777 [arXiv:2202.13596[nucl-th]]

- Insert a screen of “pinholes” with spin/isospin, that allow nucleons with corresponding spin/isospin to pass

Elhatisari, Epelbaum, Krebs, Lähde et al., PRL **119**, 222505 (2017)
Lu, Li, Elhatisari, Lee et al., Phys. Lett. B **797**, 134863 (2019)

$$Z_{a,b}(\boldsymbol{i},\boldsymbol{j},\boldsymbol{n};L_t) = \langle\Psi_a|M^{L_t/2}\rho_A(\boldsymbol{i},\boldsymbol{j},\boldsymbol{n})M^{L_t/2}|\Psi_b\rangle$$

$$\rho_A(\boldsymbol{i},\boldsymbol{j},\boldsymbol{n}) =: \rho(i_1,j_1,\boldsymbol{n}_1)\cdots\rho(i_A,j_A,\boldsymbol{n}_A):$$

$$\rho(i,j,\boldsymbol{n}) = a^\dagger_{i,j}(\boldsymbol{n})a_{i,j}(\boldsymbol{n})$$

Locations and spin/isospin updated with MC
—> see next page

- Originally introduced for proton and neutron distributions in AFQMC (relative to the center of mass of the *A*-nucleon system)

$$\langle\rho(r)\rangle = \frac{1}{A!}\sum_{\boldsymbol{n}}\langle\Psi|M^{L_t/2}\rho_A(\boldsymbol{n})M^{L_t/2}|\Psi\rangle\sum_{k=1}^{A}\delta(r-|\boldsymbol{r}_k-\boldsymbol{R}|)$$

$$\boldsymbol{R} = \frac{1}{A}\sum_{k=1}^{A}\boldsymbol{r}_k$$

Radial charge density profile

- Also computationally efficient stochastic estimator

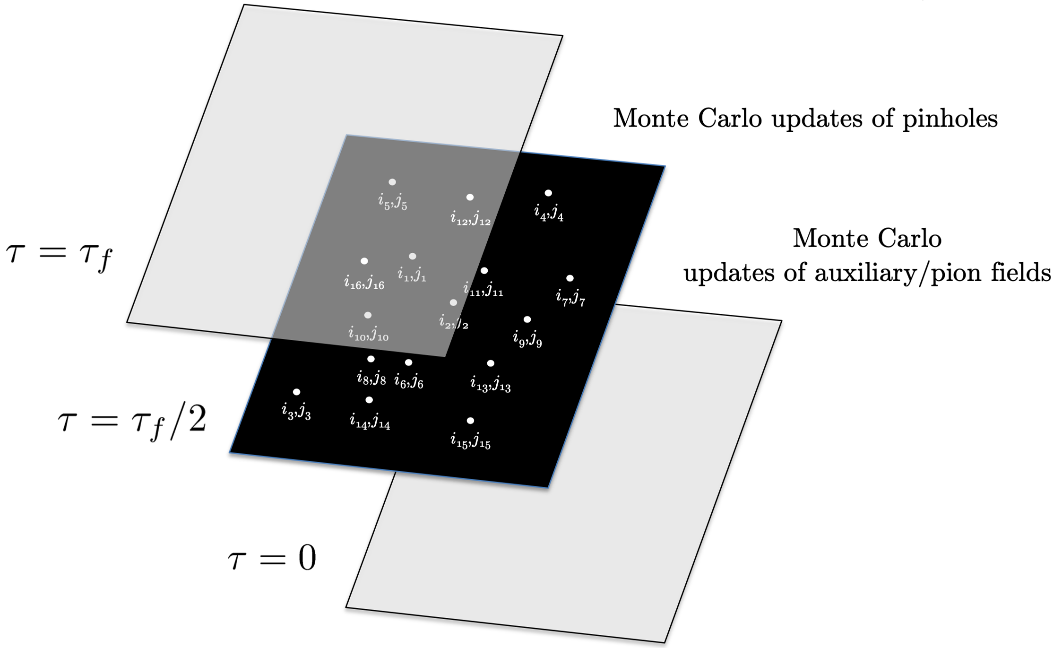
TOMOGRAPHY OF ^{12}C STATES

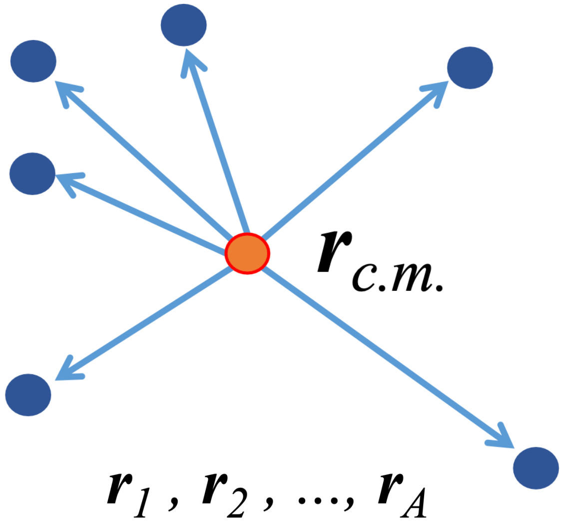
Shen, Lähde, Lee, Lu, Meißner, Nature Commun. **14** (2023) 2777 [arXiv:2202.13596[nucl-th]]

- Metropolis updates of pinhole positions/spin/isospin

$$Z_{a,b}(\boldsymbol{i},\boldsymbol{j},\boldsymbol{n};L_t) = \int \mathcal{D}s\mathcal{D}\pi \langle\Psi_a|M^{L_t/2}\{s,\pi\}\rho_A(\boldsymbol{i},\boldsymbol{j},\boldsymbol{n})M^{L_t/2}\{s,\pi\}|\Psi_b\rangle$$

$$A(s,\pi;\boldsymbol{i},\boldsymbol{j},\boldsymbol{n};L_t) = \left|\langle\Psi_a|M^{L_t/2}\{s,\pi\}\rho_A(\boldsymbol{i},\boldsymbol{j},\boldsymbol{n})M^{L_t/2}\{s,\pi\}|\Psi_b\rangle\right|$$



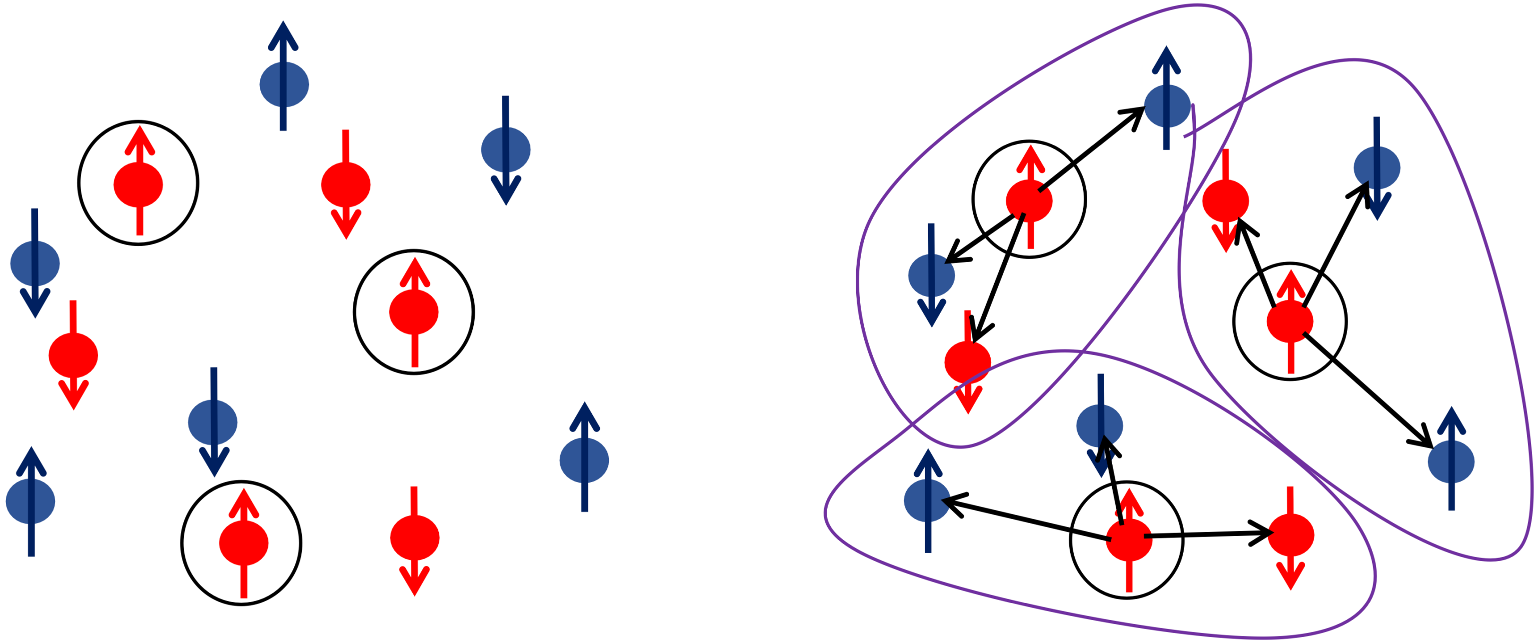


- Ensembles of configurations of *A* nucleons (relative to center of mass)

TOMOGRAPHY OF ^{12}C STATES

Shen, Lähde, Lee, Lu, Meißner, Nature Commun. **14** (2023) 2777 [arXiv:2202.13596[nucl-th]]

- Search for alpha clusters using pinhole configurations:
  1. Identify 3 spin-up protons
  2. Find the closest possible candidate of the 3 other species

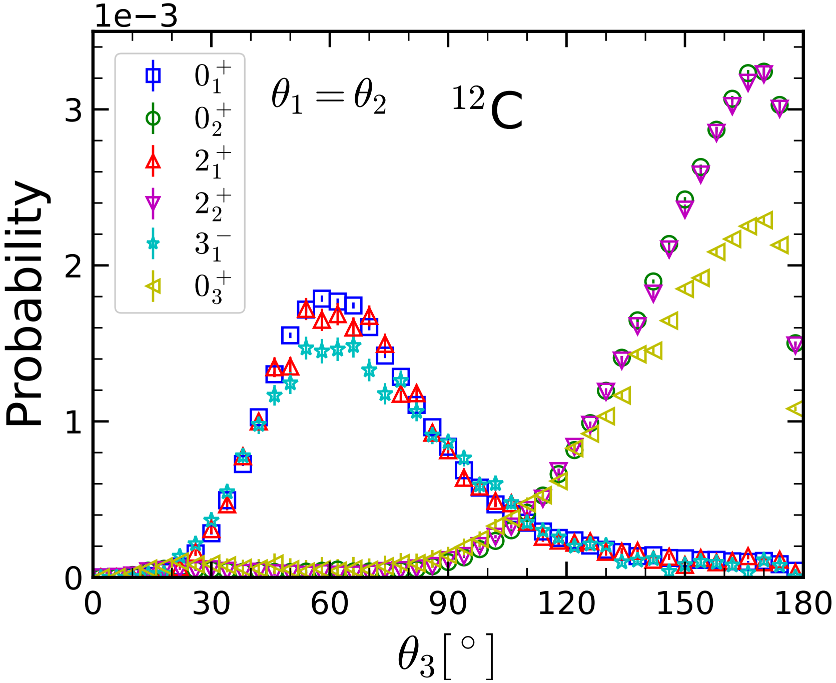


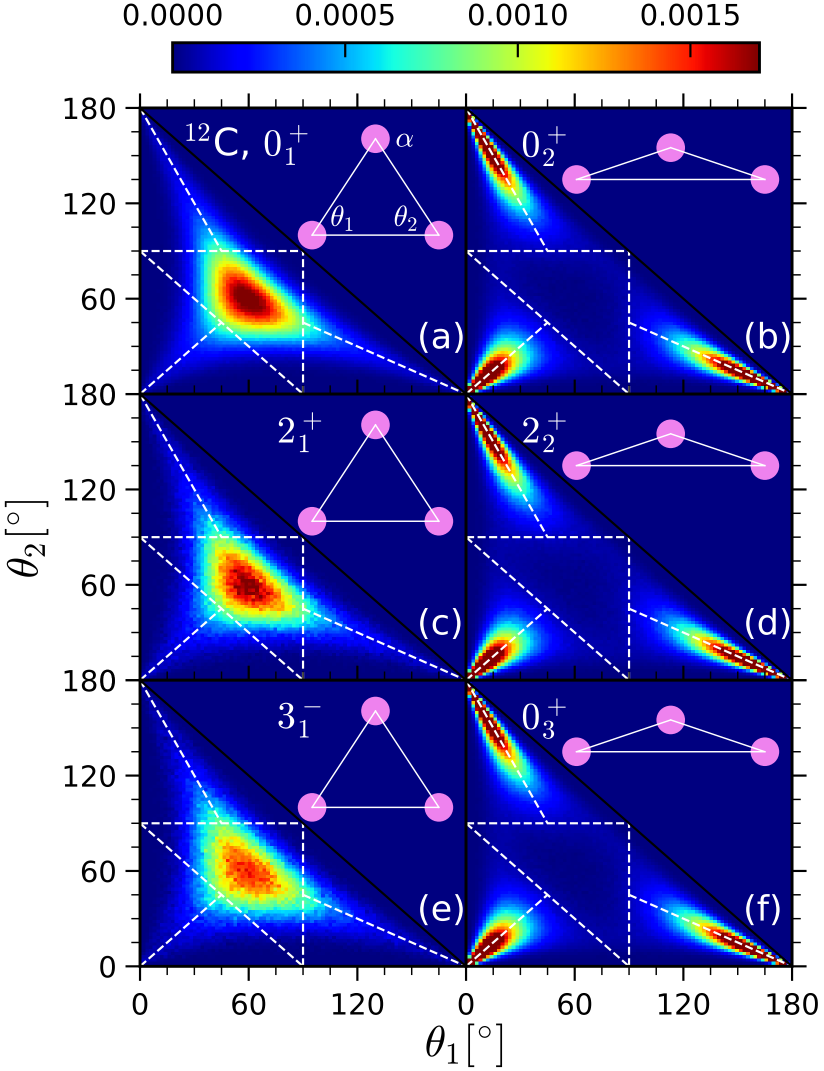
- Cluster radii (1.65 … 1.71 fm) similar to free alpha particles (1.63 fm)

TOMOGRAPHY OF ^{12}C STATES

Shen, Lähde, Lee, Lu, Meißner, Nature Commun. **14** (2023) 2777 [arXiv:2202.13596[nucl-th]]

- Study angles between alpha clusters
- Two distinct structures emerge:
  1. Equilateral triangular
  2. Obtuse large-angle triangular

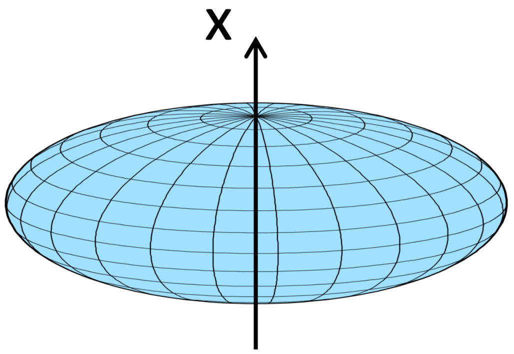


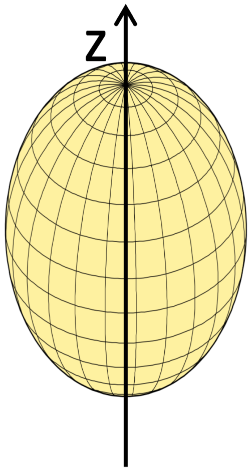


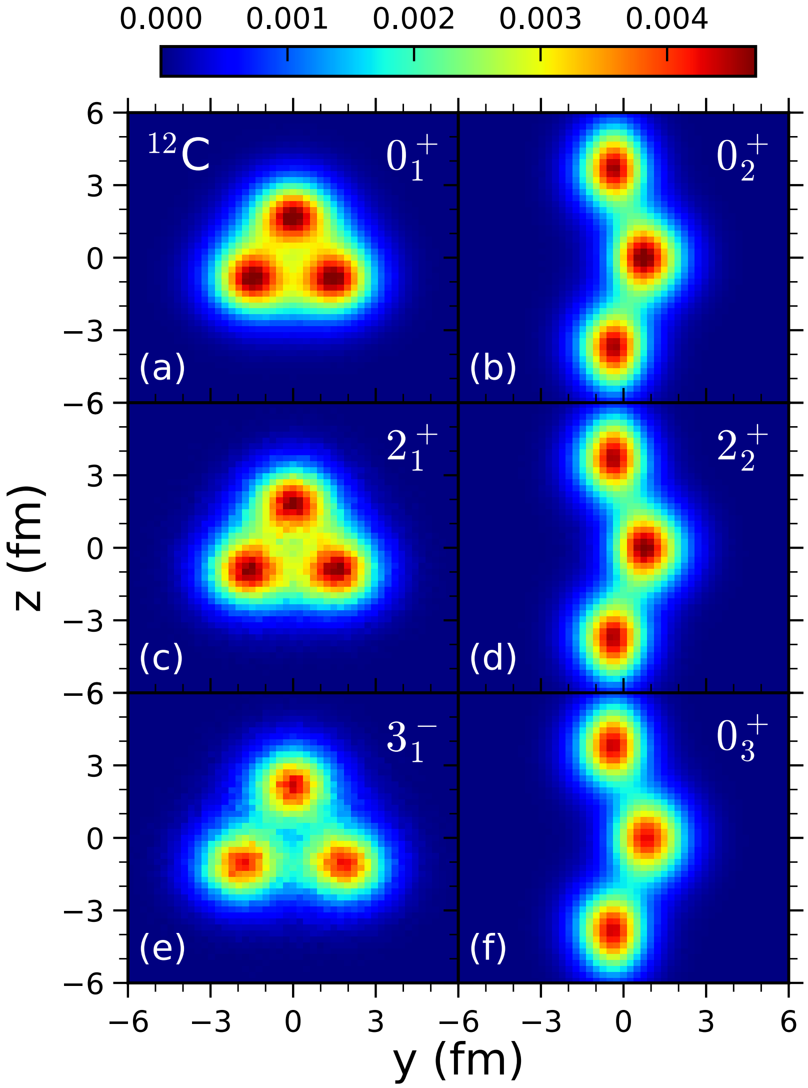
TOMOGRAPHY OF ^{12}C STATES

Shen, Lähde, Lee, Lu, Meißner, Nature Commun. **14** (2023) 2777 [arXiv:2202.13596[nucl-th]]

- Equilateral-type (Ground) states:
  1. Align shortest axis to x
  2. Rotate one α to (y = 0, z > 0)
  3. Random 120 degree rotation
- Obtuse-type (Hoyle) states:
  1. Align longest axis to z
  2. Rotate central α to (x=0, y > 0)



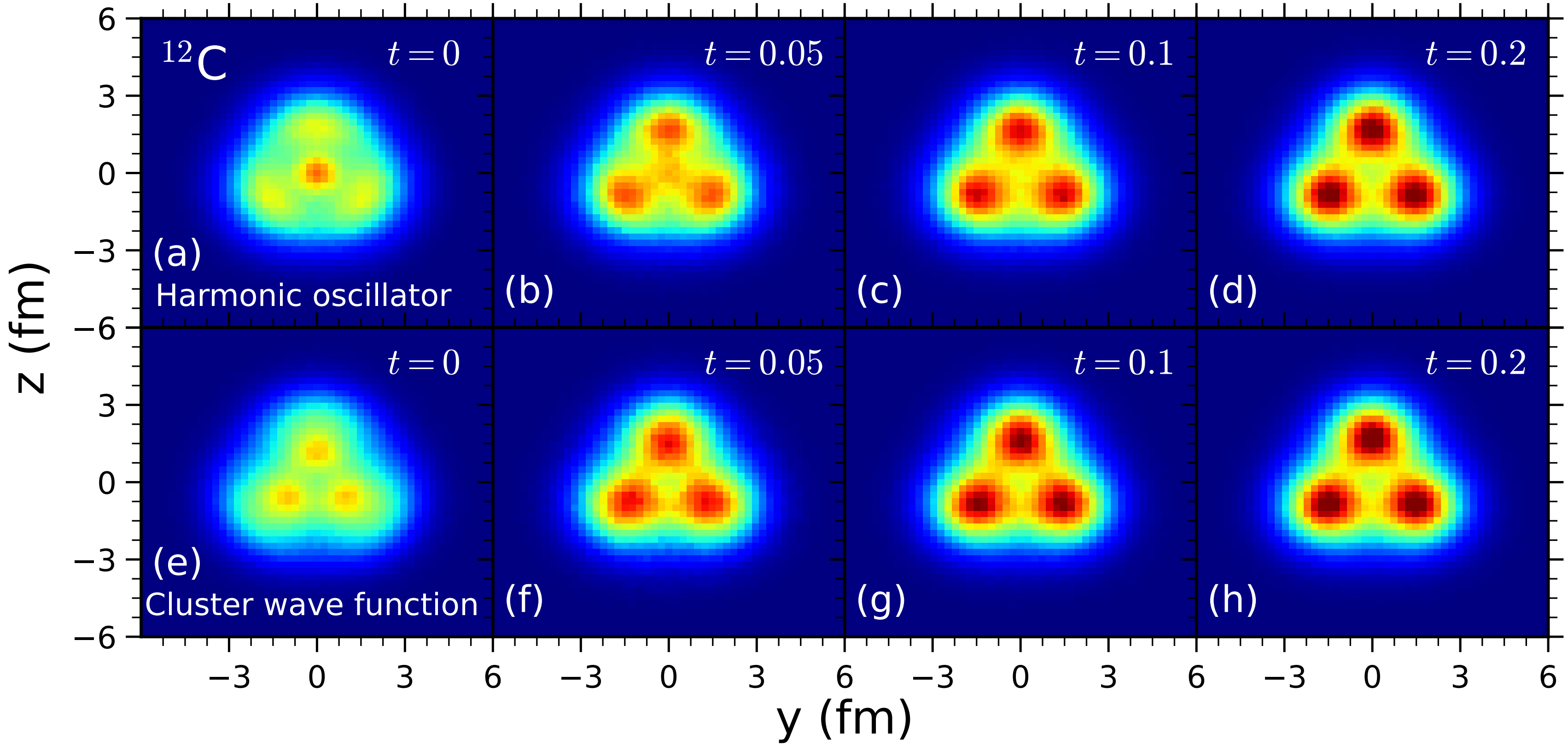




EMERGENT ALPHA CLUSTERING

Shen, Lähde, Lee, Lu, Meißner, Nature Commun. **14** (2023) 2777 [arXiv:2202.13596[nucl-th]]

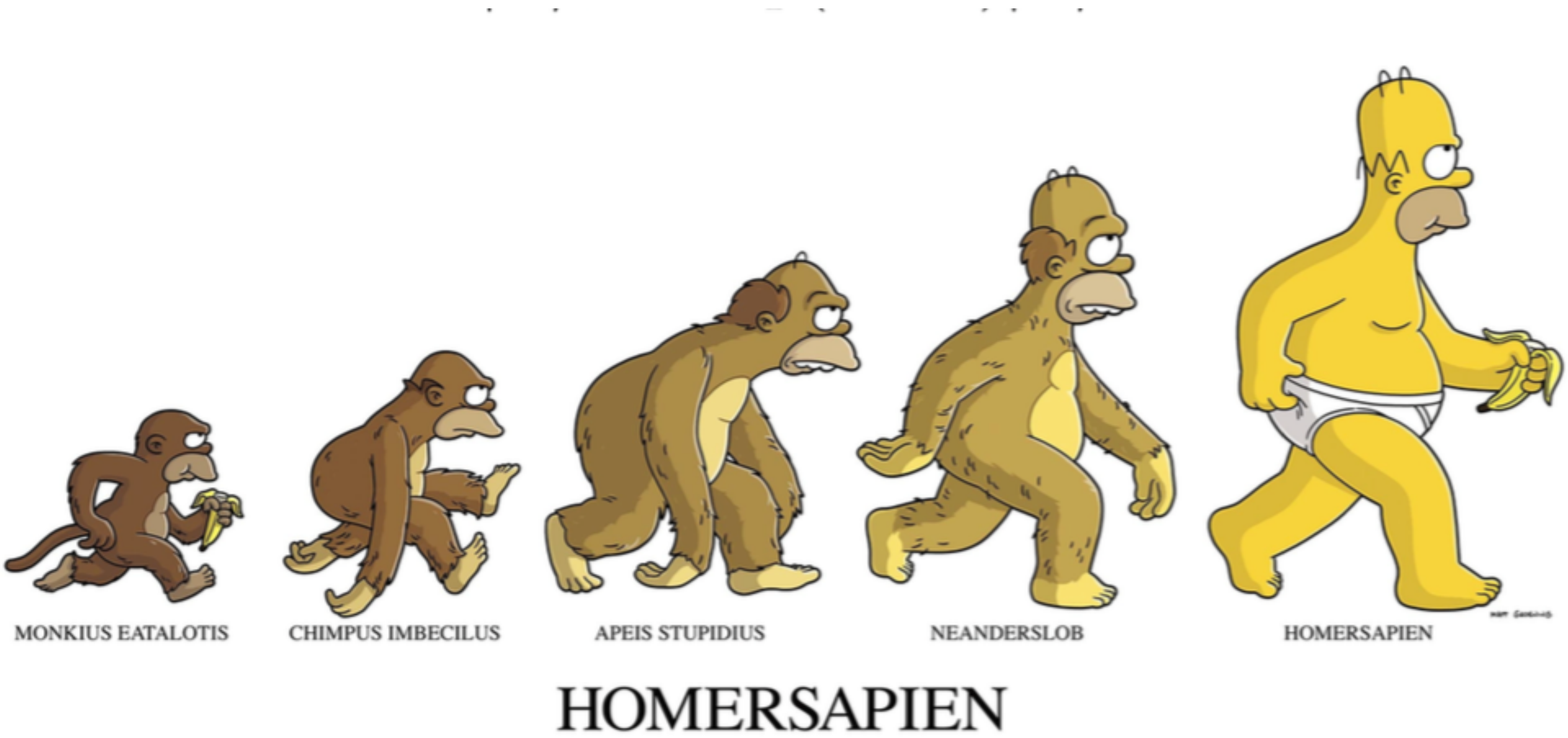
- Alpha cluster structure emerges naturally
  — not a built-in assumption



- After sufficiently large Euclidean projection time
  — memory of trial state erased

EMERGENT ALPHA CLUSTERING

Shen, Lähde, Lee, Lu, Meißner, Nature Commun. **14** (2023) 2777 [arXiv:2202.13596[nucl-th]]

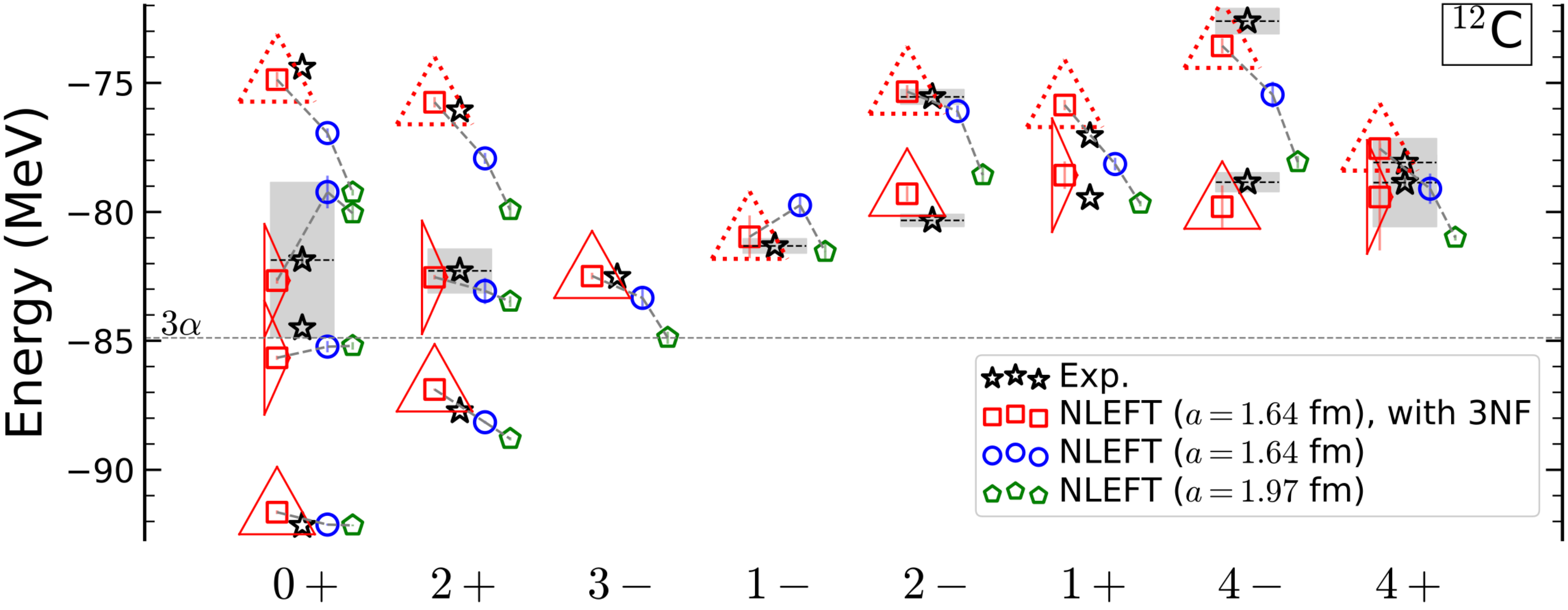


Euclidean time projection

CLUSTER/SHELL-MODEL DUALITY

Shen, Lähde, Lee, Lu, Meißner, Nature Commun. **14** (2023) 2777 [arXiv:2202.13596[nucl-th]]

- Lowest states are predominantly alpha cluster states with equilateral or obtuse (“bent-arm”) triangular arrangement



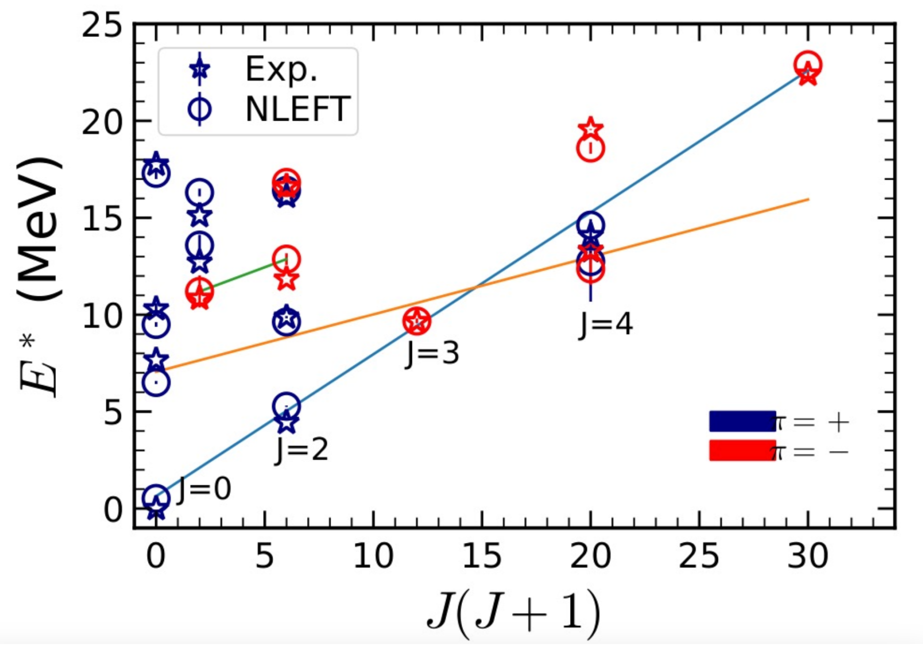
- Dashed triangles — strong 1p-1h component in the wave function, preference for shell-model trial states

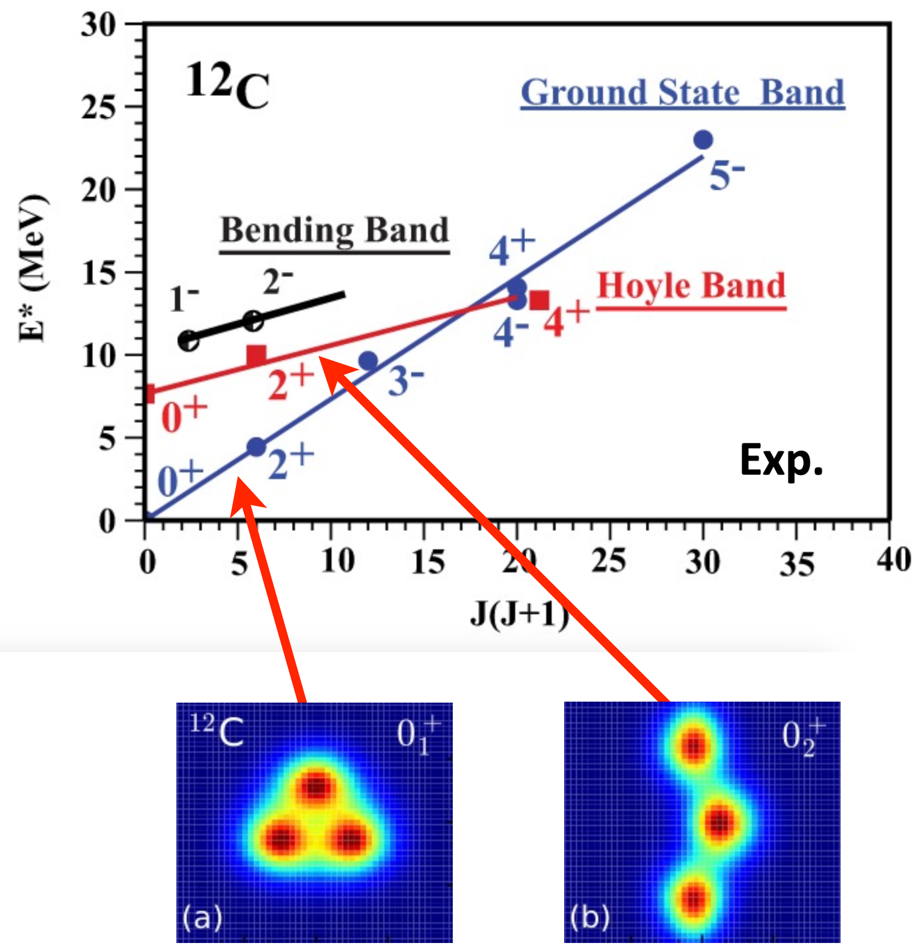
BAND STRUCTURE

Bijker, Iachello, PRC **61** (2000) 067305

Marín-Lámbarri, Bijker, Freer, Gai et al., PRL **113** (2014) 012502

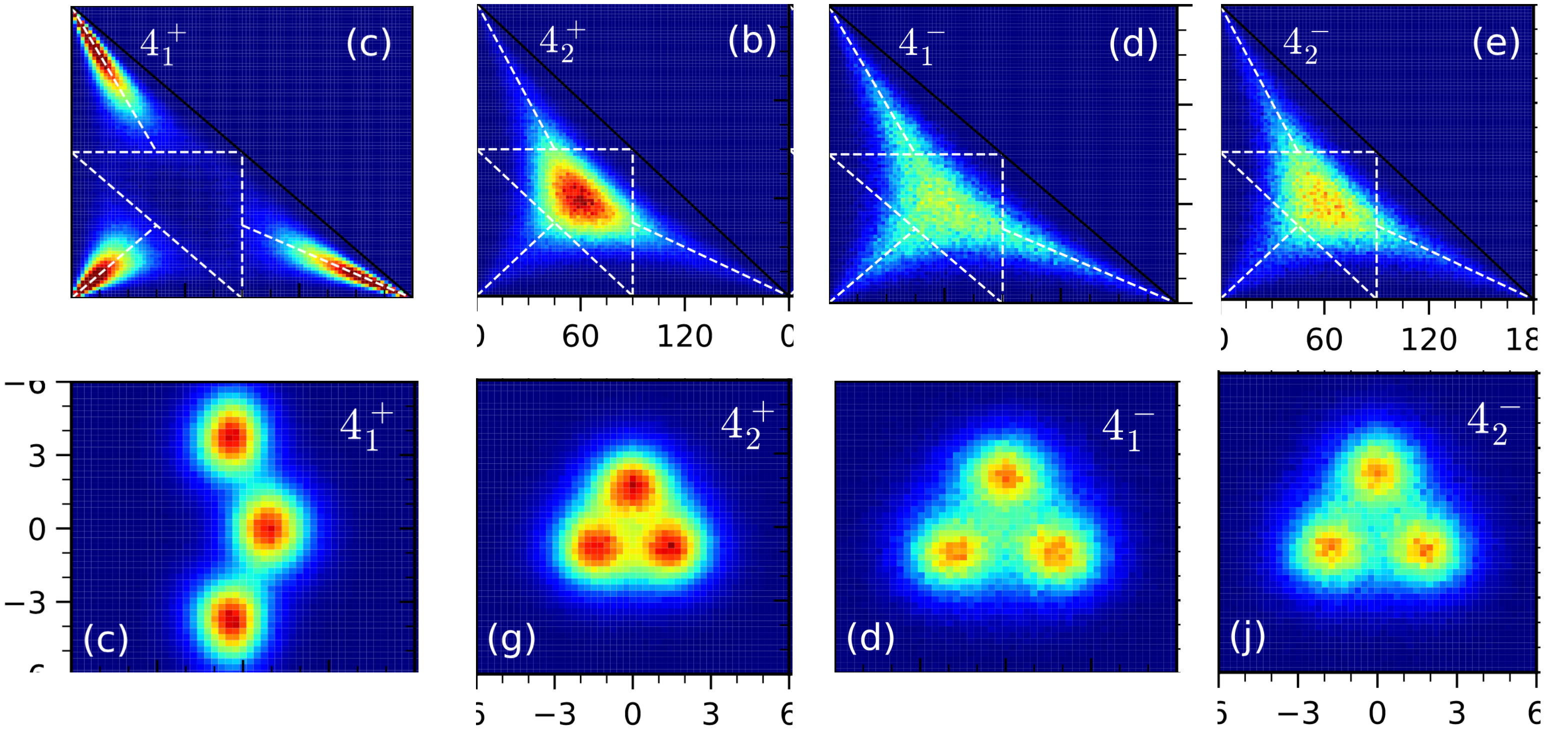
Shen, Lähde, Lee, Lu, Meißner, Nature Commun. **14** (2023) 2777 [arXiv:2202.13596[nucl-th]]



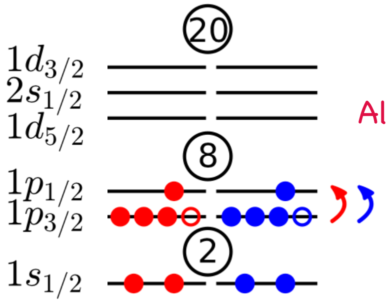


HIGHER EXCITED STATES (4+, 4-)

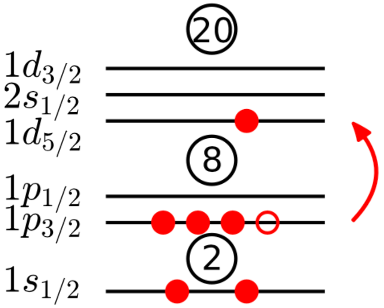
Shen, Lähde, Lee, Lu, Meißner, Nature Commun. **14** (2023) 2777 [arXiv:2202.13596[nucl-th]]



Alpha cluster trial state



Alpha cluster trial state



SUMMARY & OUTLOOK

- Successful description of low-lying ^{12}C spectrum with Wigner SU(4) symmetric interaction (starting point for higher-order NLEFT)
- Successful characterization of the emergent alpha cluster geometry in the low-lying ^{12}C states

- Now possible — NLEFT calculations to N3LO in chiral EFT (see also talk by Lukas Bovermann)

  Elhatisari, Bovermann, Ma, Epelbaum et al., Nature **630** (2024) 59

- Ab initio studies of Be isotopes from ^{7}Be to ^{12}Be

  Shen, Elhatisari, Lee, Meißner, Ren [arXiv:2411.14935 [nucl-th]]

- Nucleon distribution and shell closure in ^{22}Si

  Zhang, Elhatisari, Meißner, Shen [arXiv:2411.17462 [nucl-th]]

- Studies of ^{16}O and ^{20}Ne

  Giacalone, Bally, Nijs, Shen et al., [arXiv:2402.05995 [nucl-th]]
  Giacalone, Zhao, Bally, Shen et al., [arXiv:2405.20210 [nucl-th]]