

Lattice 2022

Structure and Geometry of ^{12}C with Wigner SU(4) Interaction

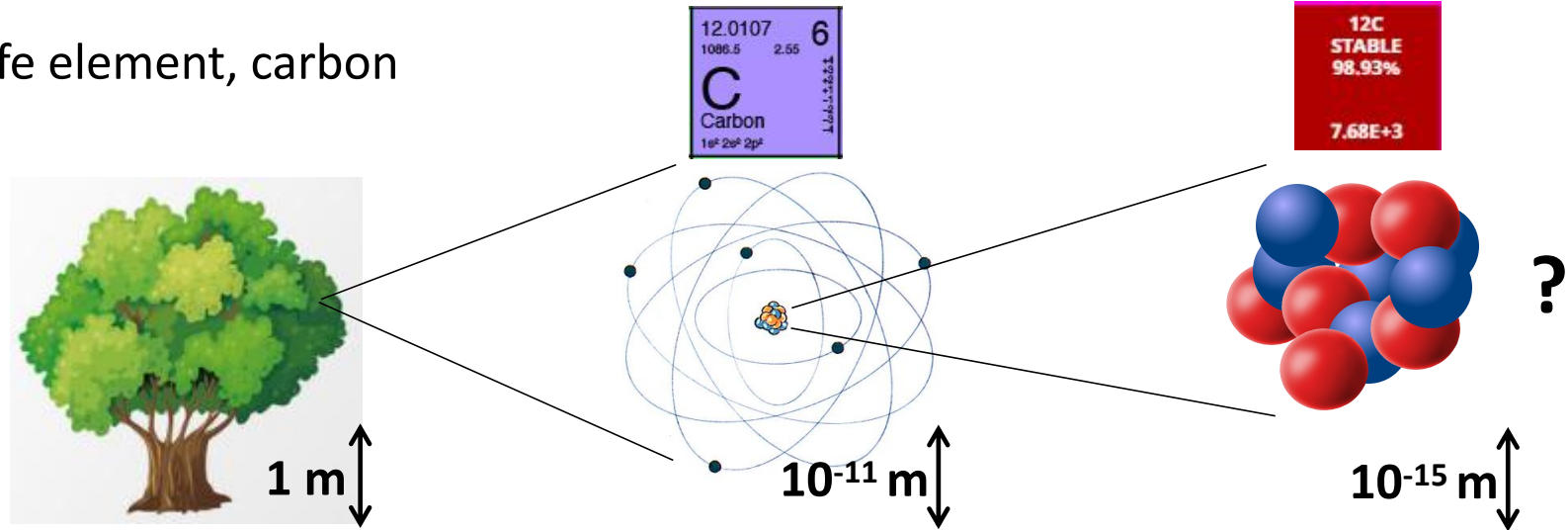
Shihang Shen
Forschungszentrum Jülich



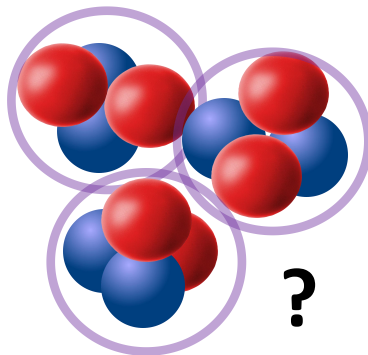
Collaborators: Timo A. Lähde, Dean Lee, Ulf-G. Meißner

What's Interesting about Carbon-12

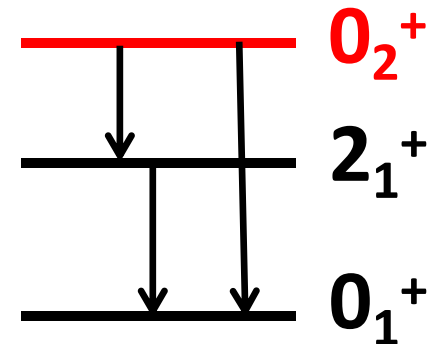
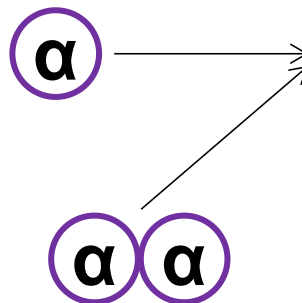
- Life element, carbon



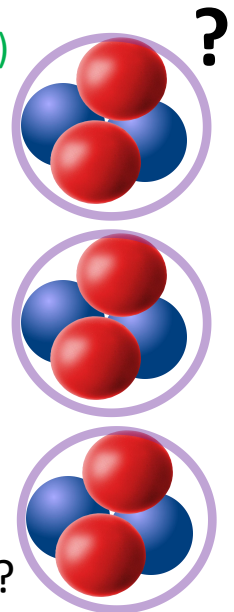
- We know little about its shape



is it like an equilateral triangle of α clusters?
or as independent particles in the shell model?



is the Hoyle state like a linear chain?



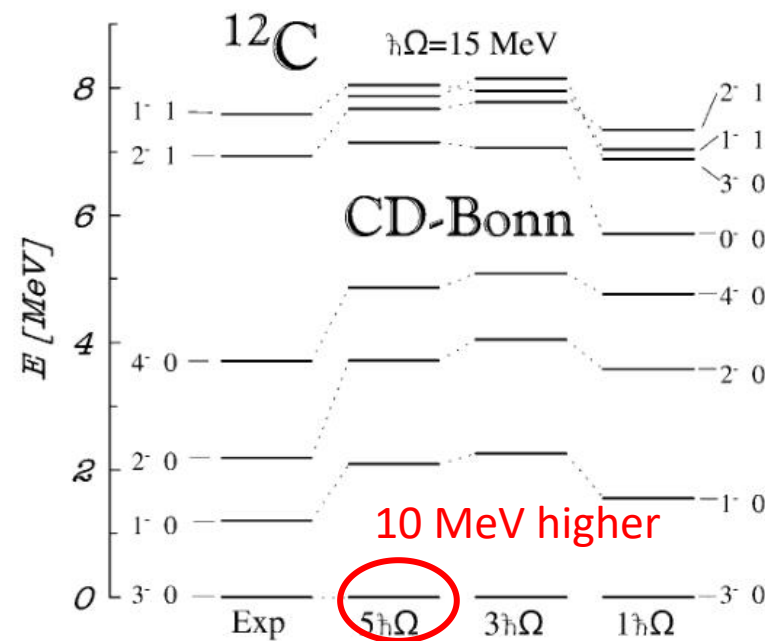
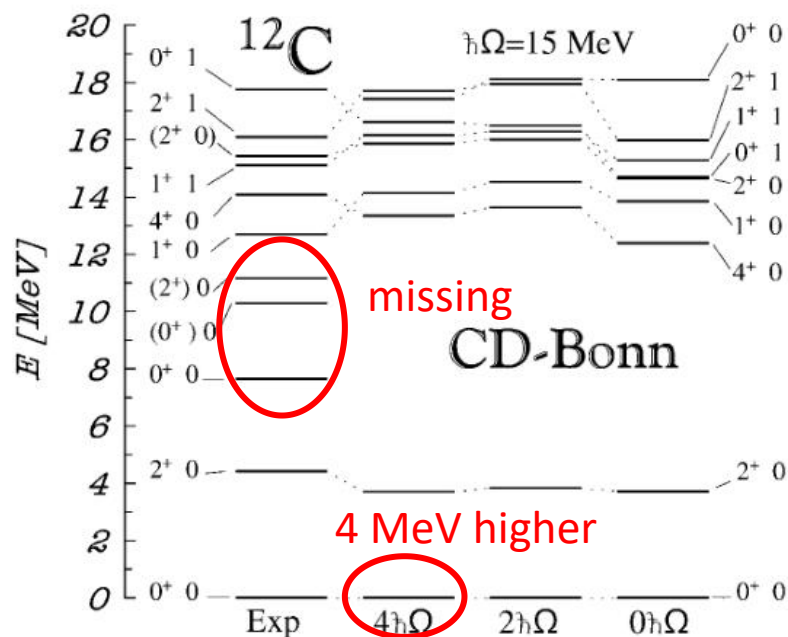
Challenge for Theoretical Calculations

➤ Microscopic cluster models

- resonating group method J. A. Wheeler, Phys. Rev. 52(11), 1083 (1937)
- generator coordinate method with Bloch–Brink cluster wave function D. M. Brink (1966)
- antisymmetrized molecular dynamics A. Ono, H. Horiuchi, T. Maruyama, and A. Ohnishi, Phys. Rev. Lett. 68(19), 2898 (1992)
- fermionic molecular dynamics H. Feldmeier, Nucl. Phys. A 515(1), 147 (1990)
-

➤ *Ab initio* calculations: solving the exact A-body problem, extremely difficult

e.g. no-core shell model Navrátil, P., J. P. Vary, and B. R. Barrett, Phys. Rev. Lett. 84, 5728 (2000)



Challenge for Theoretical Calculations

- First ab initio calculation for Hoyle state by nuclear lattice effective field theory

PRL **106**, 192501 (2011) week ending
13 MAY 2011

Selected for a **Viewpoint** in *Physics*
PHYSICAL REVIEW LETTERS



Ab Initio Calculation of the Hoyle State

Evgeny Epelbaum,¹ Hermann Krebs,¹ Dean Lee,² and Ulf-G. Meißner^{3,4}

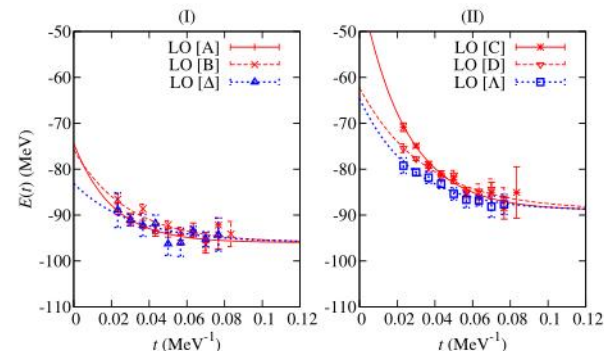
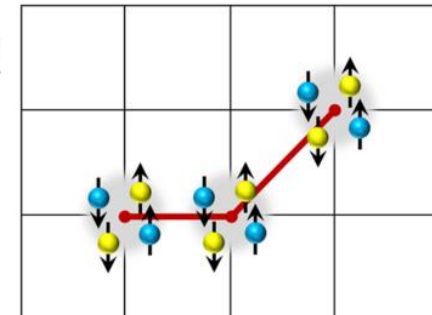
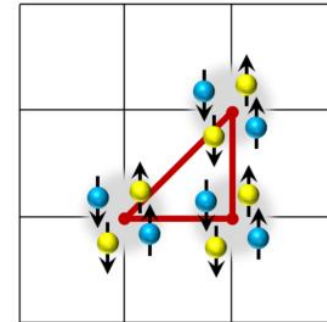
PRL **109**, 252501 (2012) week ending
21 DECEMBER 2012

PHYSICAL REVIEW LETTERS



Structure and Rotations of the Hoyle State

Evgeny Epelbaum,¹ Hermann Krebs,¹ Timo A. Lähde,² Dean Lee,⁴ and Ulf-G. Meißner^{5,2,3}



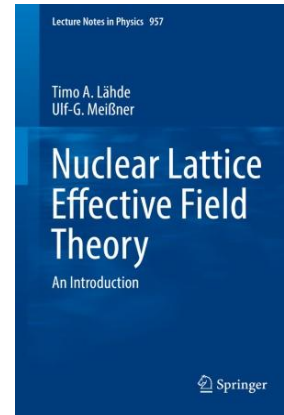
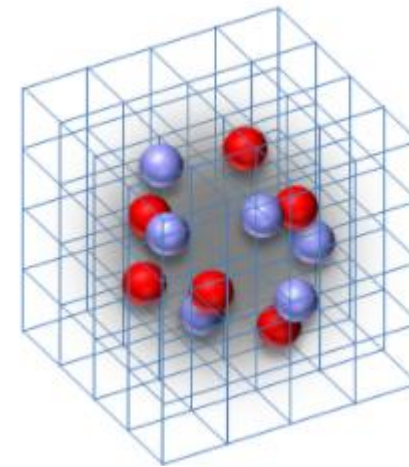
- Further questions:

- Sign problem
- Can we find a way to see the shape of the final states?
- Low-lying spectrum, cluster excitation / single-particle excitation ?

Nuclear Lattice Effective Field Theory

➤ Nuclear lattice effective field theory (NLEFT)

	2N force	3N force	4N force
LO		—	—
NLO		—	—
N ² LO			—
N ³ LO			



Progress in Particle and Nuclear Physics 63 (2009) 117–154



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journal homepage: www.elsevier.com/locate/ppnp



Review

Lattice simulations for few- and many-body systems

Dean Lee

Department of Physics, North Carolina State University, Raleigh, NC 27695, United States

- ^{16}O , E. Epelbaum et al., PRL 112, 102501 (2014)
- α - α scattering, S. Elhatisari et al., Nature 528, 111 (2015)
- thermodynamics, B.-N. Lu et al., PRL 125, 192502 (2020)
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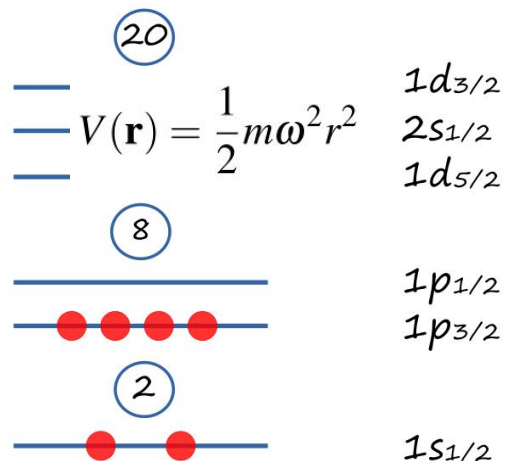
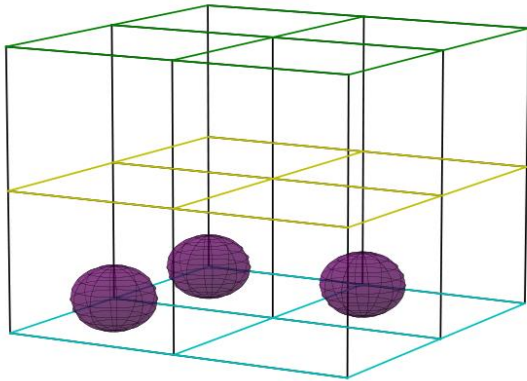
lattice figure from <https://www.physics.ncsu.edu/ntg/leegroup/research.html>

Theoretical Framework

- Starting from an initial many-body wave function:

$$|\Phi_0\rangle = \mathcal{A}[\phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2)\dots\phi_A(\mathbf{r}_A)]$$

$$\phi(\mathbf{r}) = \exp\left(-(\mathbf{r}-\mathbf{r}_0)^2/2w^2\right)$$

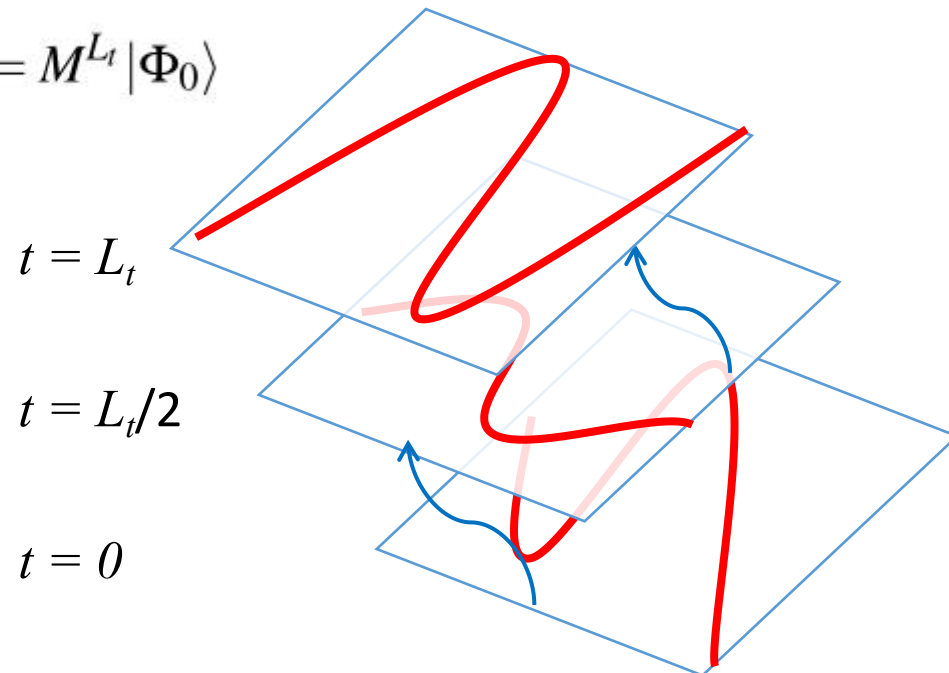


- Euclidean time projection with transfer matrix:

$$M =: \exp(-\alpha_t H) : \quad \alpha_t = a_t/a$$

with H the many-body Hamiltonian, a_t and a the temporal and spatial lattice spacing.

$$|\Phi_{L_t}\rangle = M^{L_t} |\Phi_0\rangle$$



Theoretical Framework

- Hamiltonian consists of kinetic energy and nucleon-nucleon interaction

$$H = T + V$$

- In this work we adopt the leading-order simplest possible interaction, Wigner SU(4) symmetric interaction (spin and isospin independent):

$$V = \frac{C_2}{2!} \sum_{\mathbf{n}} \tilde{\rho}(\mathbf{n})^2 + \frac{C_3}{3!} \sum_{\mathbf{n}} \tilde{\rho}(\mathbf{n})^3,$$
$$\tilde{\rho}(\mathbf{n}) = \sum_{i=1}^A \tilde{a}_i^\dagger(\mathbf{n}) \tilde{a}_i(\mathbf{n}) + s_L \sum_{|\mathbf{n}' - \mathbf{n}|=1} \sum_{i=1}^A \tilde{a}_i^\dagger(\mathbf{n}') \tilde{a}_i(\mathbf{n}'),$$
$$\tilde{a}_i(\mathbf{n}) = a_i(\mathbf{n}) + s_{\text{NL}} \sum_{|\mathbf{n}' - \mathbf{n}|=1} a_i(\mathbf{n}').$$

Sign problem is largely suppressed [J.W. Chen, D. Lee, T. Schäfer, PRL, 93, 242302 \(2004\)](#)

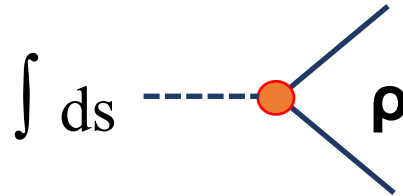
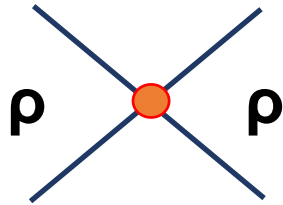
Four parameters C_2 , C_3 , s_L , and s_{NL} will be fitted to binding energy of ^4He and ^{12}C , radius of ^{12}C , and to some extent transition properties.

Interaction seems too simple? Let's wait to see how the descriptions look like

Theoretical Framework

- Auxiliary field with Monte-Carlo sampling

$$\exp\left(-\frac{C\alpha_t}{2}\rho^2\right) := \sqrt{\frac{1}{2\pi}} \int_{-\infty}^{\infty} ds : \exp\left(-\frac{1}{2}s^2 + \sqrt{-C\alpha_t}s\rho\right) :$$



- Final states are a superposition of millions of configurations (Slater determinants)

$$|\Phi_{L_t}\rangle = \sum_{s_i} |\Phi_{s_i, L_t}\rangle$$

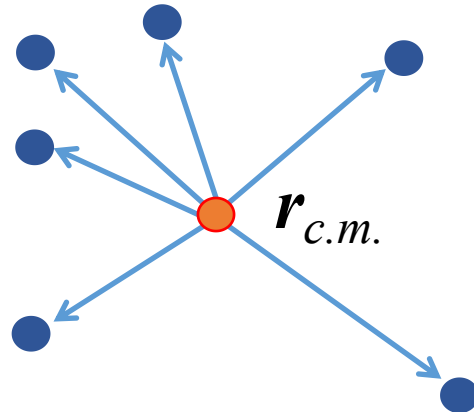
$$|\Phi_{s_i, L_t}\rangle = M_{s_i}^{L_t} |\Phi_0\rangle = \mathcal{A}[\phi_{s_i,1}(\mathbf{r}_1)\phi_{s_i,2}(\mathbf{r}_2)\dots\phi_{s_i,A}(\mathbf{r}_A)]$$

Theoretical Framework

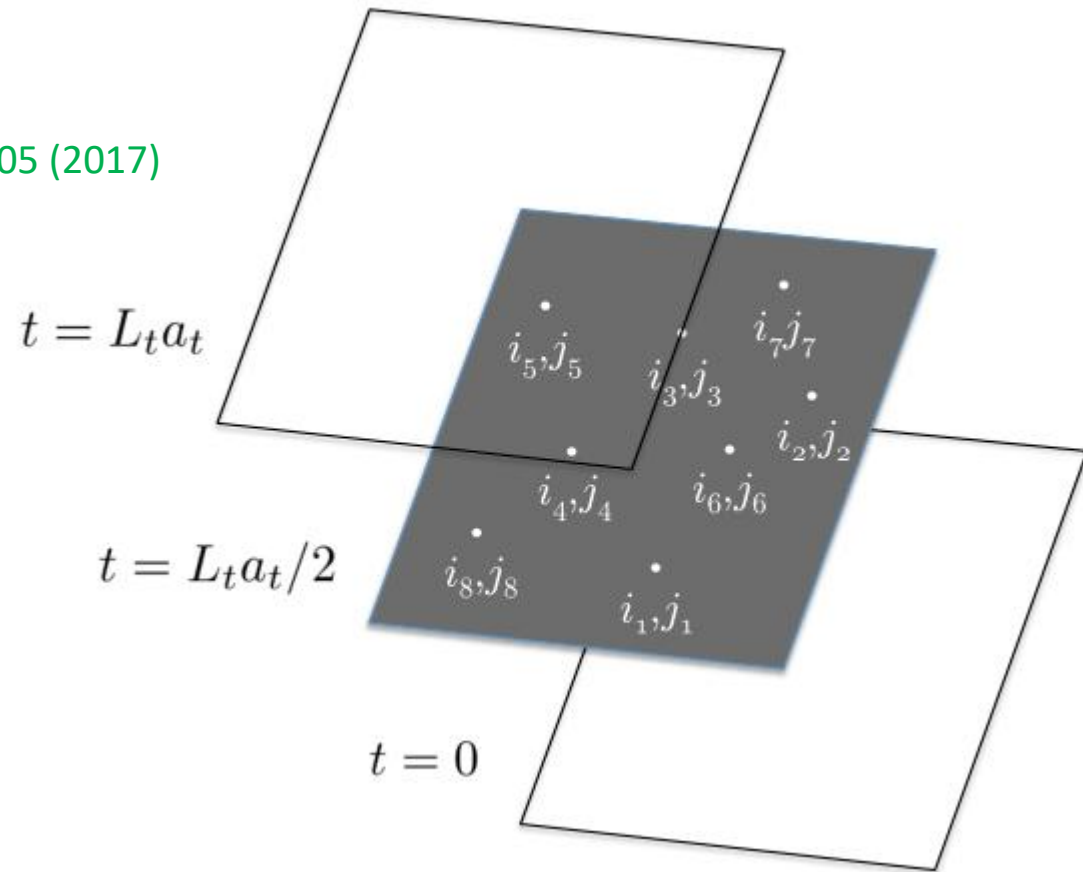
➤ Pinhole algorithm

S. Elhatisari et al., PRL 119, 222505 (2017)

A time slice is inserted to sample the positions and spin-isospin indices in the middle time step.



$\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A$



- Density distribution $\rho(\mathbf{r})$ can be obtained by counting how many times the nucleons appear at position \mathbf{r} over millions of configurations.

Numerical Details

- Lattice length $L = 14.8$ fm with spacing $a = 1.64$ fm; temporal lattice spacing $a_t = 0.55$ fm/c.
- Fitted results for SU(4) interaction

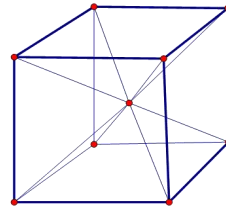
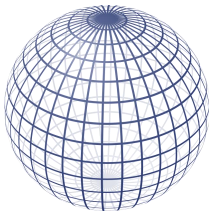
C_2 [MeV ⁻²]	C_3 [MeV ⁻⁵]	s_L	s_{NL}
-2.15×10^{-5}	6.17×10^{-12}	0.08	0.05

	NLEFT	Exp.
$E(^4\text{He})$ [MeV]	-28.1 (1)	-28.3
$E(^{12}\text{C})$ [MeV]	-91.6 (1)	-92.2
$r_c(^{12}\text{C})$ [fm]	2.52 (1)	2.47 (2)

Calculation of the Hoyle state

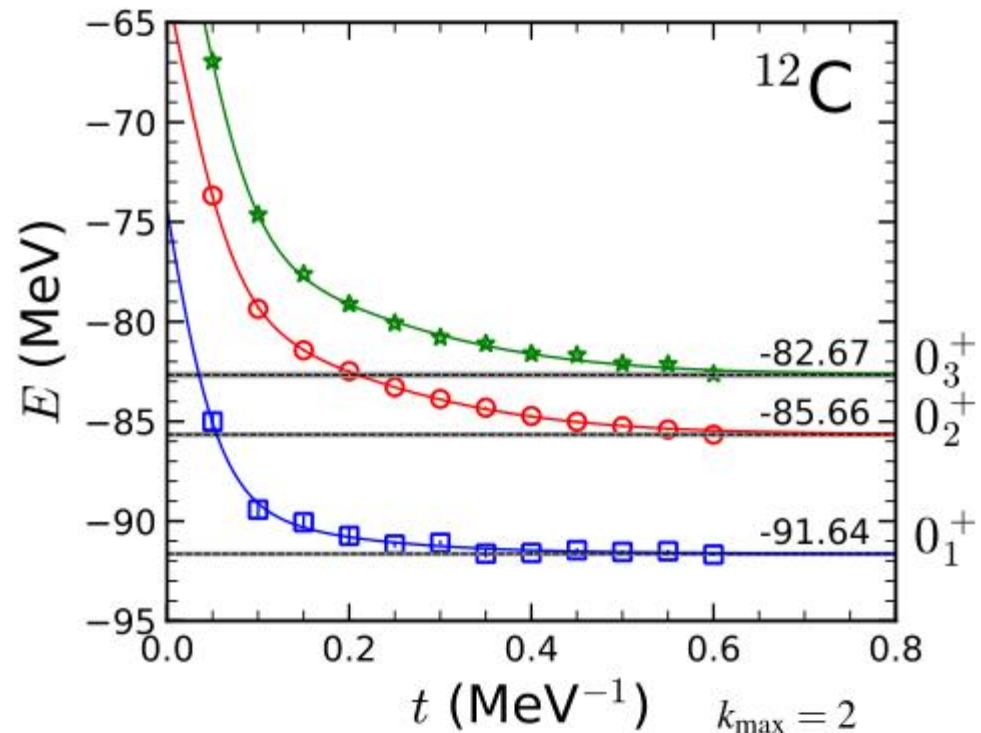
➤ Hoyle state

Angular momentum projection: SO(3) group reduced to cubic group O



J	irrepresentation
0	A ₁
1	T ₁
2	E + T ₂
3	A ₂ + T ₁ + T ₂
4	A ₁ + E + T ₁ + T ₂

$$\phi(\mathbf{r}) = \exp\left(-(\mathbf{r} - \mathbf{r}_0)^2/2w^2\right)$$

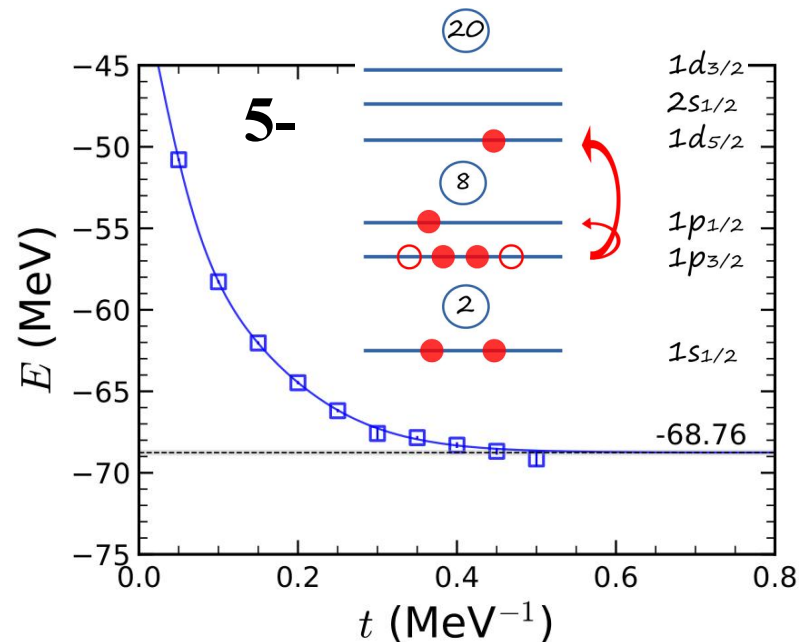
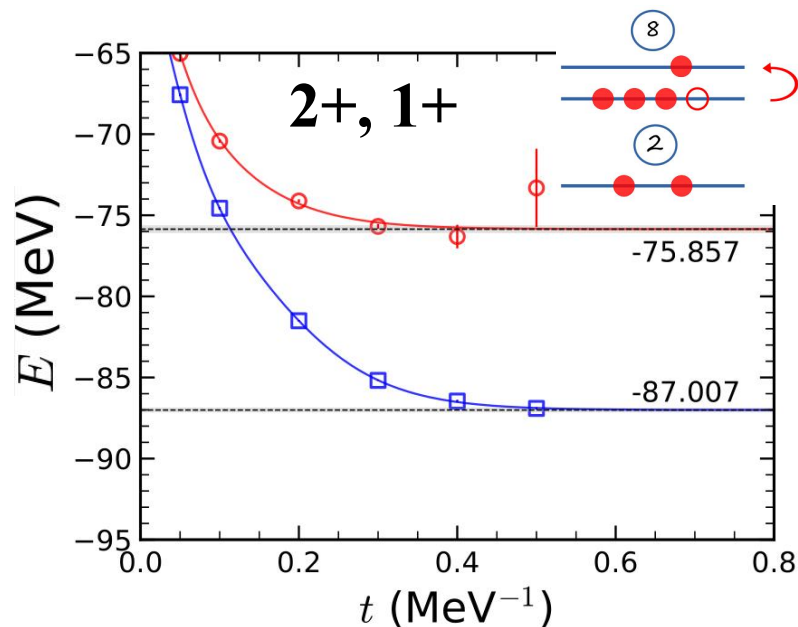
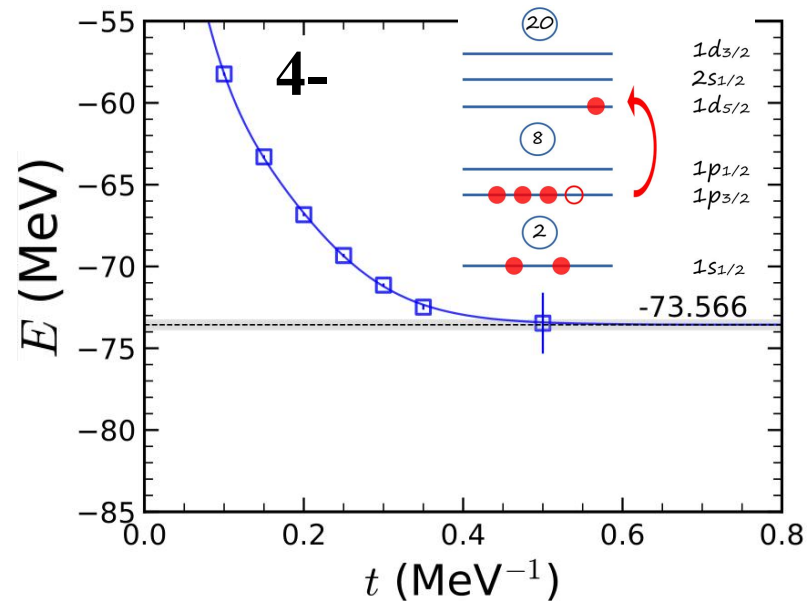
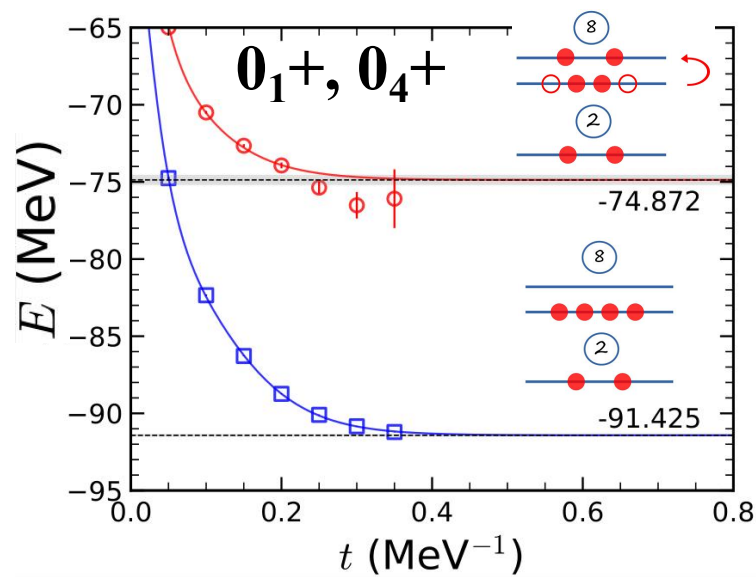


$$E_i(t) = \frac{E_i + \sum_{k=1}^{k_{\max}} (E_i + \Delta E_{i,k}) c_{i,k} e^{-\Delta E_{i,k} t}}{1 + \sum_{k=1}^{k_{\max}} c_{i,k} e^{-\Delta E_{i,k} t}}$$

T. A. Lähde et al., JPG 42 (2015) 034012

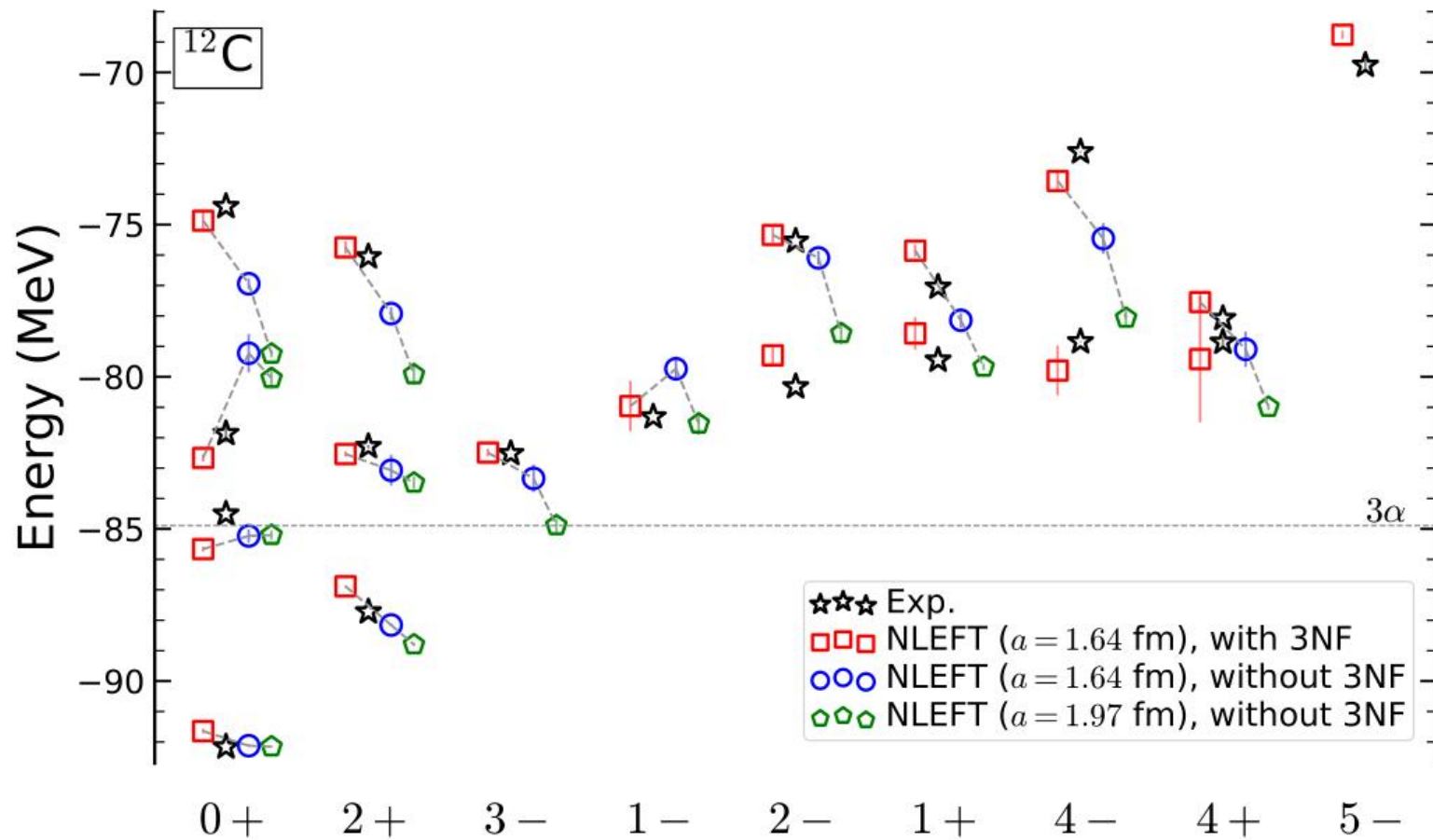
Web figures from: <https://en.wikipedia.org/wiki/Sphere>
<https://math.ucr.edu/home/baez/icosidodecahedron/7.html>

Shell-Model States Used as Initial Wave



Low-lying Spectrum

- Spectrum of ^{12}C calculated by NLEFT using SU(4) interaction in comparison with experimental data.



S. Shen, T. A. Lähde, D. Lee, U.-G. Meißner, arXiv:2202.13596
S. Shen, T. A. Lähde, D. Lee, U.-G. Meißner, EPJA 57, 276 (2021)

Electromagnetic Properties

- Quadrupole moment and transition rates of ^{12}C calculated by NLEFT, comparing with other theoretical calculations and Experiments. Units for Q and $M(E0)$ are $e\text{ fm}^2$ and for $B(E2)$ $e^2\text{ fm}^4$.

	NLEFT	FMD	α cluster	NCSM	GCM	Exp.
$Q(2_1^+)$	6.8(3)(1.2)	—	—	6.3(3)	—	8.1(2.3)
$Q(2_2^+)$	−35(1)(1)	—	—	—	—	—
$M(E0, 0_1^+ \rightarrow 0_2^+)$	4.8(3)	6.5	6.5	—	6.2	5.4(2)
$M(E0, 0_1^+ \rightarrow 0_3^+)$	0.4(3)	—	—	—	3.6	—
$M(E0, 0_2^+ \rightarrow 0_3^+)$	7.4(4)	—	—	—	47.0	—
$B(E2, 2_1^+ \rightarrow 0_1^+)$	11.4(1)(4.3)	8.7	9.2	8.7(9)	—	7.9(4)
$B(E2, 2_1^+ \rightarrow 0_2^+)$	2.4(2)(7)	3.8	0.8	—	—	2.6(4)

Future Experiments can be used as a test.

fermion molecular dynamics (FMD) [M. Chernykh et al., PRL 98, 032501 \(2007\)](#)

α cluster [M. Chernykh et al., PRL 98, 032501 \(2007\)](#)

BEC [Y. Funaki et al., PRC 67, 051306 \(2003\); EPJA 24, 321 \(2005\)](#)

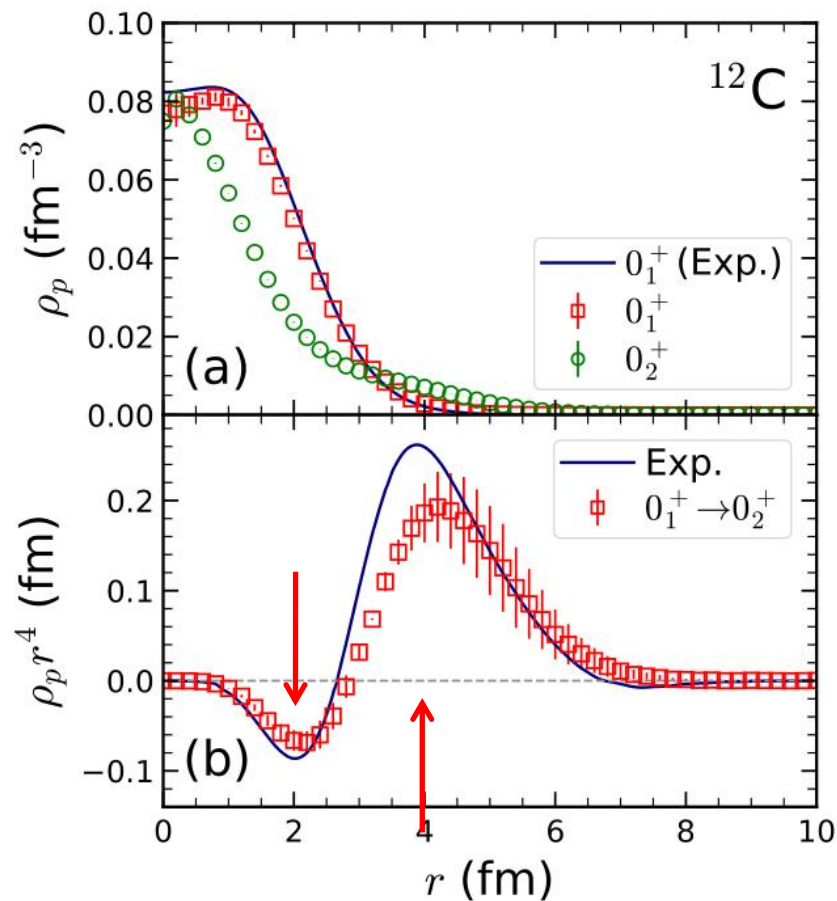
in-medium no-core shell model (NCSM) [A. D'Alessio et al., PRC 102, 011302 \(2020\)](#)

generator coordinate method (GCM) [B. Zhou, PRC 94, 044319 \(2016\)](#)

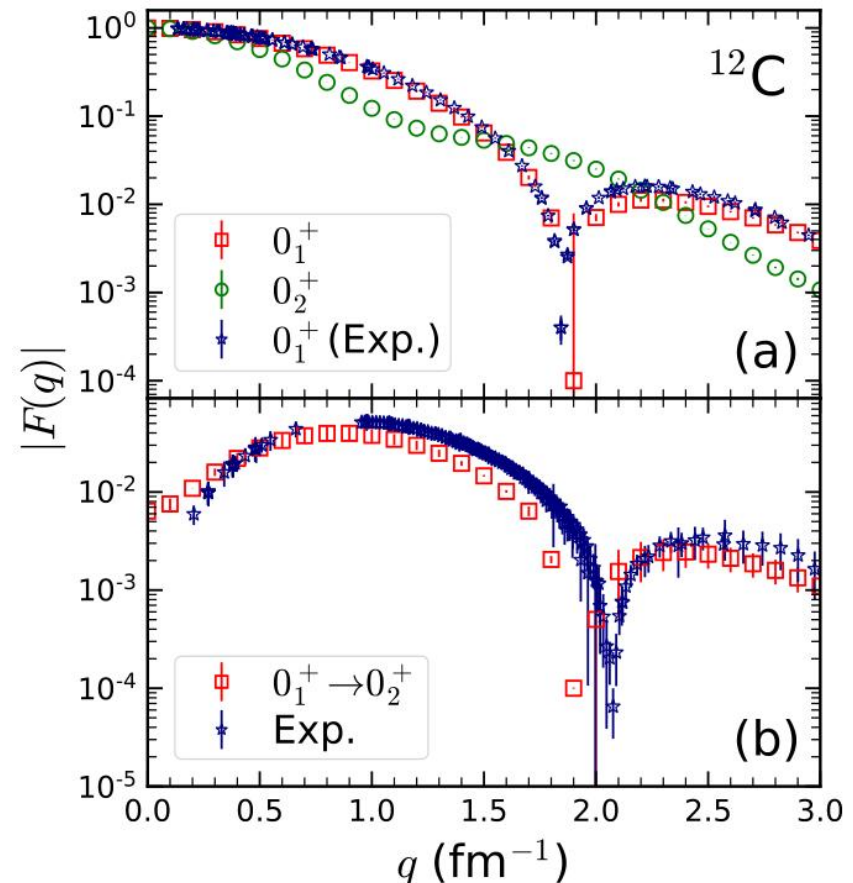
Exp. [F. Ajzenberg-Selove, NPA 506, 1 \(1990\); J. Saiz Lomas, PhD thesis, University of York, UK \(2021\)](#)

Density Profiles

- Charge density distributions (left) and form factors (right) of ground state, Hoyle state, and transitions between them.



$$F(q) = \frac{4\pi}{Z} \int dr r^2 \rho_p(r) j_0(qr)$$



Exp. M. Chernykh et al., PRL 105, 022501 (2010)

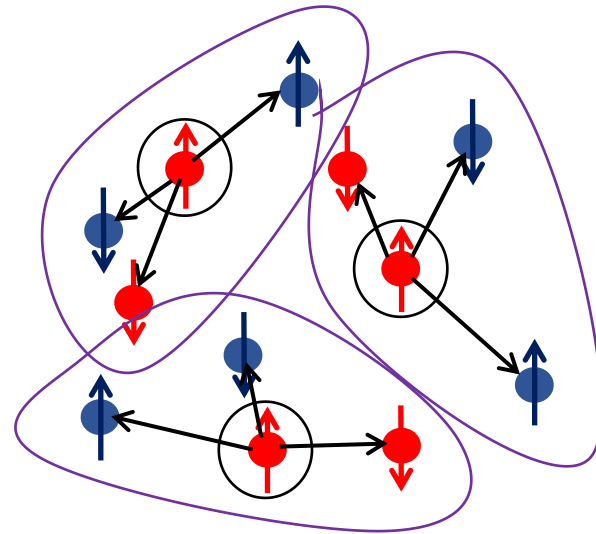
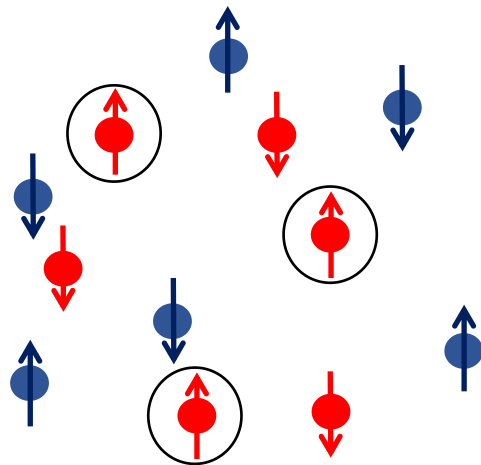
I. Sick and J. S. McCarthy, NPA 150, 631 (1970)

P. Strehl, Z. Phys. 234 (1970) 416; H. Crannell et al., NPA 758, 399 (2005)

Investigation of the Geometry

➤ Define α cluster

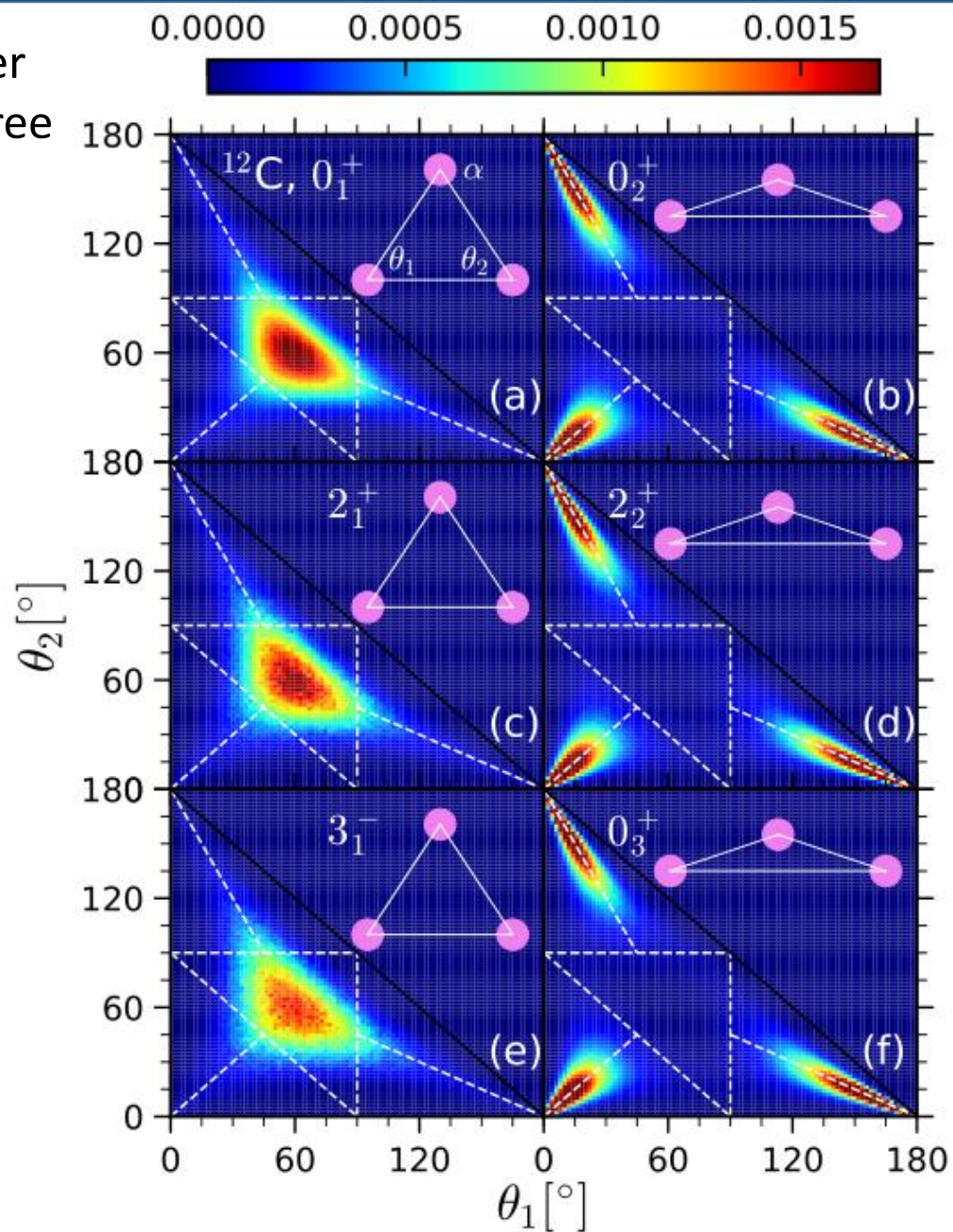
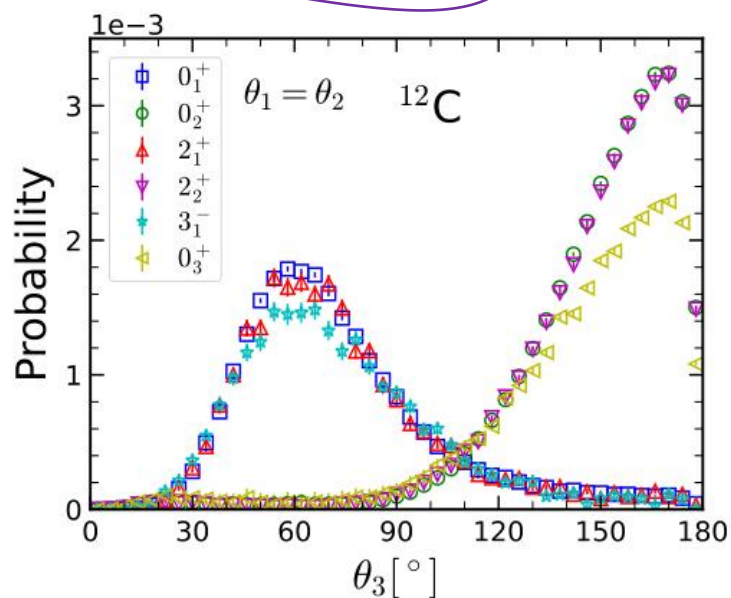
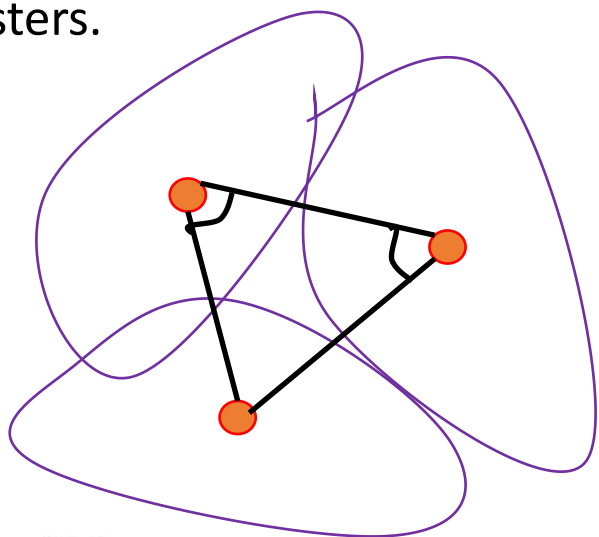
1. Identify 3 spin-up protons;
2. Find the closest possible of the other 3 types of particles (spin-down proton, spin-up neutron, spin-down neutron);
3. Calculate the rms radius of α cluster defined this way and compare with 4He calculation.



	$12\text{C}, 0_1^+$	$12\text{C}, 0_2^+$	4He
rms α cluster [fm]	1.65	1.71	1.63

Distribution of Angles

Probability distribution for the two inner angles of the triangle formed by the three α clusters.



Density Distribution

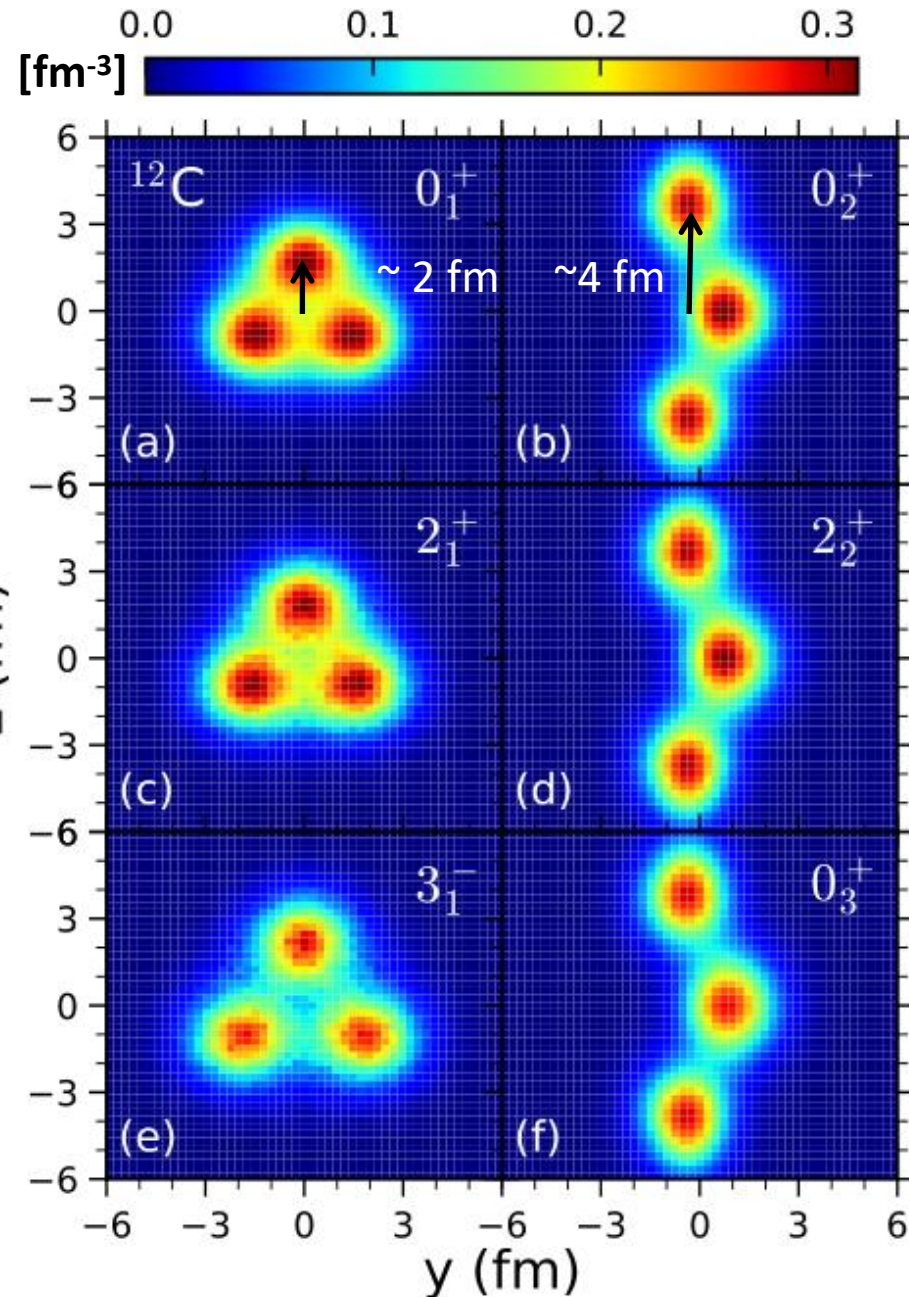
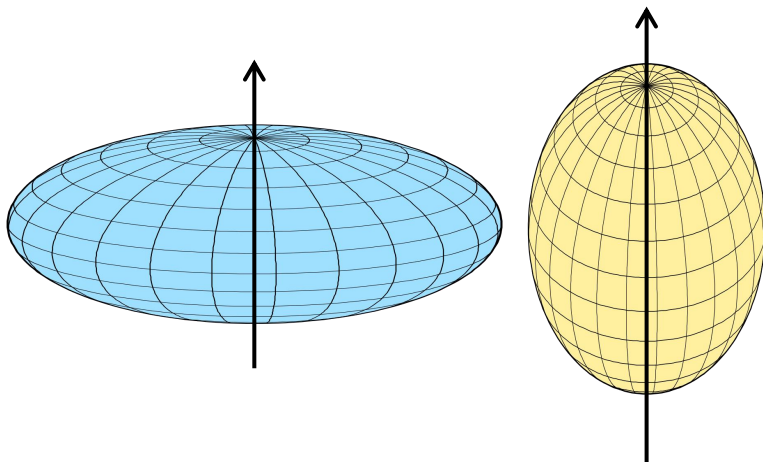
➤ Alignment of configurations:

For equilateral triangle type:

1. Align shortest principal axis to x
2. Rotate 1 α to $y = 0$ (positive z), and (randomly) $\pm 120^\circ$.

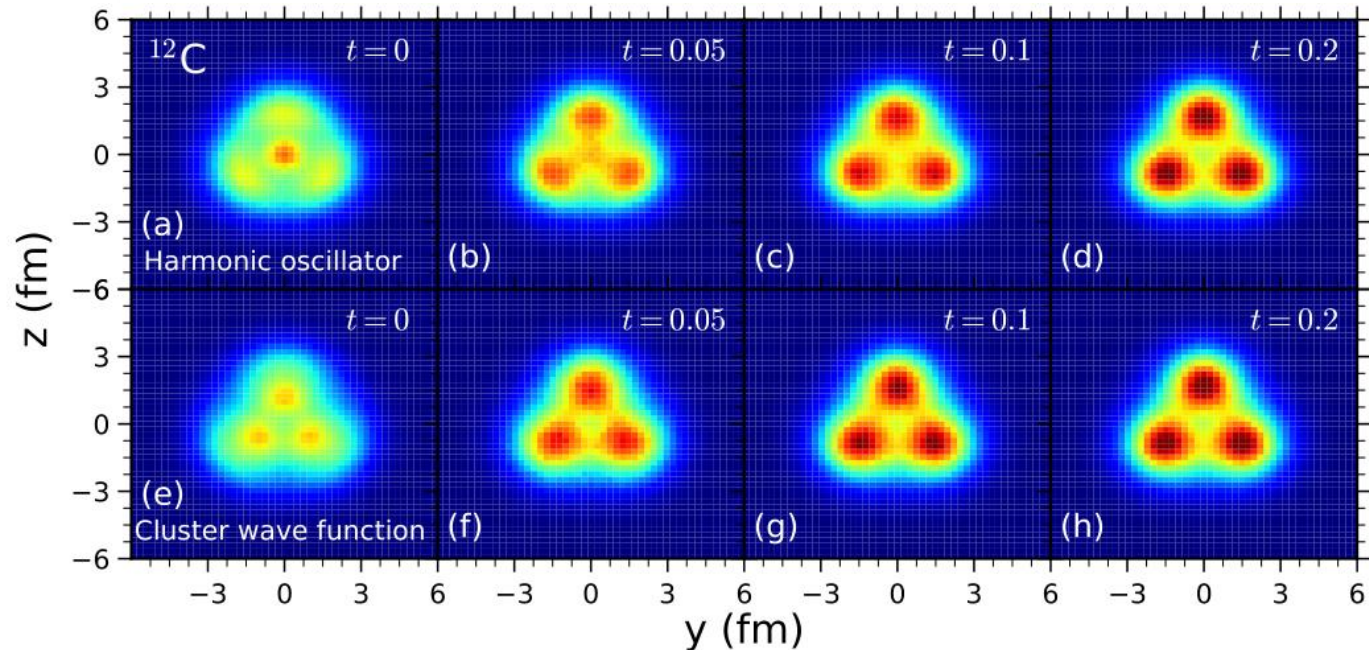
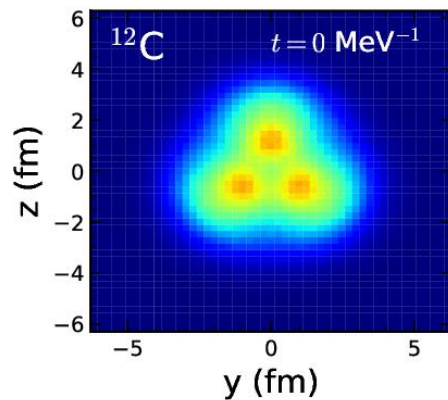
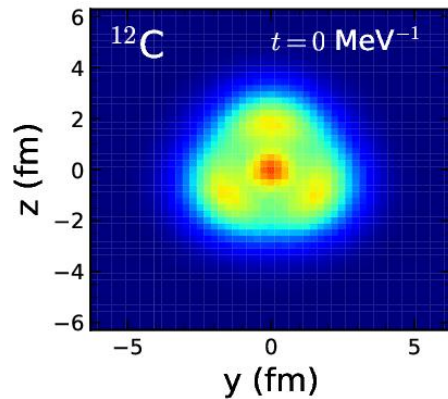
For obtuse triangle type:

1. Align longest principal axis to z;
2. Rotate central α to $x = 0$ (positive y).

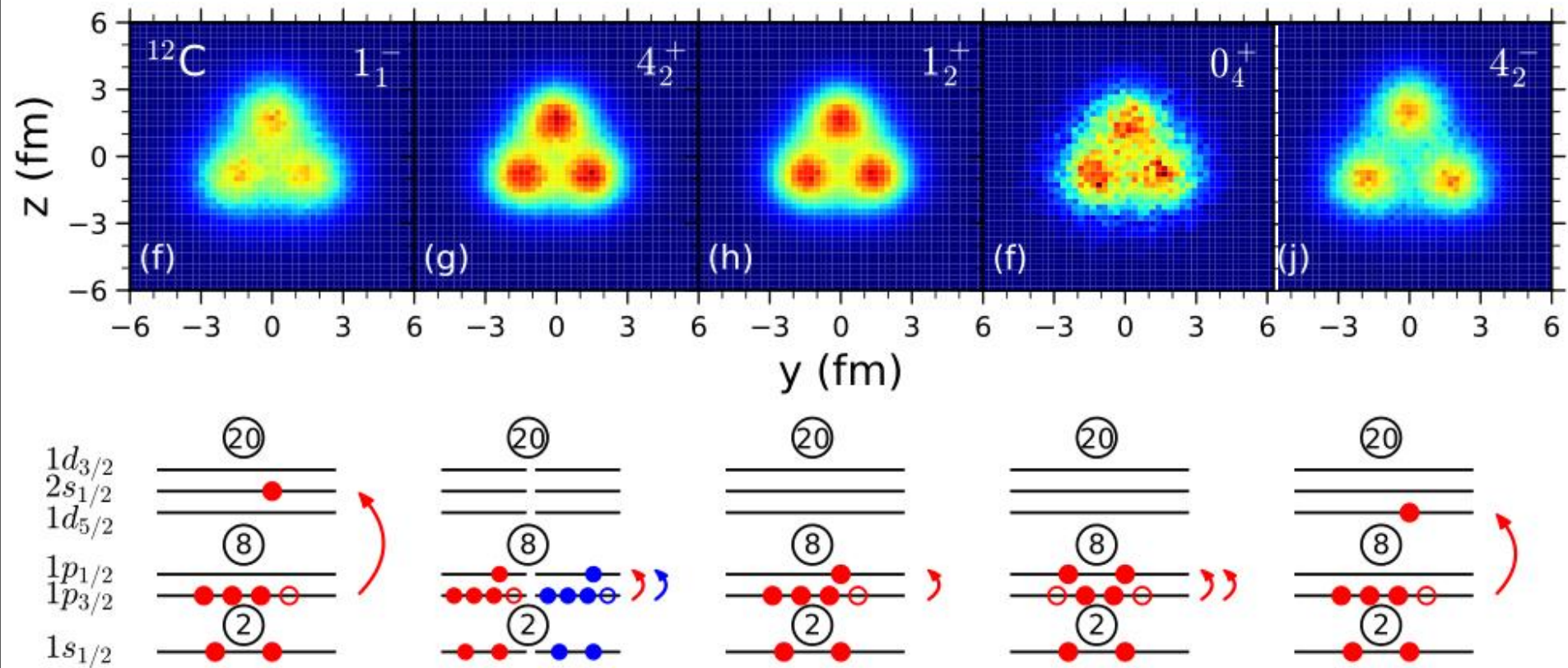


Cluster Formation

- Density distribution of ^{12}C ground state using (a-d) harmonic oscillator or (e-h) cluster wave function as initial states, with Euclidean projection time ranging from $t = 0$ to 0.2 MeV^{-1} .

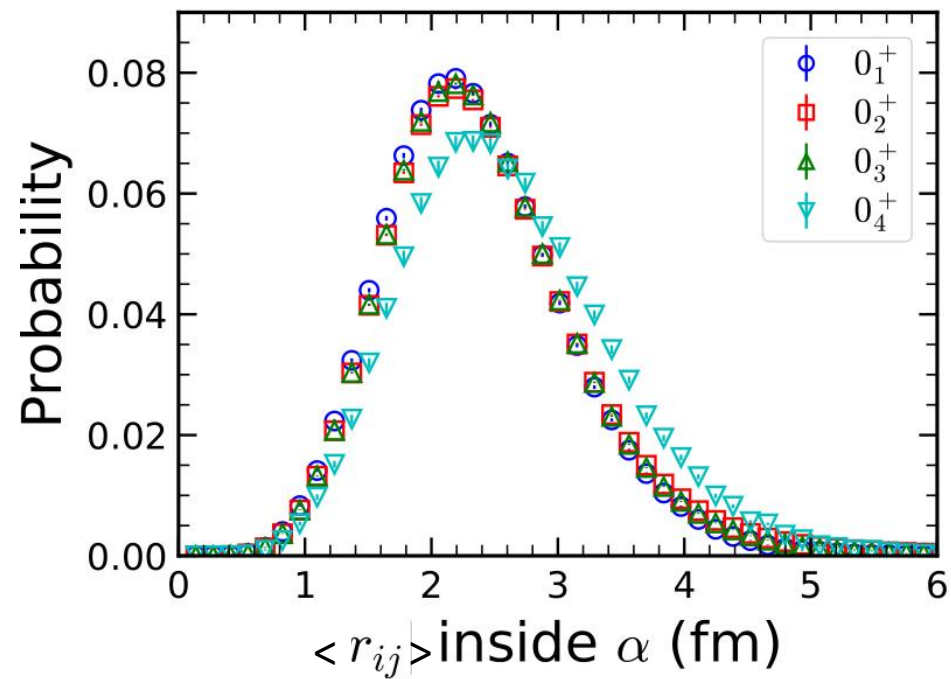
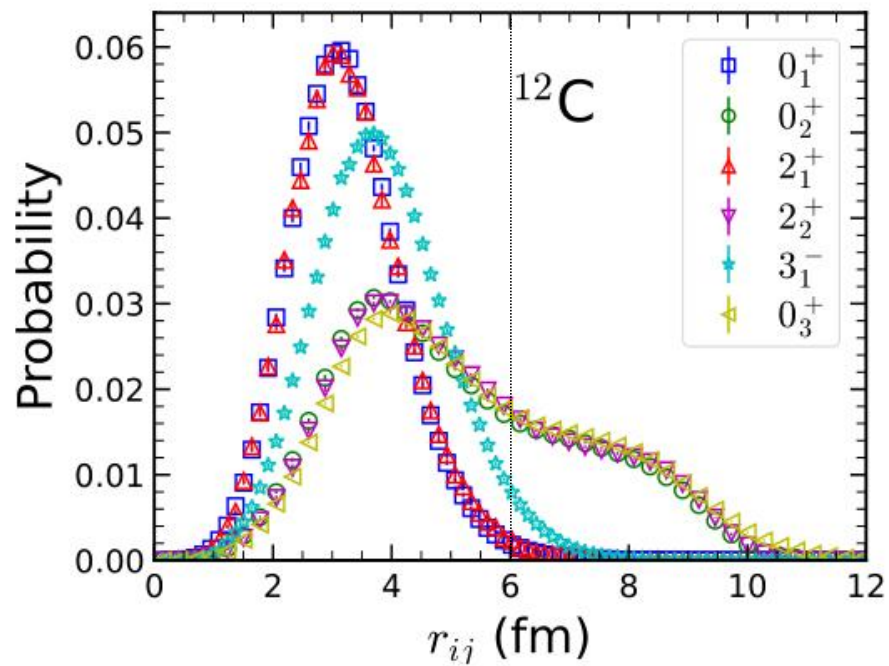
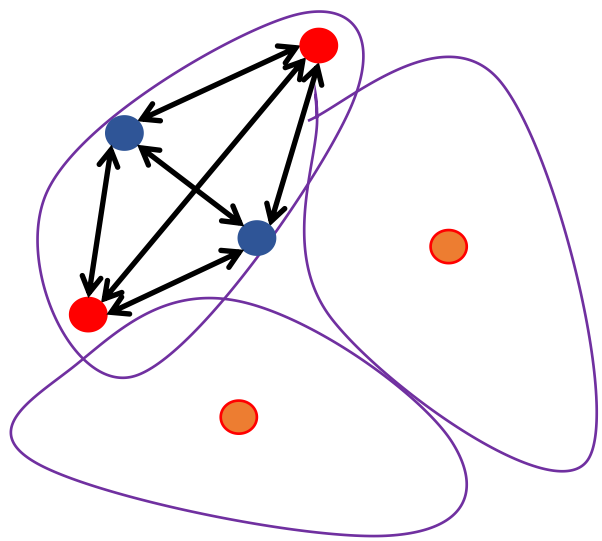
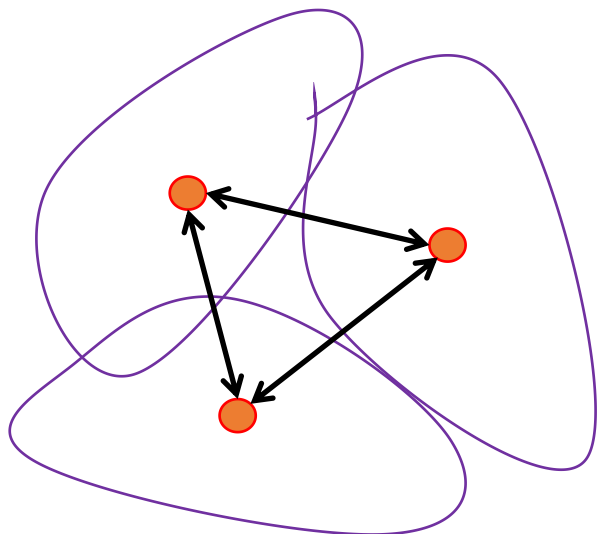


Shell-Model States as Initial Wave



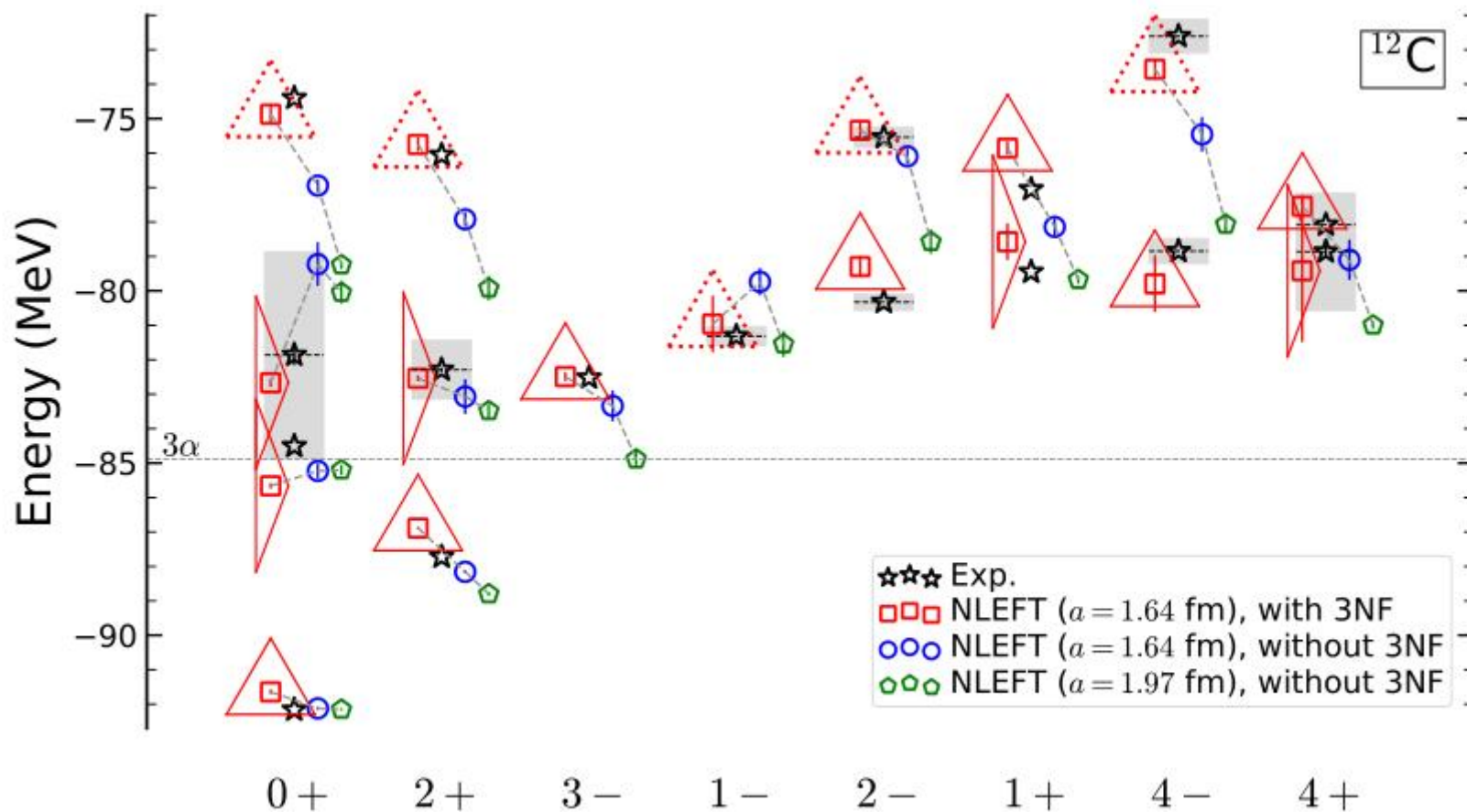
- α cluster structure is less clear due to single-particle excitation, especially when excited to the next shell.

Cluster Excitation? Single-Particle Excitation?



Geometry Information in the Low-Lying Spectrum

- To summarize the geometry properties of each states in the low-lying spectrum of ^{12}C calculated by NLEFT:
- 2 types of shape: equilateral or large angle obtuse triangle.
 - α cluster is well maintained (solid triangles) or diminished (dashed ones).



Summary

Summary

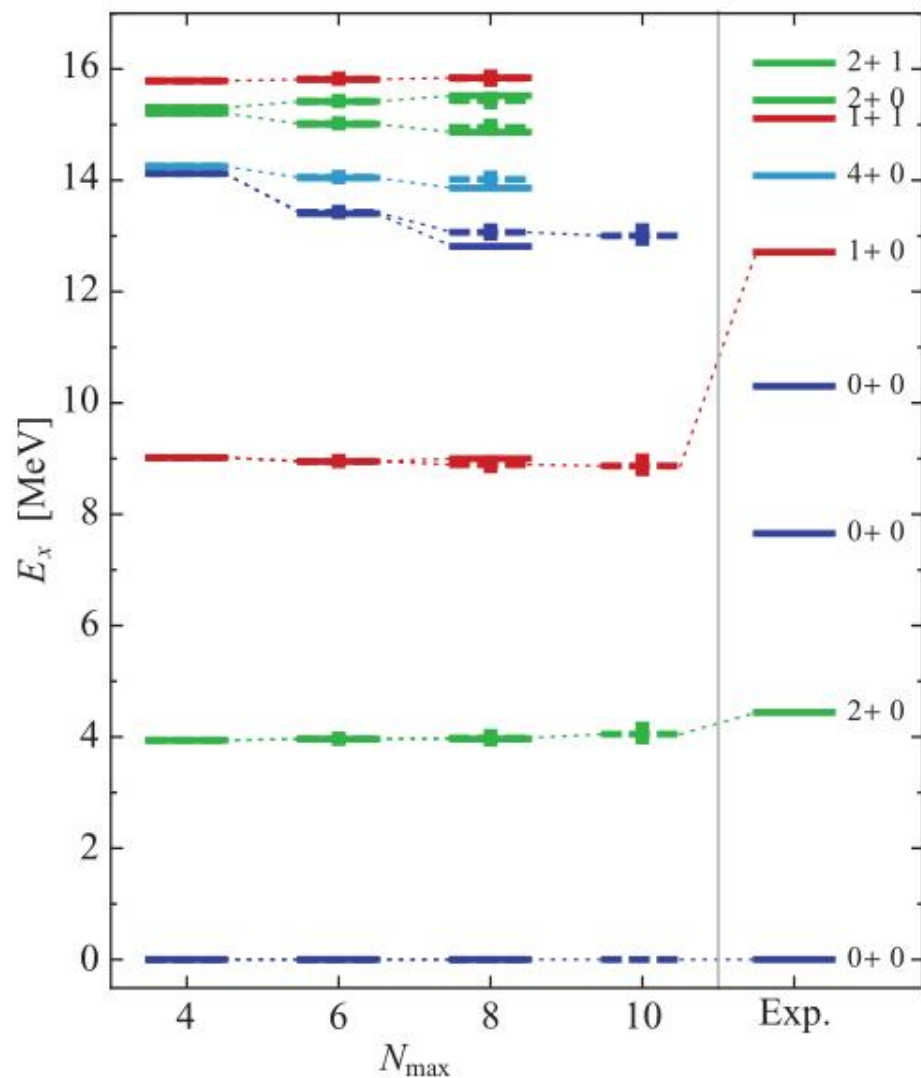
- ❑ Low-lying spectrum of ^{12}C have been studied by NLEFT using SU(4) interaction, the agreement with experiment is impressive, not only energies, but also electromagnetic transitions and density profiles.
- ❑ A model-independent tomographic scan of the three-dimensional geometry of the nuclear states has been introduced. The Hoyle state and its rotational/vibrational excitations, as already stated in [E. Epelbaum et al., PRL 109, 252501 \(2012\)](#), are found to be an obtuse isosceles triangle with large angle.

Perspectives

- ❑ ^{16}O
- ❑ full N3LO interaction
- ❑

THANK YOU!

Maris P, Vary JP, Calci A, Langhammer J, Binder S, Roth R., Phys Rev C. (2014) 90:014314
D. R. Entem and R. Machleidt, Phys. Rev. C 68, 041001 (2003)



PHYSICAL REVIEW C **90**, 014314 (2014)

^{12}C properties with evolved chiral three-nucleon interactions

P. Maris,^{1,*} J. P. Vary,^{1,†} A. Calci,^{2,‡} J. Langhammer,^{2,§} S. Binder,^{2,||} and R. Roth^{2,¶}

