Dr. Klaus Erkelenz Prize Colloquium, 26 April 2022

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

Shihang Shen
Forschungszentrum Jülich

Special thanks to Dr. Gabriele Erkelenz and the prize committe

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

Acquaintance with Dr. Klaus Erkelenz's Work

- My PhD work: Relativistic Brueckner-Hartree-Fock Theory for Finite Nuclei

Progress in Particle and Nuclear Physics 109 (2019) 103713

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Progress in Particle and Nuclear Physics

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

Review

Towards an *ab initio* covariant density functional theory for nuclear structure

Shihang Shen [a,b,c], Haozhao Liang [d,e], Wen Hui Long [f,g], Jie Meng [a,h,i,*], Peter Ring [a,j]

[51] K. Erkelenz, Phys. Rep. 13 (1974) 191–258

Bonn potential, one of the most successful models for nuclear interaction in the framework of one-boson-exchange, is one of the very few choices that is also suitable for relativistic *ab initio* calculations.

PHYSICS REPORTS (Section C of Physics Letters) 13, no. 5 (1974) 191–258. NORTH-HOLLAND PUBLISHING COMPANY

CURRENT STATUS OF THE RELATIVISTIC TWO-NUCLEON ONE BOSON EXCHANGE POTENTIAL

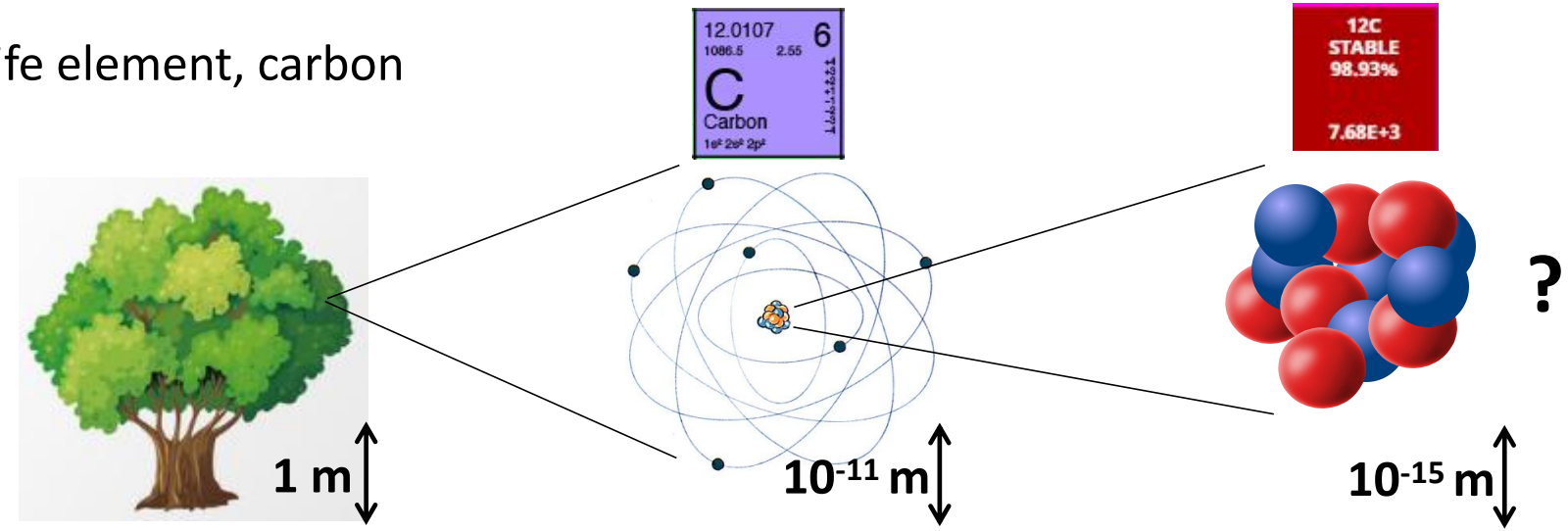
K. ERKELENZ

Institut für Theoretische Kernphysik, Bonn, W.-Germany

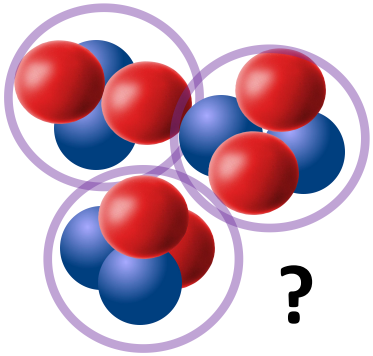
Received April 1974

What's Interesting about Carbon-12

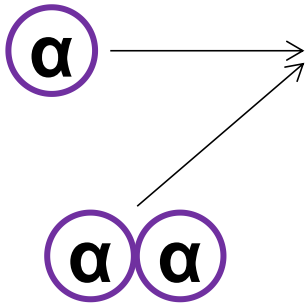
- Life element, carbon

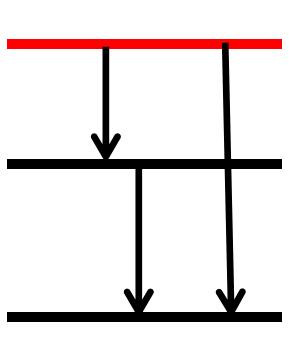


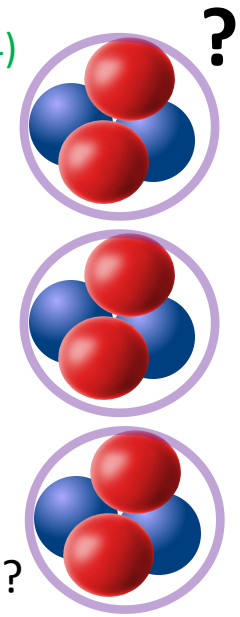
- We know little about its shape



F. Hoyle, Astrophys. J. Suppl. Ser. 1, 121 (1954)
H. Morinaga, Phys. Rev. 101, 254 (1956)







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

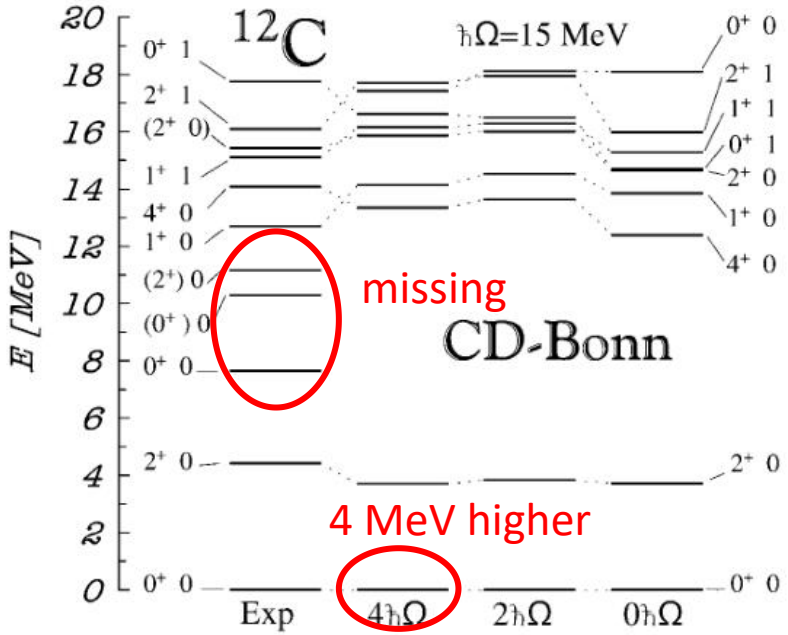
is the Hoyle state like a linear chain?

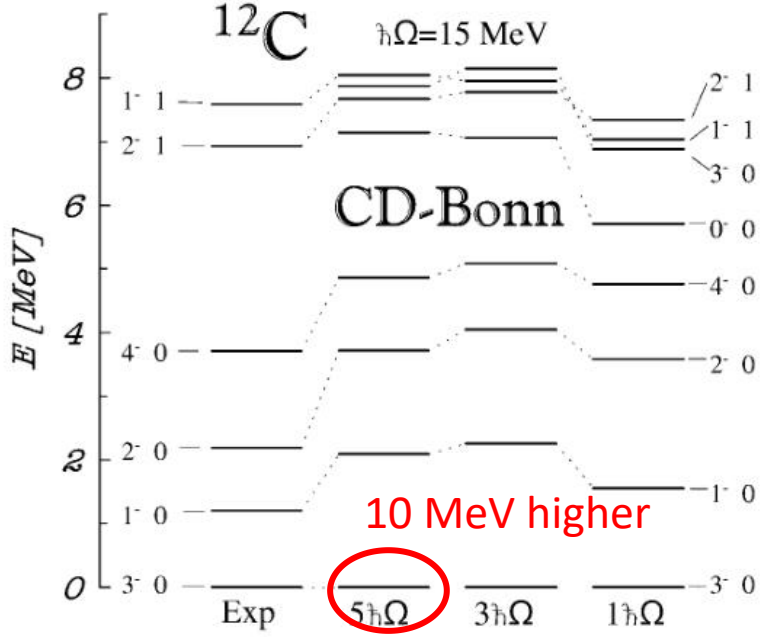
Challenge for Theoretical Calculations

- 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 dynamces H. Feldmeier, Nucl. Phys. A 515(1), 147 (1990)
  - … …

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

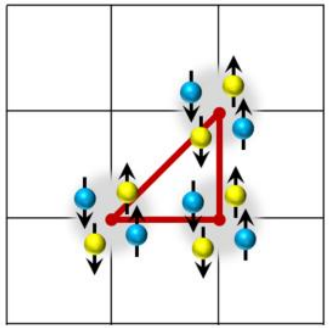
e.g. no-core shell model Navrátil, P., J. P. Vary, and B. R. Barrett, Phys. Rev. Lett. 84, 5728 (2000)

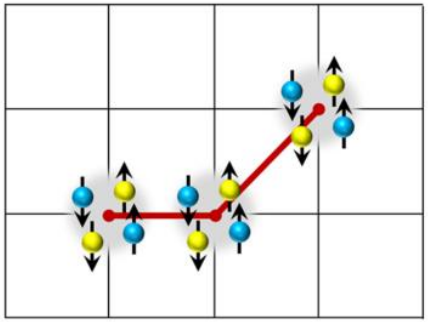




Challenge for Theoretical Calculations

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





Selected for a Viewpoint in *Physics*
PRL **106,** 192501 (2011) PHYSICAL REVIEW LETTERS week ending 13 MAY 2011

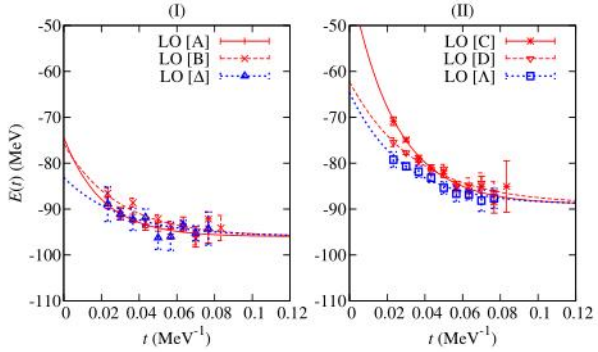
Ab Initio Calculation of the Hoyle State

Evgeny Epelbaum,[1] Hermann Krebs,[1] Dean Lee,[2] and Ulf-G. Meißner[3,4]

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

Structure and Rotations of the Hoyle State

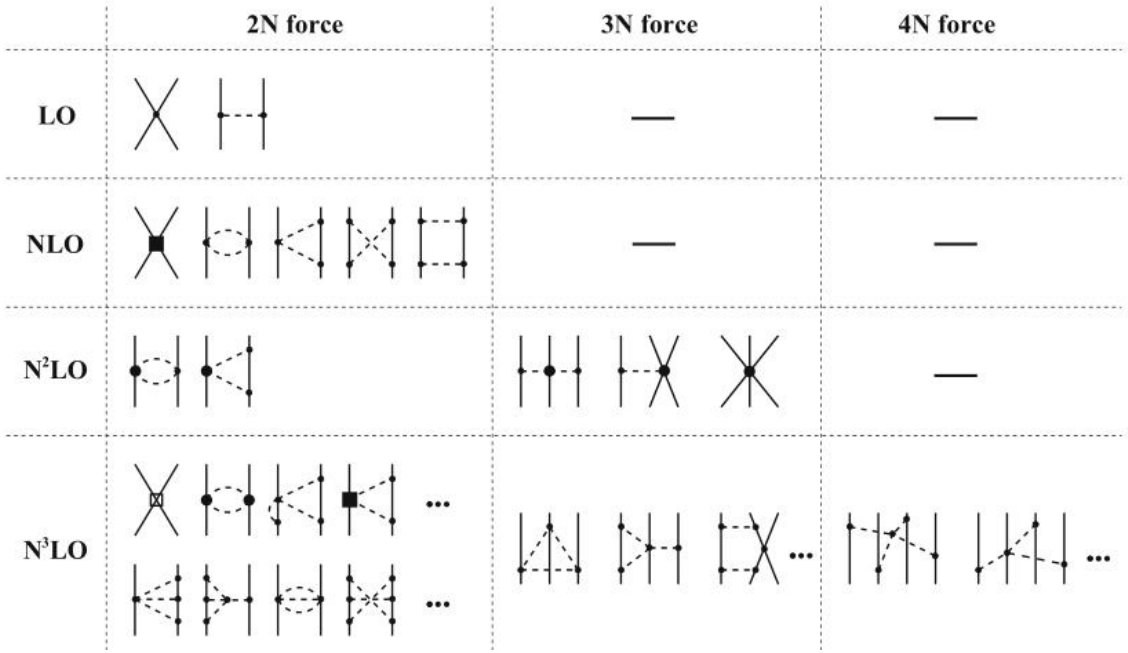
Evgeny Epelbaum,[1] Hermann Krebs,[1] Timo A. Lähde,[2] Dean Lee,[4] and Ulf-G. Meißner[5,2,3]

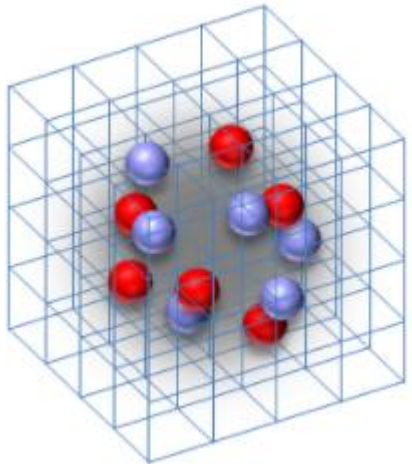


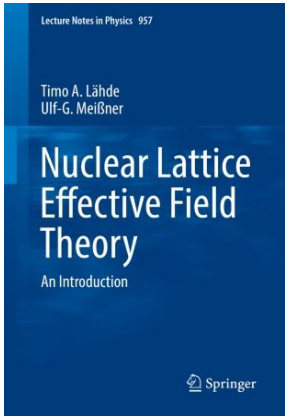
- Further questions:
  - Sign problem
  - Can we find a way to see the shape of the final states?
  - Low-lying spectrum, cluster excitation / single-particle excitation ?

Nuclear Lattice Effective Field Theory

- Nuclear lattice effective field theory (NLEFT)







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

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Review

Lattice simulations for few- and many-body systems

Dean Lee

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

- 16O, 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)
- … …

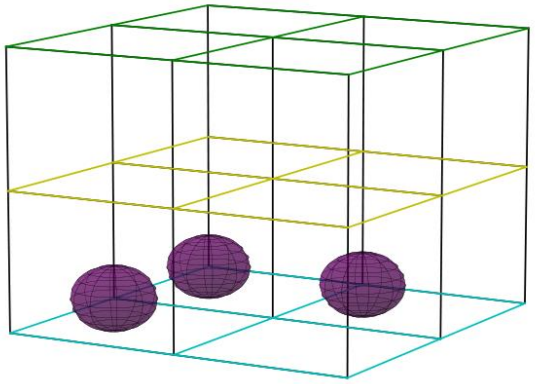
lattice figure from https://www.physics.ncsu.edu/ntg/leegroup/research.html

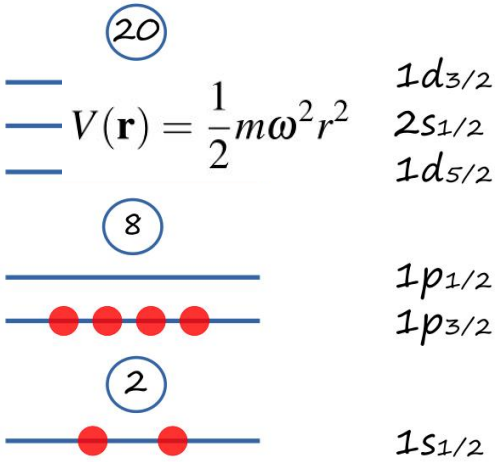
Theoretical Framework

- Starting from an initial many-body wave function:

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

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



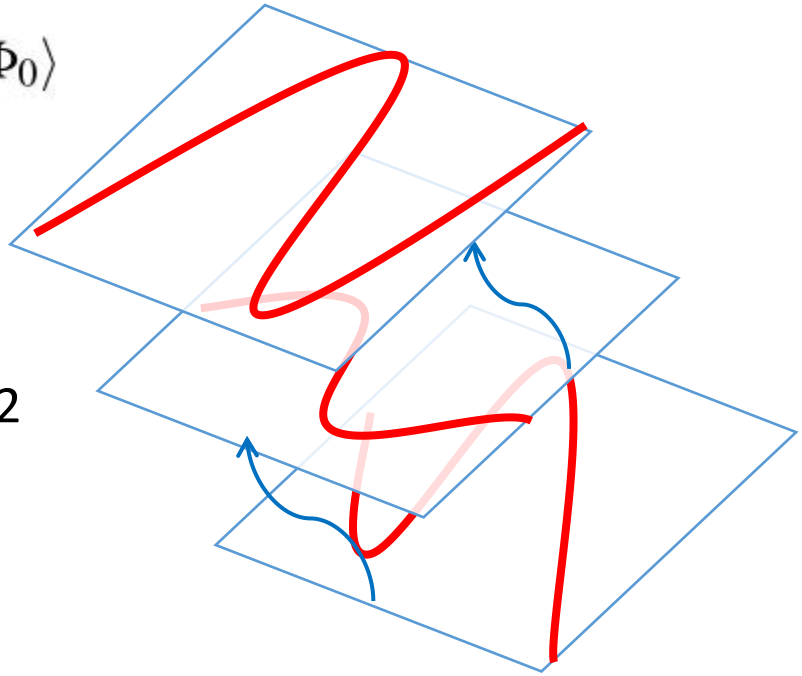


- Eculidean time projection with transfer matrix:

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

with H the many-body Hamiltonian, a_t and a the tempral 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):

$$V = \frac{C_2}{2!}\sum_{\mathbf{n}}\tilde{\rho}(\mathbf{n})^2 + \frac{C_3}{3!}\sum_{\mathbf{n}}\tilde{\rho}(\mathbf{n})^3,$$

$$\tilde{\rho}(\mathbf{n}) = \sum_{i=1}^{A}\tilde{a}_i^{\dagger}(\mathbf{n})\tilde{a}_i(\mathbf{n}) + s_L\sum_{|\mathbf{n}'-\mathbf{n}|=1}\sum_{i=1}^{A}\tilde{a}_i^{\dagger}(\mathbf{n}')\tilde{a}_i(\mathbf{n}'),$$

$$\tilde{a}_i(\mathbf{n}) = a_i(\mathbf{n}) + s_{\mathrm{NL}}\sum_{|\mathbf{n}'-\mathbf{n}|=1}a_i(\mathbf{n}').$$

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

Four parametes C_2, C_3, s_L, and s_{NL} will be fitted to binding energy of ^{4}He 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

- Auxilary 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 is a superposition of millions of configurations (Slater determinants)

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

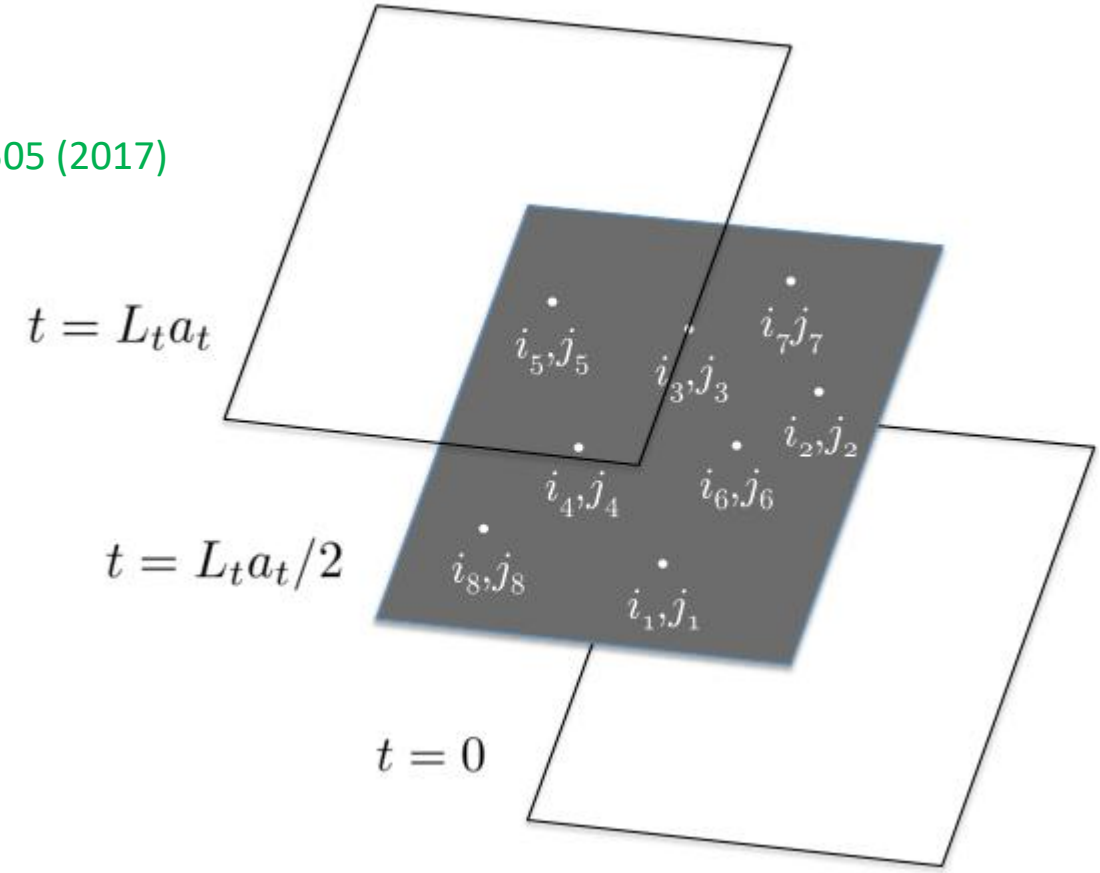
$$|\Phi_{s_i,L_t}\rangle = M_{s_i}^{L_t}|\Phi_0\rangle = \mathscr{A}[\phi_{s_i,1}(\mathbf{r}_1)\phi_{s_i,2}(\mathbf{r}_2)\ldots\phi_{s_i,A}(\mathbf{r}_A)]$$

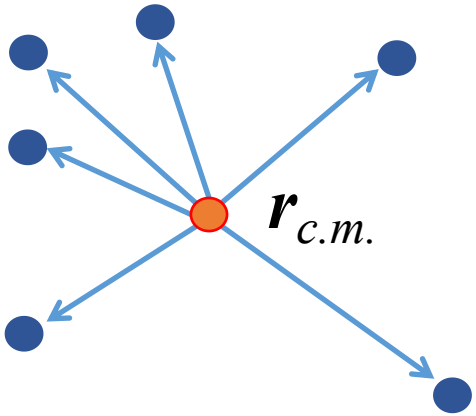
Theoretical Framework

- 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.





$\boldsymbol{r}_1$, $\boldsymbol{r}_2$, …, $\boldsymbol{r}_A$

- Density distribution ρ(***r***) can be obtained by counting how many times the nucleons appears at position ***r*** over millons 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

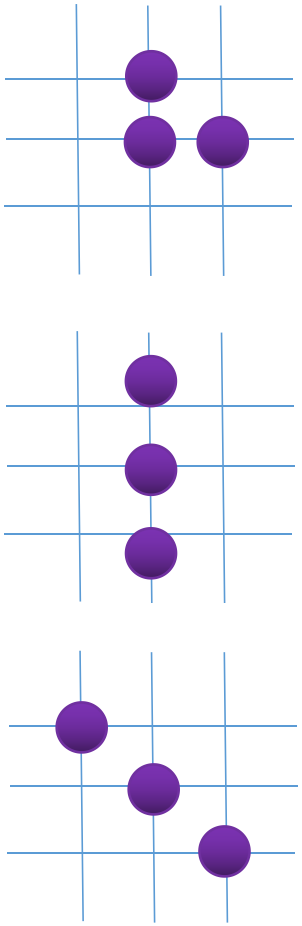
C_2 [MeV^{-2}]	C_3 [MeV^{-5}]	s_L	s_{NL}
-2.15×10^{-5}	6.17×10^{-12}	0.08	0.05

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

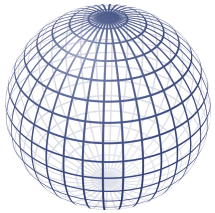
S. Shen, T. A. Lähde, D. Lee, U.-G. Meißner, arXiv:2202.13596

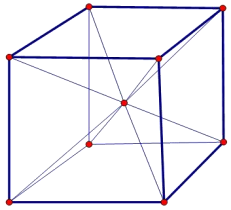
Calculation for Hoyle State

- Hoyle state



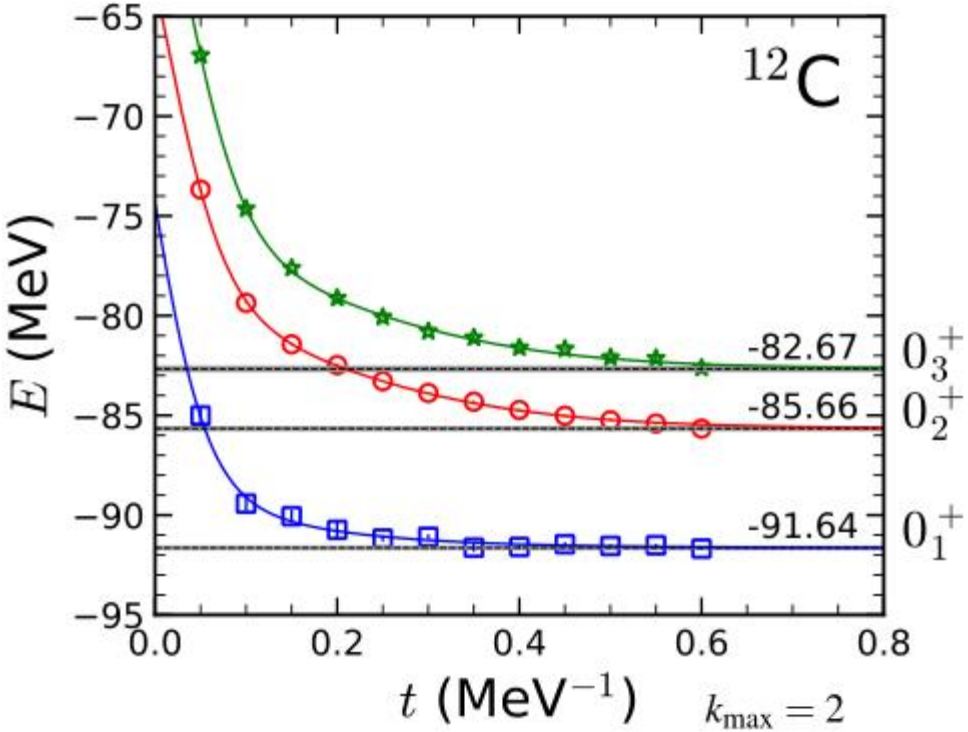
Angular momentum projection: SO(3) group reducted to cubic group O





J	irrepresentation
0	A_1
1	T_1
2	$E + T_2$
3	$A_2 + T_1 + T_2$
4	$A_1 + E + T_1 + T_2$

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

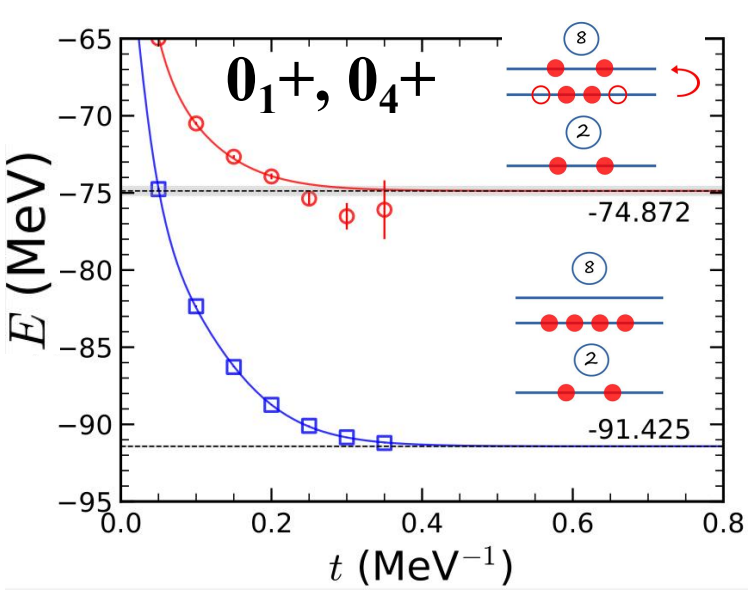


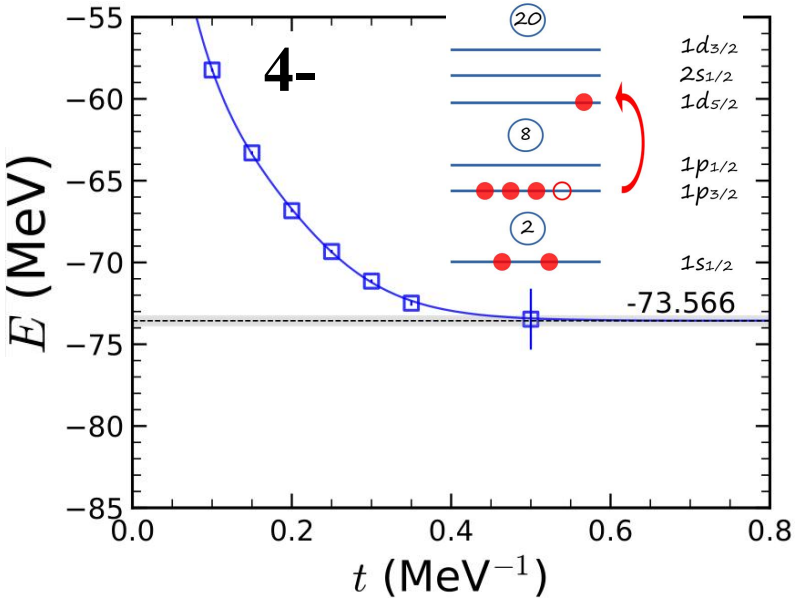
$$E_i(t) = \frac{E_i + \sum_{k=1}^{k_{\max}} (E_i + \Delta E_{i,k}) c_{i,k} e^{-\Delta E_{i,k} t}}{1 + \sum_{k=1}^{k_{\max}} c_{i,k} e^{-\Delta E_{i,k} t}}$$

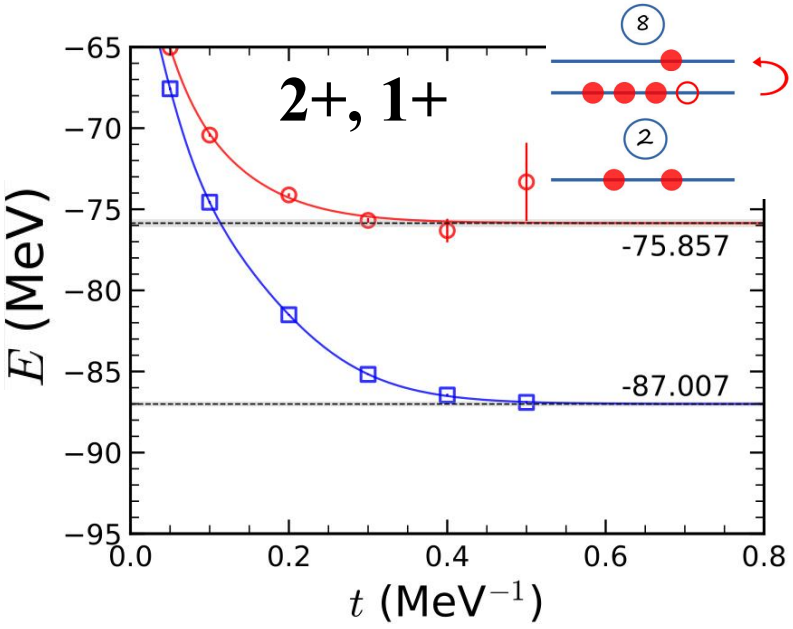
T. A. Lähde et al., JPG 42 (2015) 034012

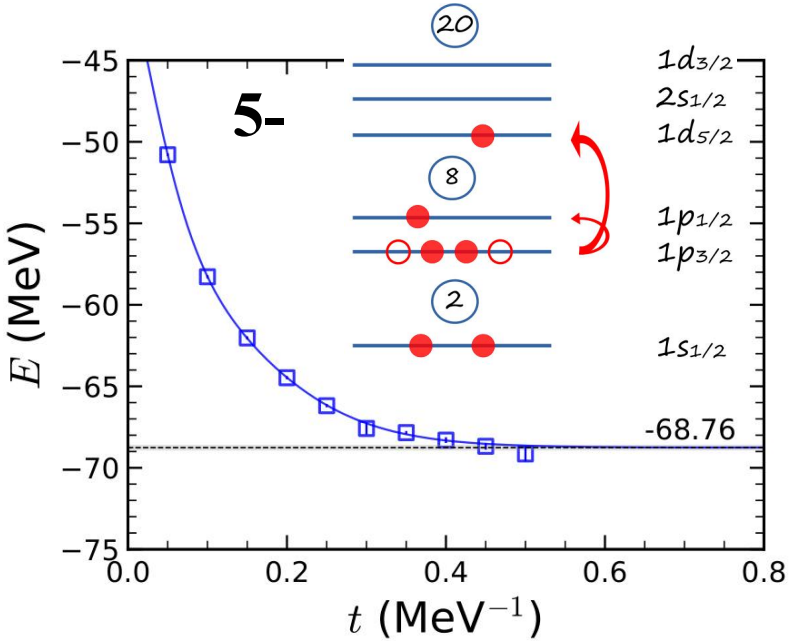
Web figures from: https://en.wikipedia.org/wiki/Sphere
https://math.ucr.edu/home/baez/icosidodecahedron/7.html

Shell-Model States Used as Initial Wave



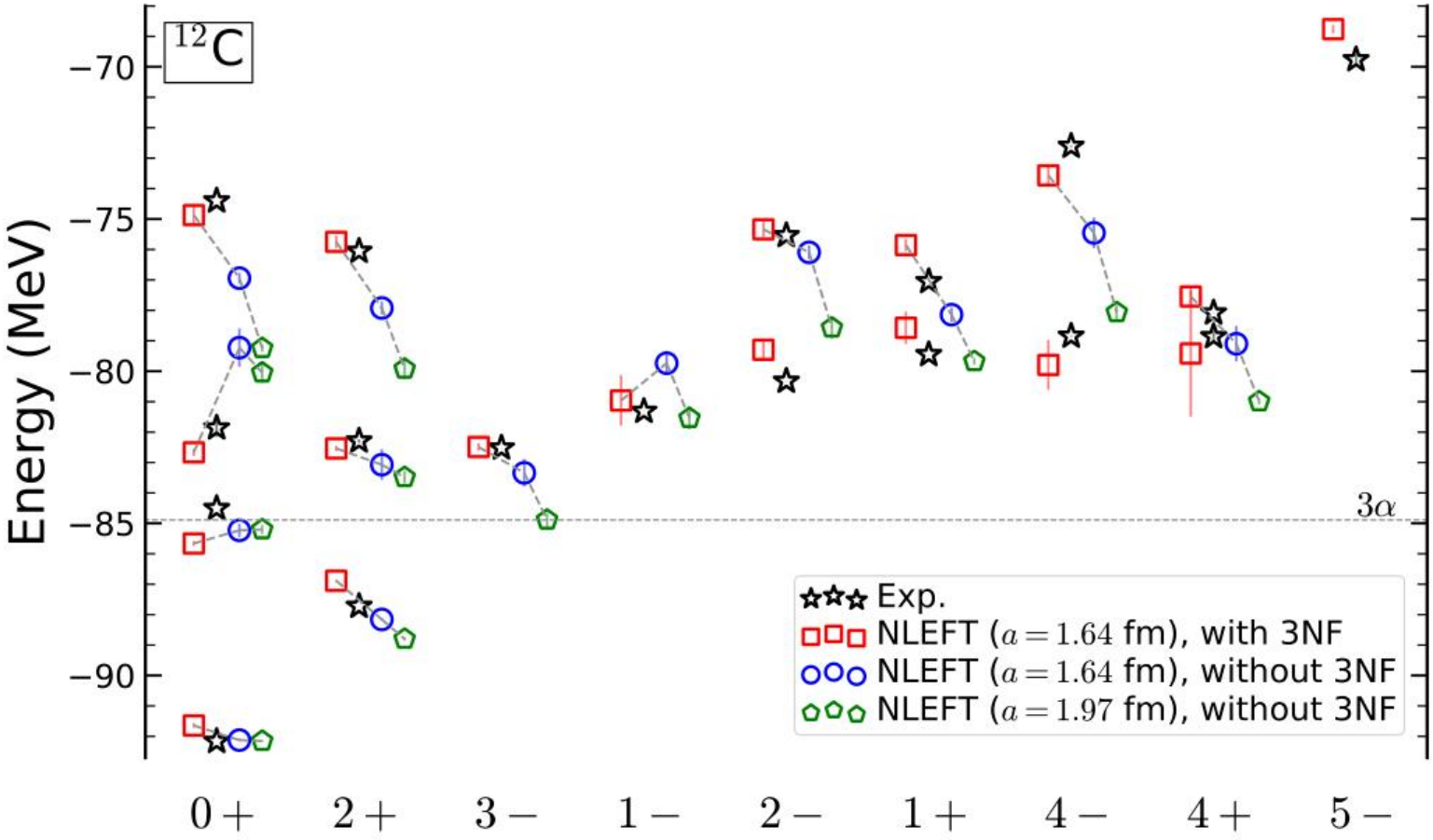






Low-lying Spectrum

- 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.

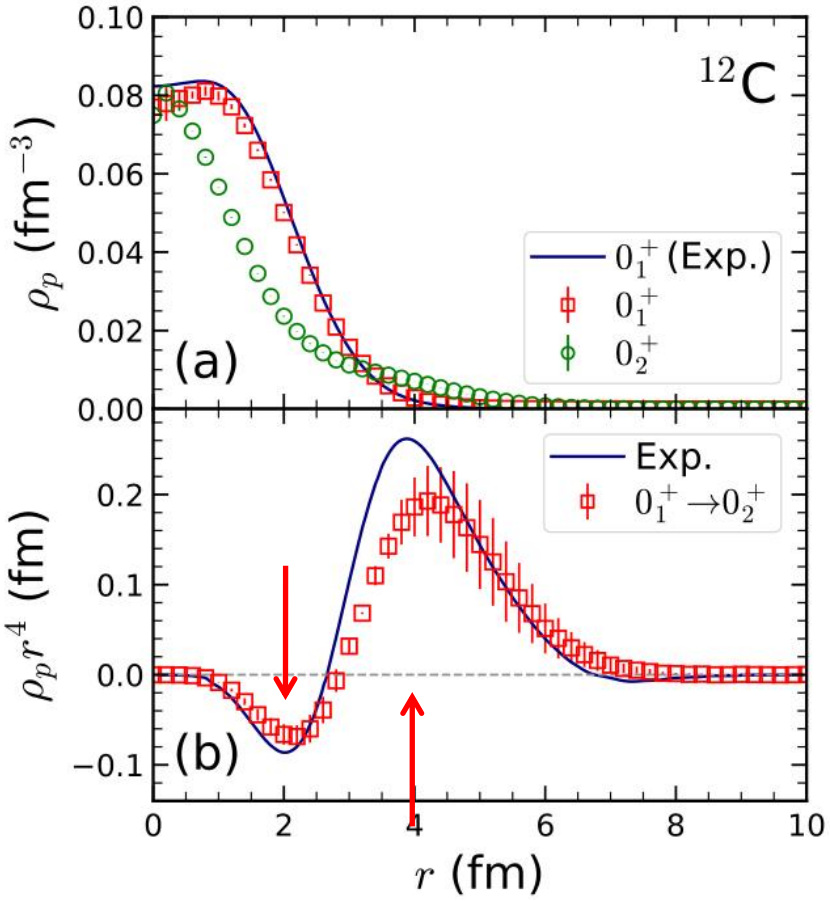
	NLEFT	FMD	α cluster	NCSM	GCM	Exp.
$Q(2_1^+)$	6.8(3)(1.2)	–	–	6.3(3)	–	8.1(2.3)
$Q(2_2^+)$	−35(1)(1)	–	–	–	–	–
$M(E0, 0_1^+ \to 0_2^+)$	4.8(3)	6.5	6.5	–	6.2	5.4(2)
$M(E0, 0_1^+ \to 0_3^+)$	0.4(3)	–	–	–	3.6	–
$M(E0, 0_2^+ \to 0_3^+)$	7.4(4)	–	–	–	47.0	–
$B(E2, 2_1^+ \to 0_1^+)$	11.4(1)(4.3)	8.7	9.2	8.7(9)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

Future Experiments can be used as a test.

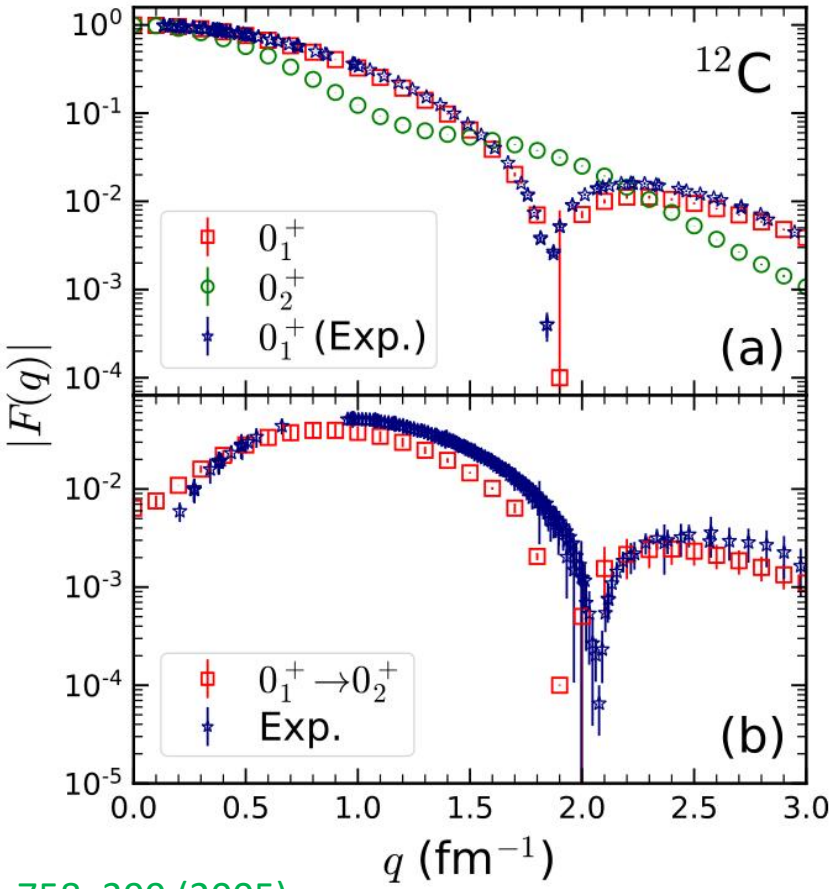
fermion molecular dynamics (FMD) M. Chernykh et al., PRL 98, 032501 (2007)
α cluster M. Chernykh et al., PRL 98, 032501 (2007)
BEC Y. Funaki et al., PRC 67, 051306 (2003); EPJA 24, 321 (2005)
in-medium no-core shell model (NCSM) A. D'Alessio et al., PRC 102, 011302 (2020)
generator coordinate method (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.



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



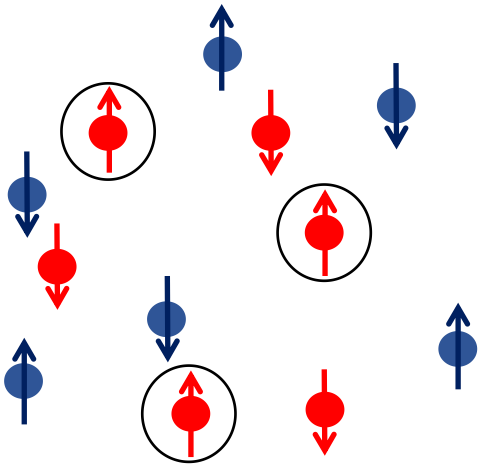
Exp. M. Chernykh et al., PRL 105, 022501 (2010)

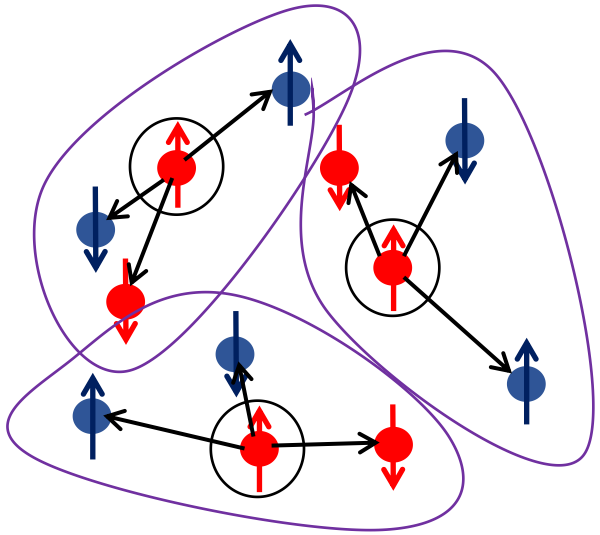
I. Sick and J. S. Mccarthy, NPA 150, 631 (1970)

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.

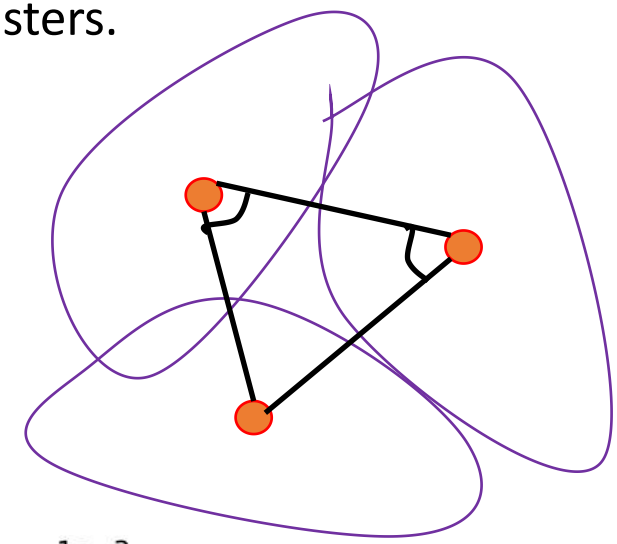


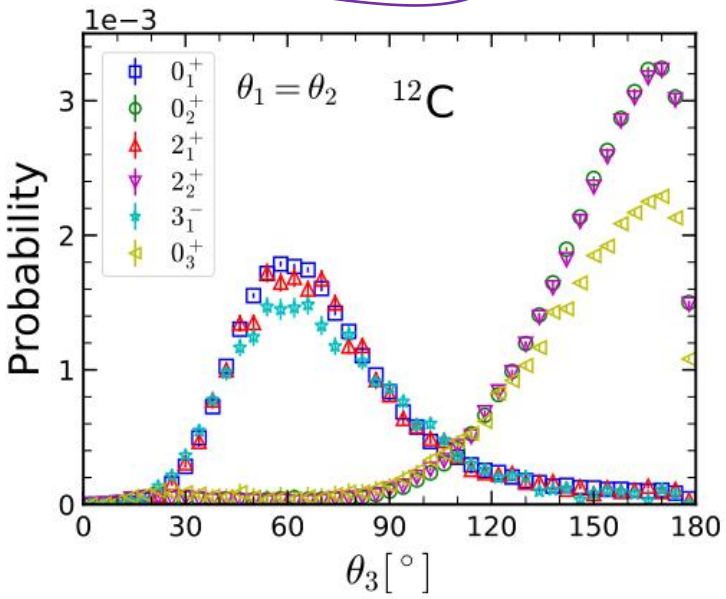


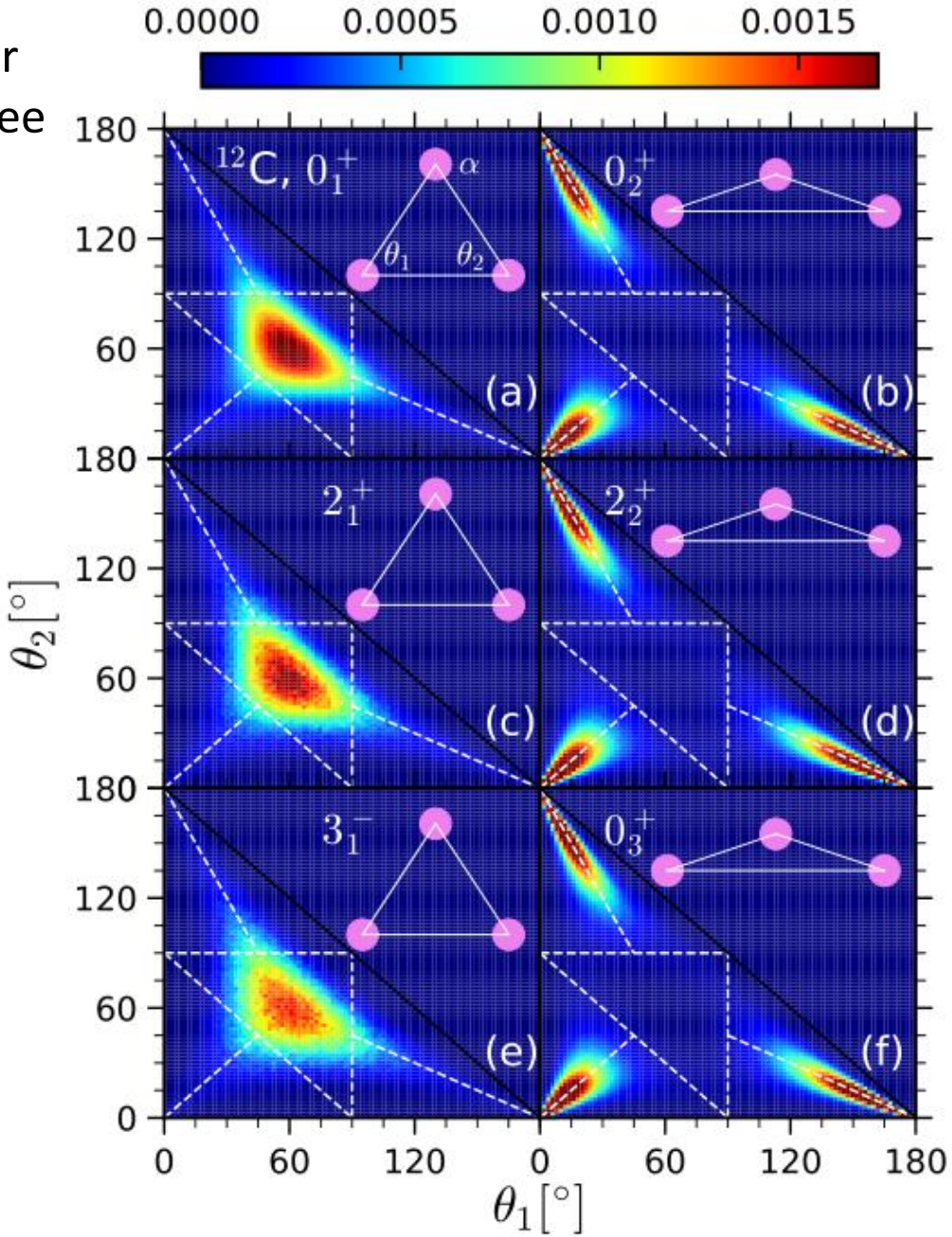
	12C, 0_1+	12C, 0_2+	4He
rms α cluster [fm]	1.65	1.71	1.63

Distribution of Angles

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







Density Distribution

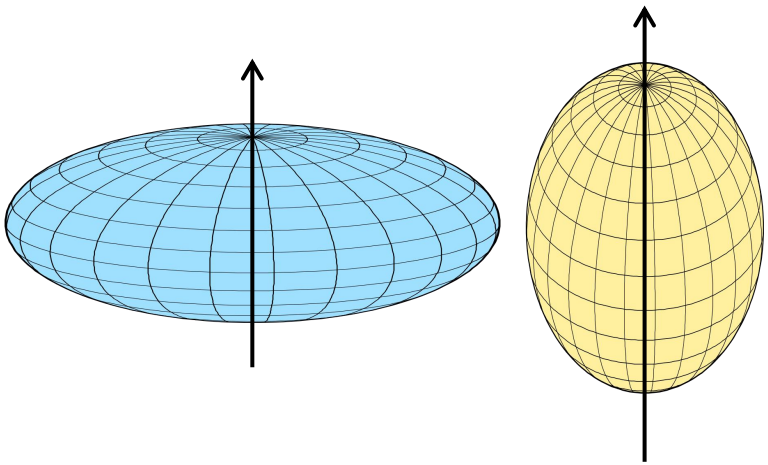
- Alignment of configurations:

For equilateral triangle type:

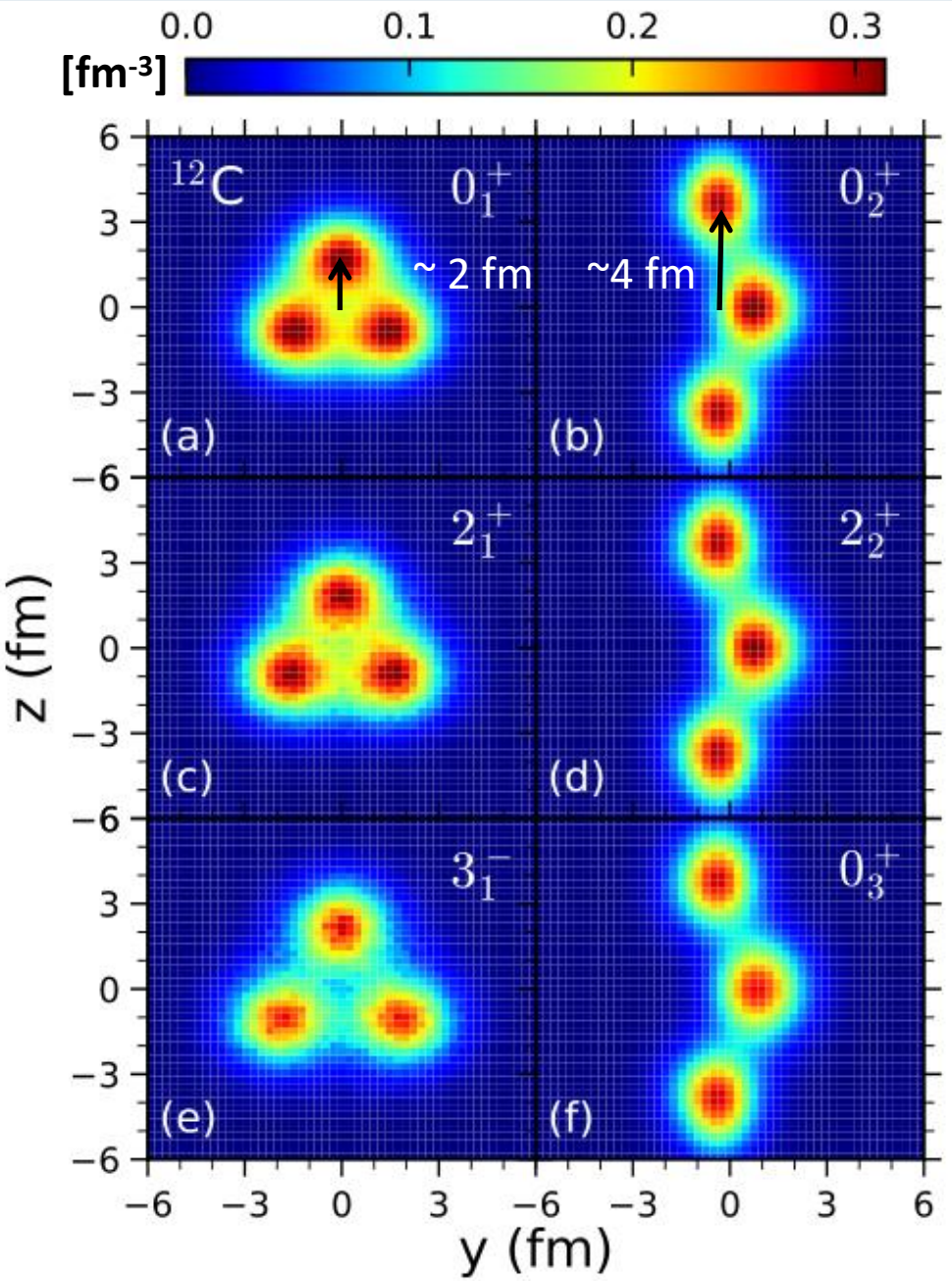
1. Align shortest principal axis to x
2. Rotate 1 α to y = 0 (positive z), and (randomly) +/- 120° .

For obtuse triangle type:

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

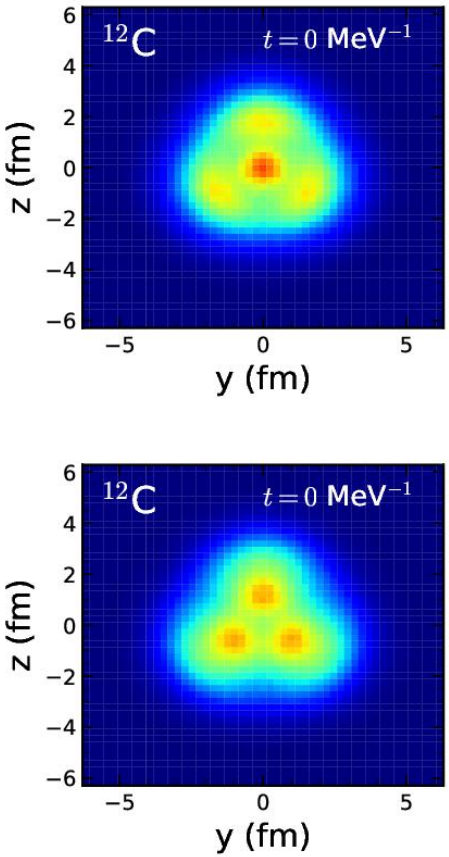


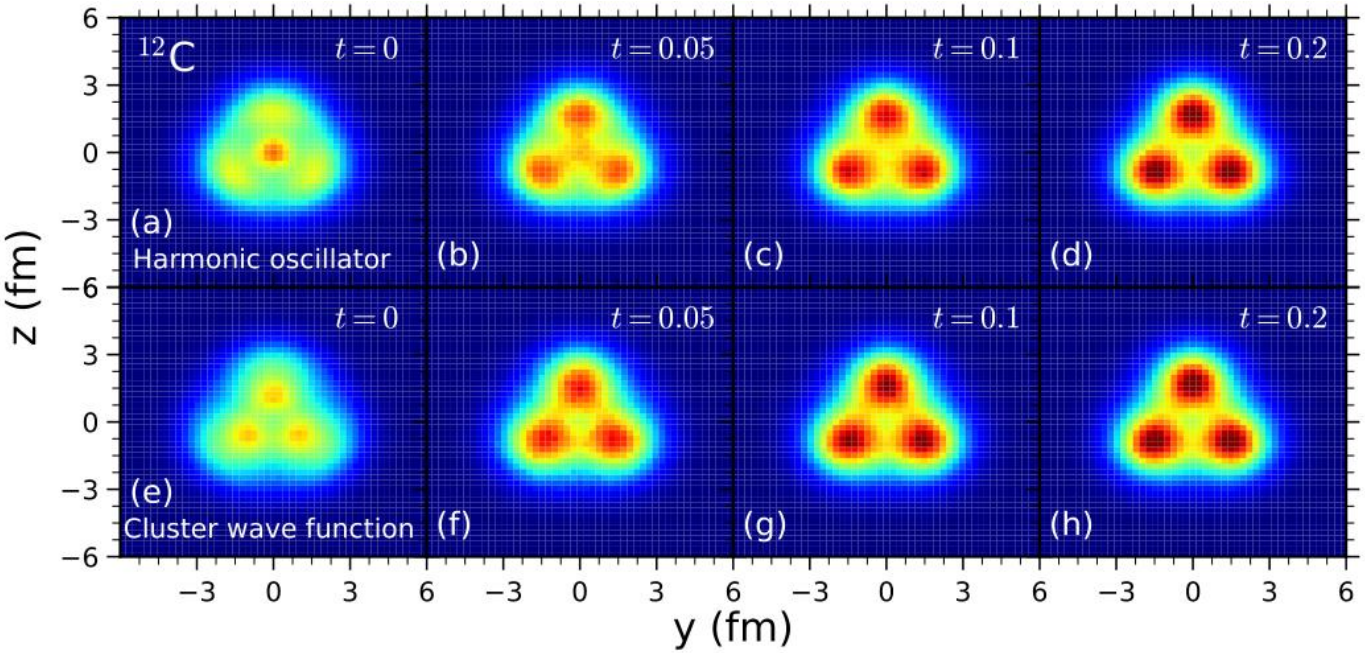
Web figure from: https://en.wikipedia.org/wiki/Spheroid



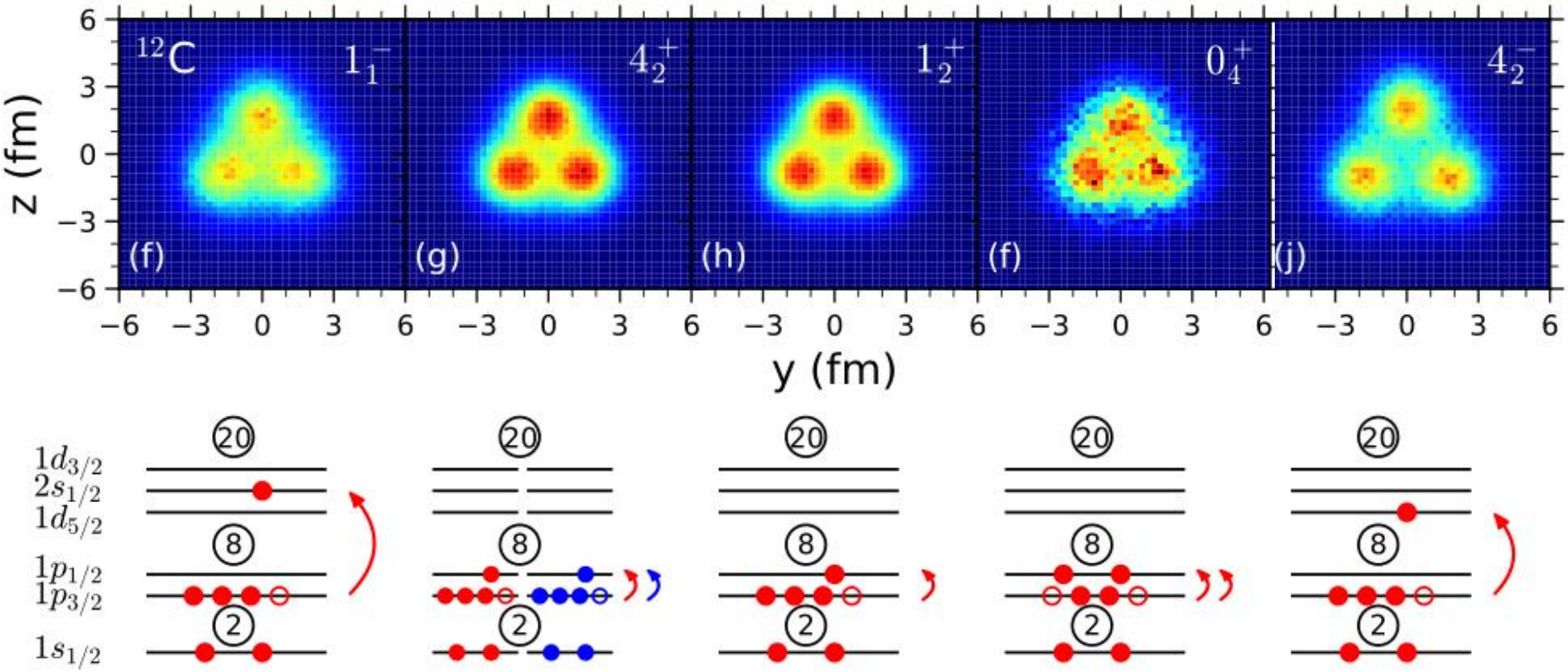
Cluster Formation

- 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}.



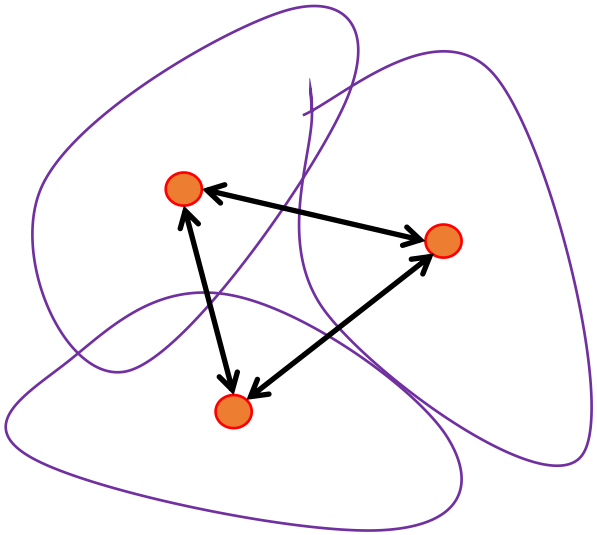


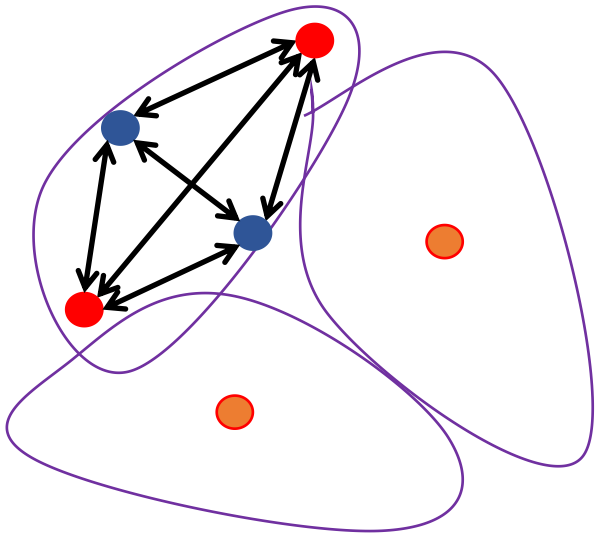
Shell-Model States as Initial Wave

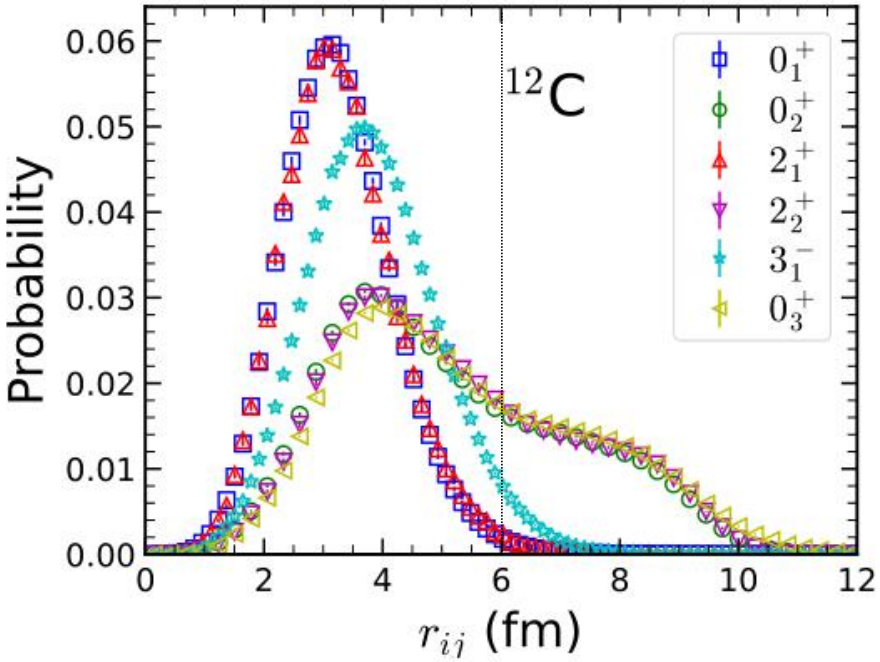


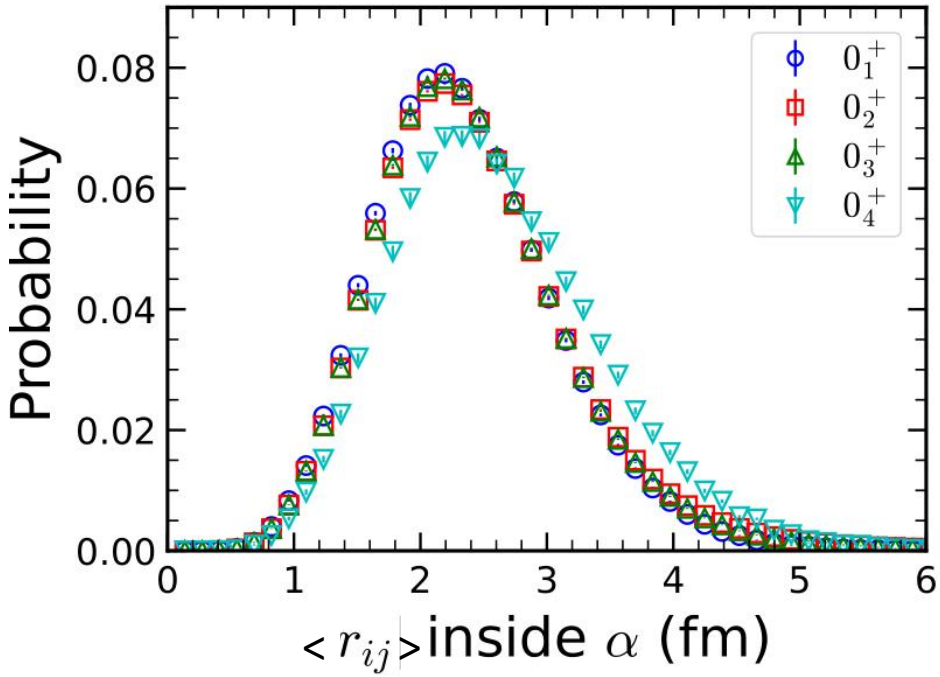
- α cluster structure is less clear due to single-particle excitation, especially when excited to the next shell.

Cluster Excitation? Single-Particle Excitation?



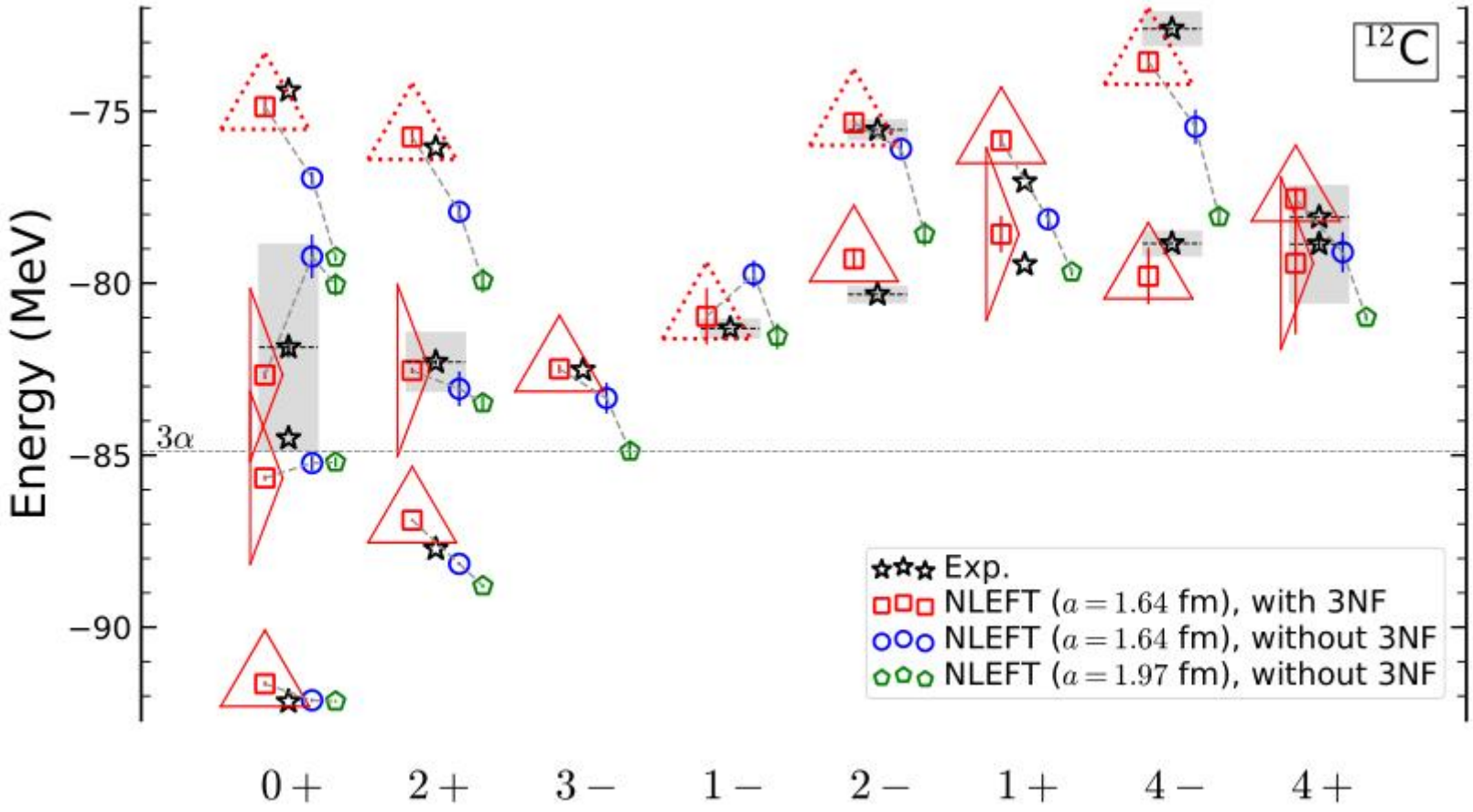






Geometry Information in the Low-Lying Spectrum

- 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

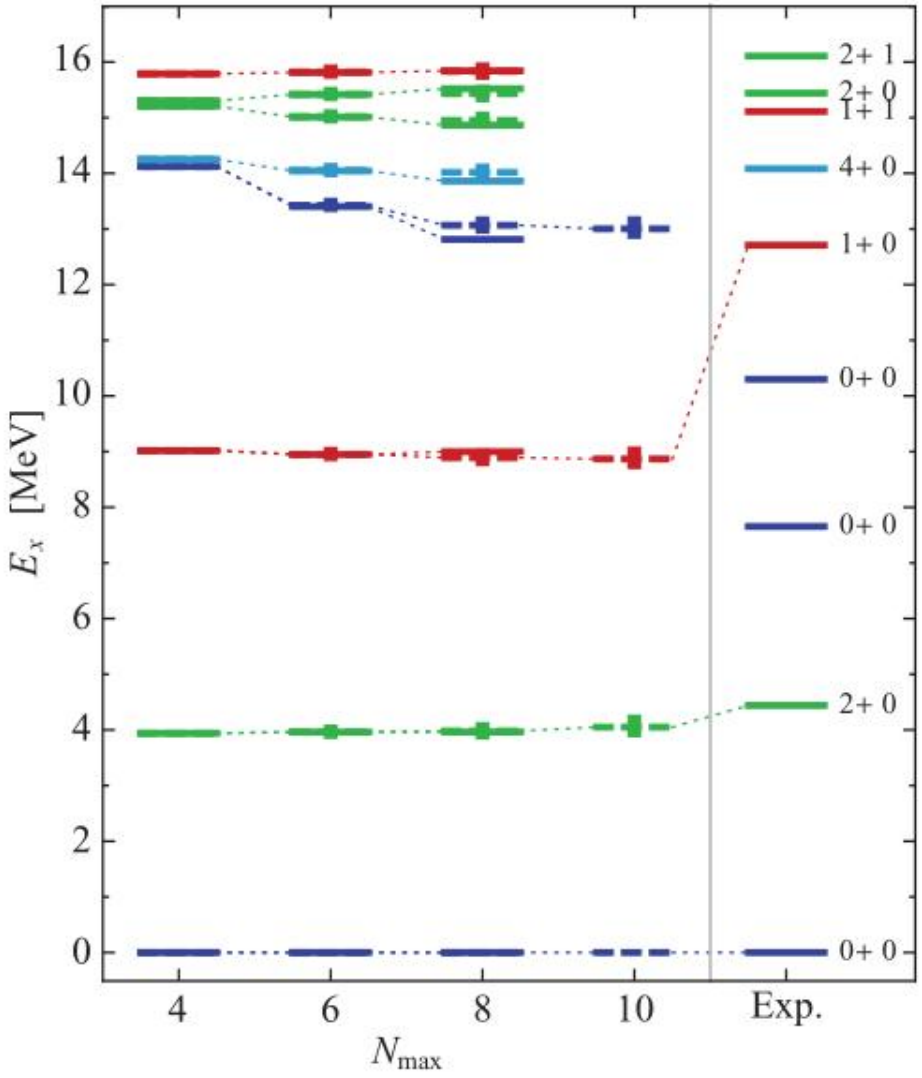
- Low-lying spectrum of ^{12}C have been studied by NLEFT using SU(4) interaction, the agreement with experiment is impressive, not only energies, but also electromanetic transitions and density profiles.
- A model-independent tomographic scan of the three-dimensional geometry of the nuclear states has 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)



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^{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,¶]