2nd Rencontre PhyNuBE

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

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European Research Council
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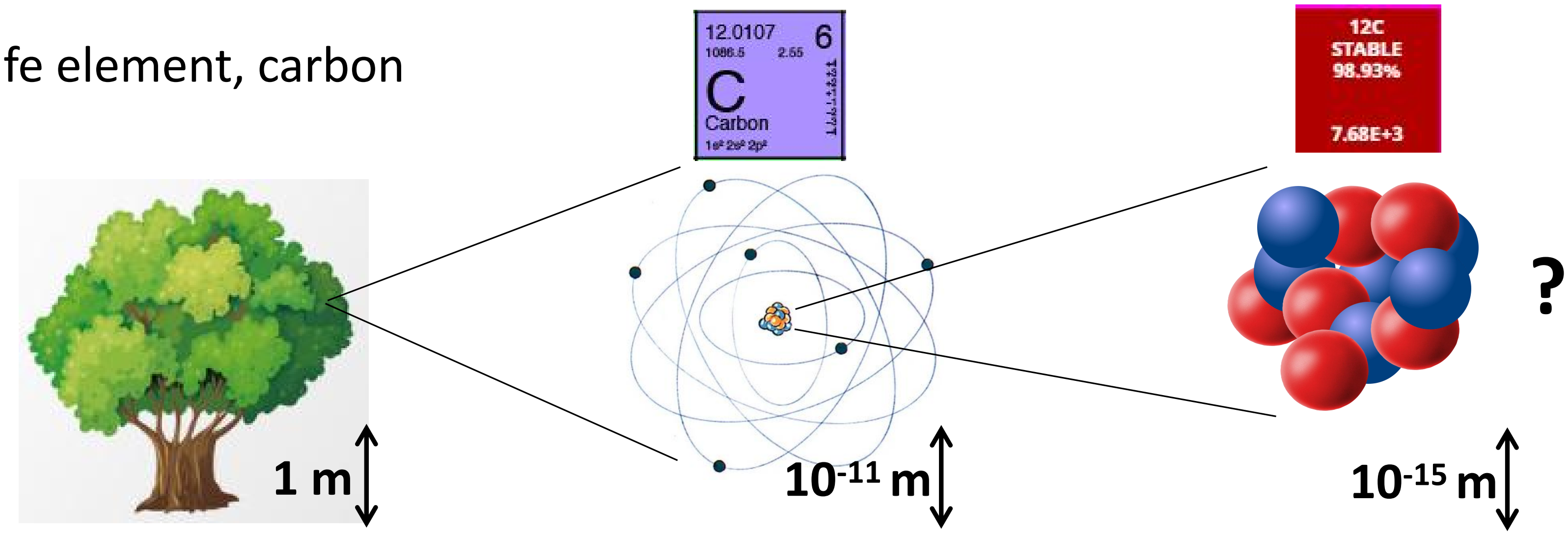
Collaborators: Serdar Elhatisari, Timo A. Lähde, Dean Lee, Bing-Nan Lu, and Ulf-G. Meißner

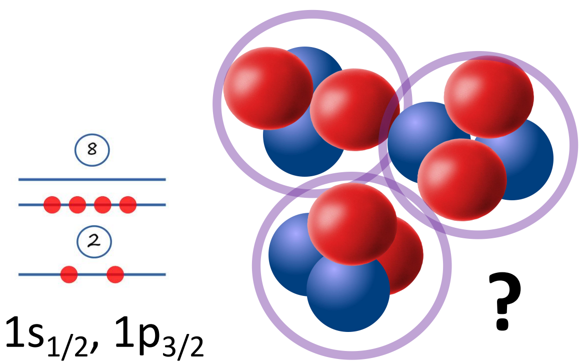
What's Interesting about Carbon-12

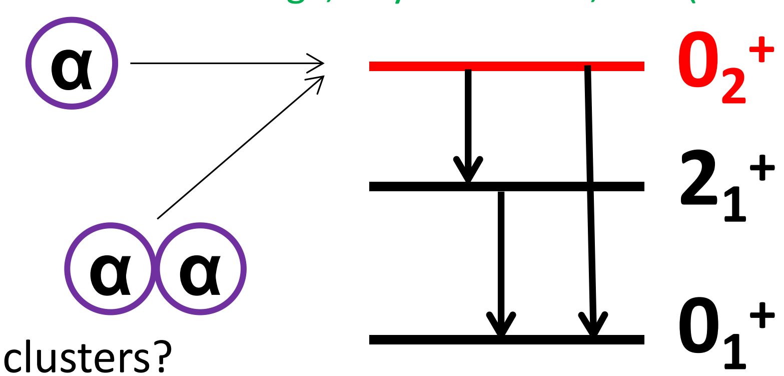
➢ Life element, carbon

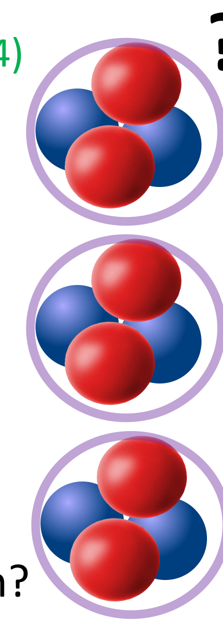


➢ We know little about its shape

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







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

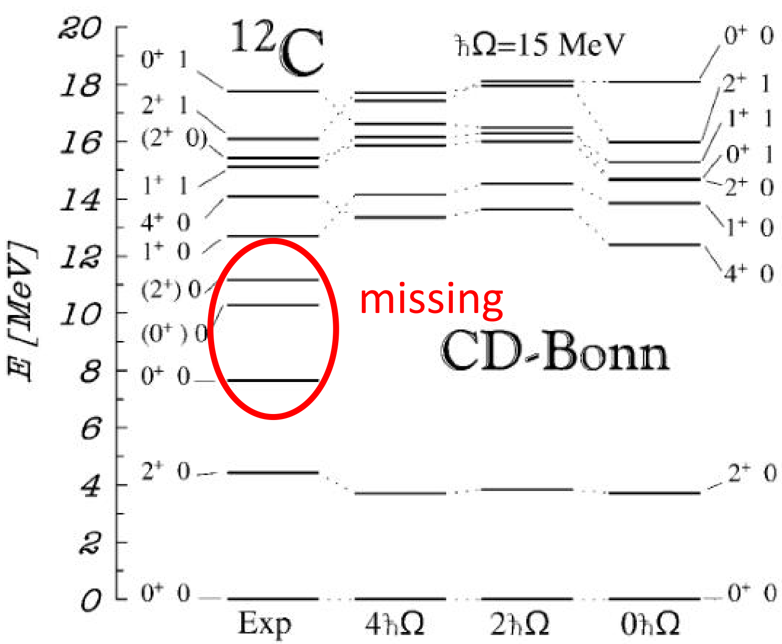
is the Hoyle state like a linear chain?

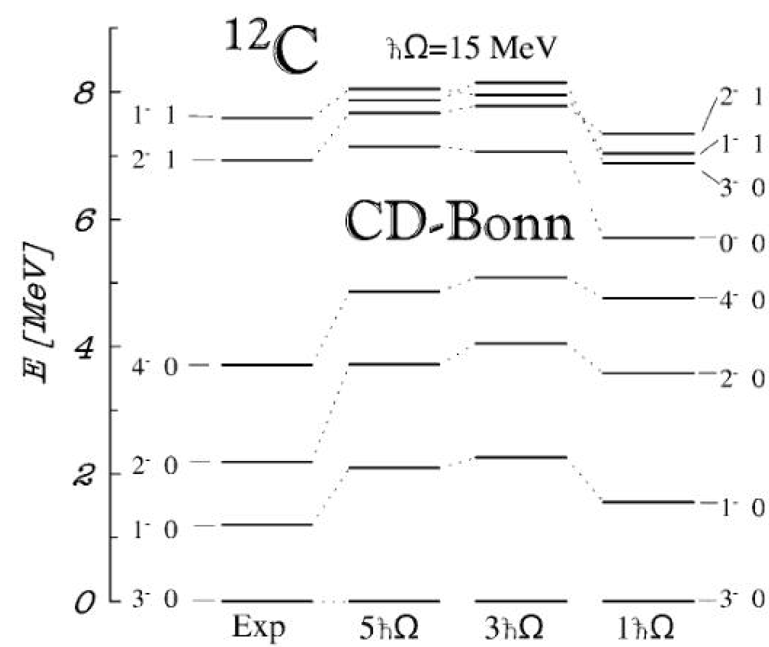
Challenge for Theoretical Calculations

- Microscopic models
  - density functional theory — P. Marevic, J.-P. Ebran, E. Khan, T. Nikšic, and D. Vretenar, Phys. Rev. C 99, 034317 (2019)
  - Tohsaki-Horiuchi-Schuck-Röpke wave function — Y. Funaki, Phys. Rev. C 92, 021302 (2015)
  - antisymmetrized molecular dynamics — Y. Kanada-En'yo, Prog. Theor. Phys. 117, 655 (2007)
  - fermionic molecular dynamces — M. Chernykh et al., Phys. Rev. Lett. 98, 032501 (2007)
  - … …

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

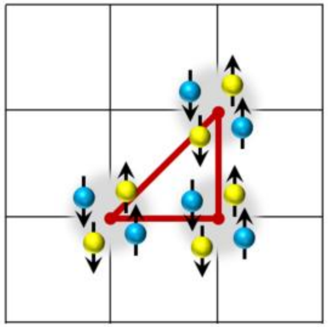
e.g. no-core shell model   Navrátil, P., J. P. Vary, and B. R. Barrett, Phys. Rev. Lett. 84, 5728 (2000)





Challenge for Theoretical Calculations

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

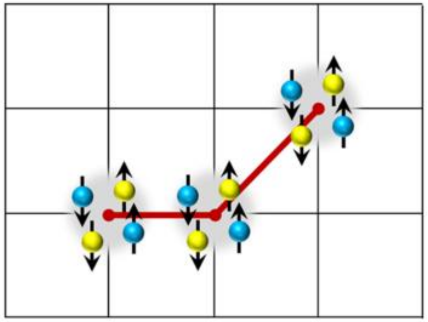


Selected for a Viewpoint in *Physics*

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

Ab Initio Calculation of the Hoyle State

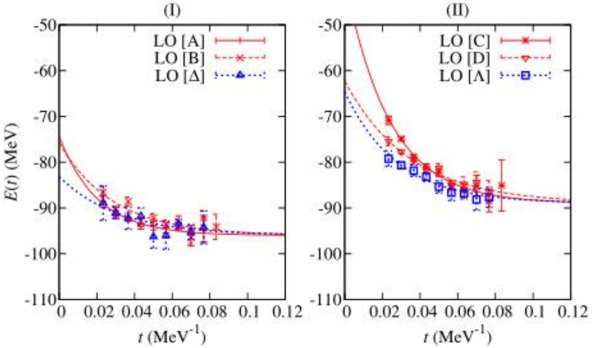
Evgeny Epelbaum,[1] Hermann Krebs,[1] Dean Lee,[2] and Ulf-G. Meißner[3,4]



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]

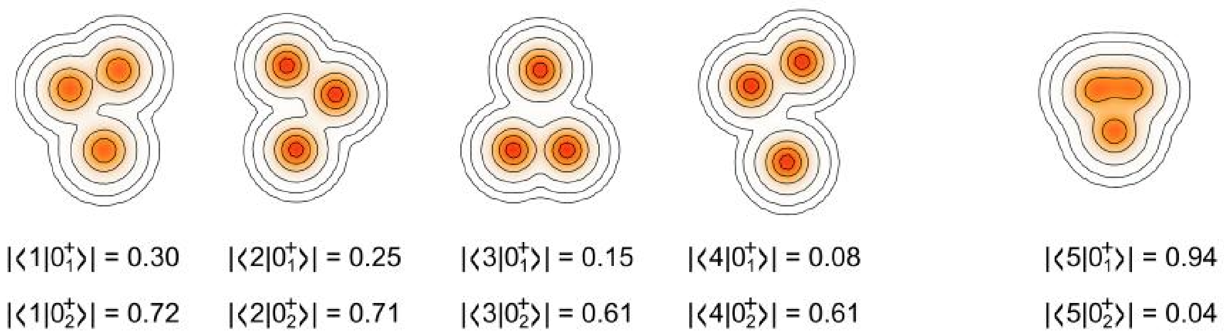


➢ Further questions:

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

Debate on the Shape of Hoyle State

- Study of the geometry, decomposition of basis states



M. Chernykh et al., Phys. Rev. Lett. 98, 032501 (2007)

U(7) model and fermionic molecular dynamic model: equilateral triangle

R. Bijker and F. Iachello Ann. Phys. 298, 334 (2002), M. Chernykh et al., Phys. Rev. Lett. 98, 032501 (2007)

Configuration-mixing method: superposition of many Slater determinants

Y. Fukuoka et al., Phys. Rev. C 88, 014321 (2013)

Green's function Monte Carlo: possibly approximately linear distribution

J. Carlson et al., Rev. Mod. Phys. 87, 1067 (2015)

Monte-Carlo Shell model: α-like clusters 2/3 and 1/3 liquid (modestly ellipsoidal)

T. Otsuka et al., Nature Commu. 13, 2234 (2022)

... ...

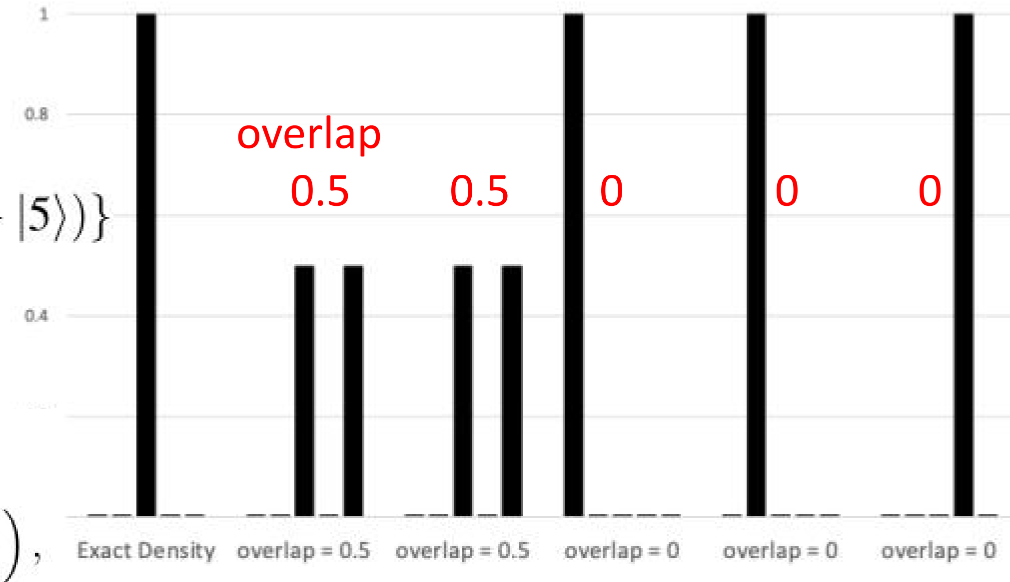
Density Snapshots for the Important Basis

courtesy of D. Lee

- Consider 1D linear lattice sites $|1\rangle, |2\rangle, |3\rangle, |4\rangle, |5\rangle$ and let $|3\rangle$ be the answer

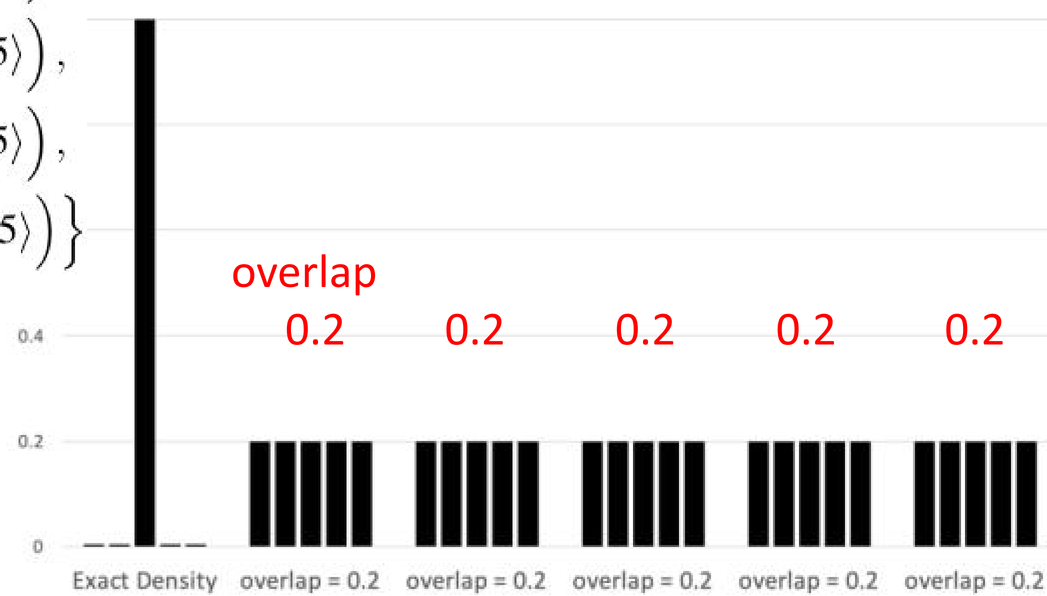
Basis set 1

$$\{|1\rangle, |2\rangle, |4\rangle, 1/\sqrt{2}(|3\rangle + |5\rangle), 1/\sqrt{2}(|3\rangle - |5\rangle)\}$$



Basis set 2

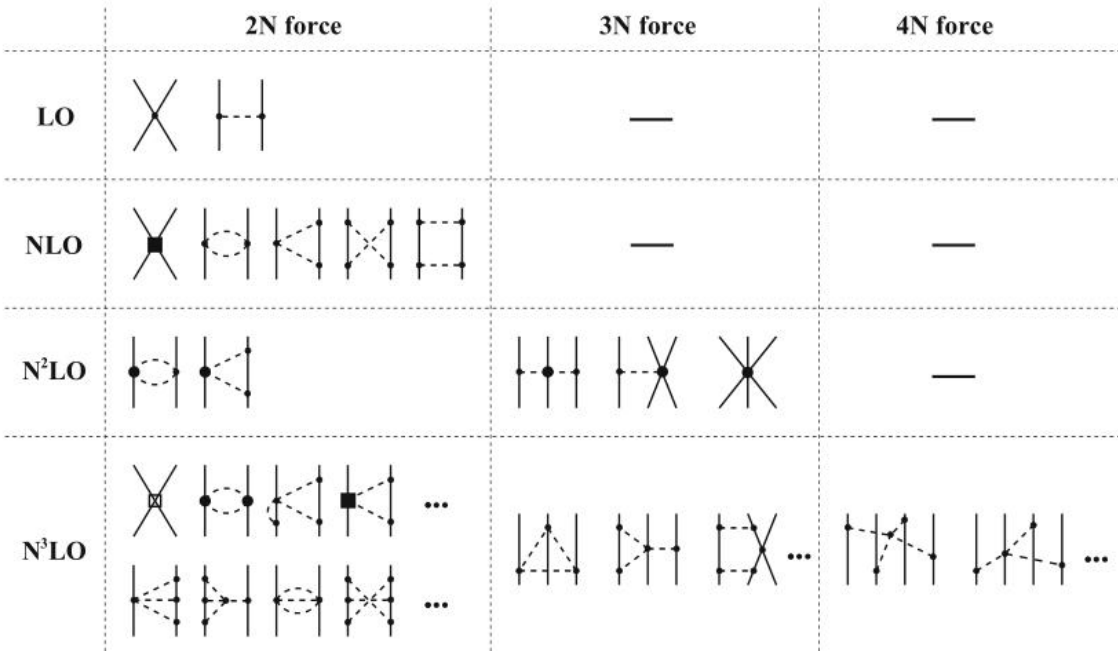
$$\Big\{1/\sqrt{5}\left(|1\rangle + |2\rangle + |3\rangle + |4\rangle + |5\rangle\right),$$
$$1/\sqrt{5}\left(|1\rangle + e^{i\theta_5}|2\rangle + e^{i2\theta_5}|3\rangle + e^{i3\theta_5}|4\rangle + e^{i4\theta_5}|5\rangle\right),$$
$$1/\sqrt{5}\left(|1\rangle + e^{i2\theta_5}|2\rangle + e^{i4\theta_5}|3\rangle + e^{i\theta_5}|4\rangle + e^{i3\theta_5}|5\rangle\right),$$
$$1/\sqrt{5}\left(|1\rangle + e^{i3\theta_5}|2\rangle + e^{i\theta_5}|3\rangle + e^{i4\theta_5}|4\rangle + e^{i2\theta_5}|5\rangle\right),$$
$$1/\sqrt{5}\left(|1\rangle + e^{i4\theta_5}|2\rangle + e^{i3\theta_5}|3\rangle + e^{i2\theta_5}|4\rangle + e^{i\theta_5}|5\rangle\right)\Big\}$$

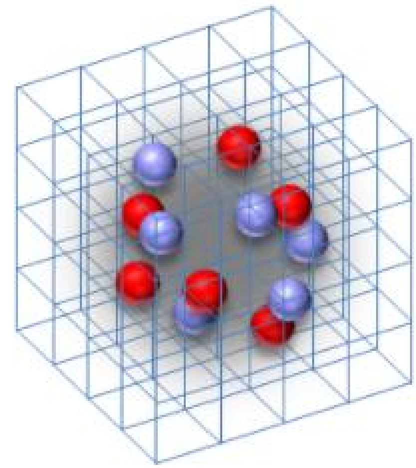


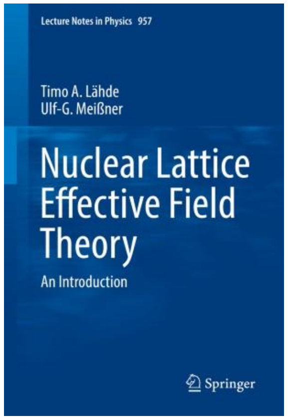
An even more substantial distortion of the basis-state density snapshots can be made using non-orthogonal basis states.

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

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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)
- ... ...

Upper left figure is in courtesy of E. Epelbaum

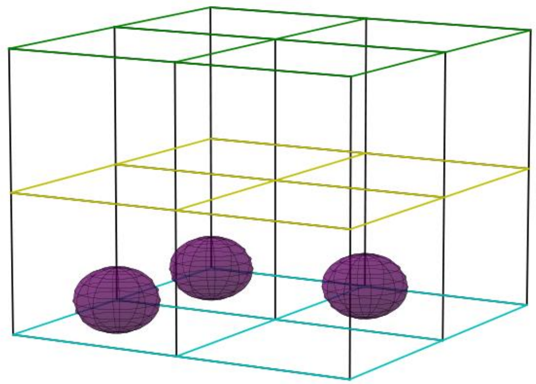
lattice figure from https://www.physics.ncsu.edu/ntg/leegroup/research.html

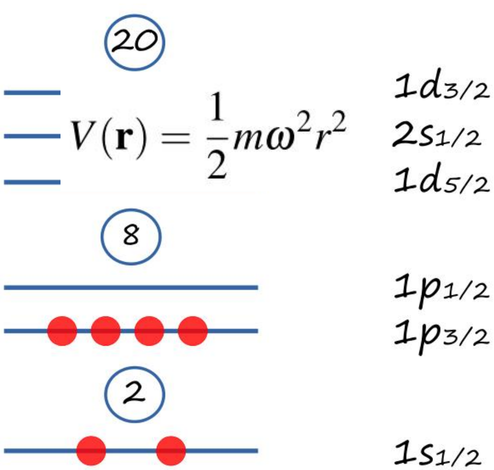
Theoretical Framework

- Starting from an initial many-body wave function:

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

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



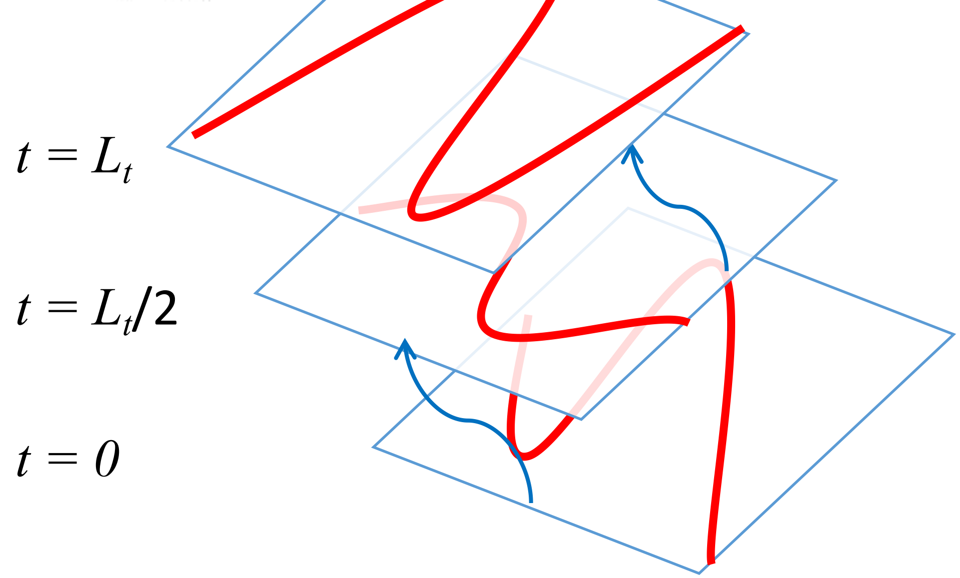


- Euclidean time projection with transfer matrix:

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

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):

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

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

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

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

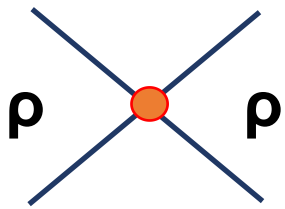
Four parametes C_2, C_3, s_{L}, and s_{NL} will be fitted to binding energy of ^{4}He and ^{12}C, radius of ^{12}C, and to some extent transition properties.

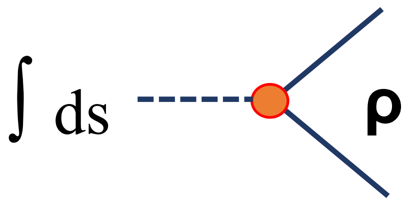
Interaction seems too simple? Let's wait to see how the descriptions look like

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 are a superposition of millions of configurations (Slater determinants)

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

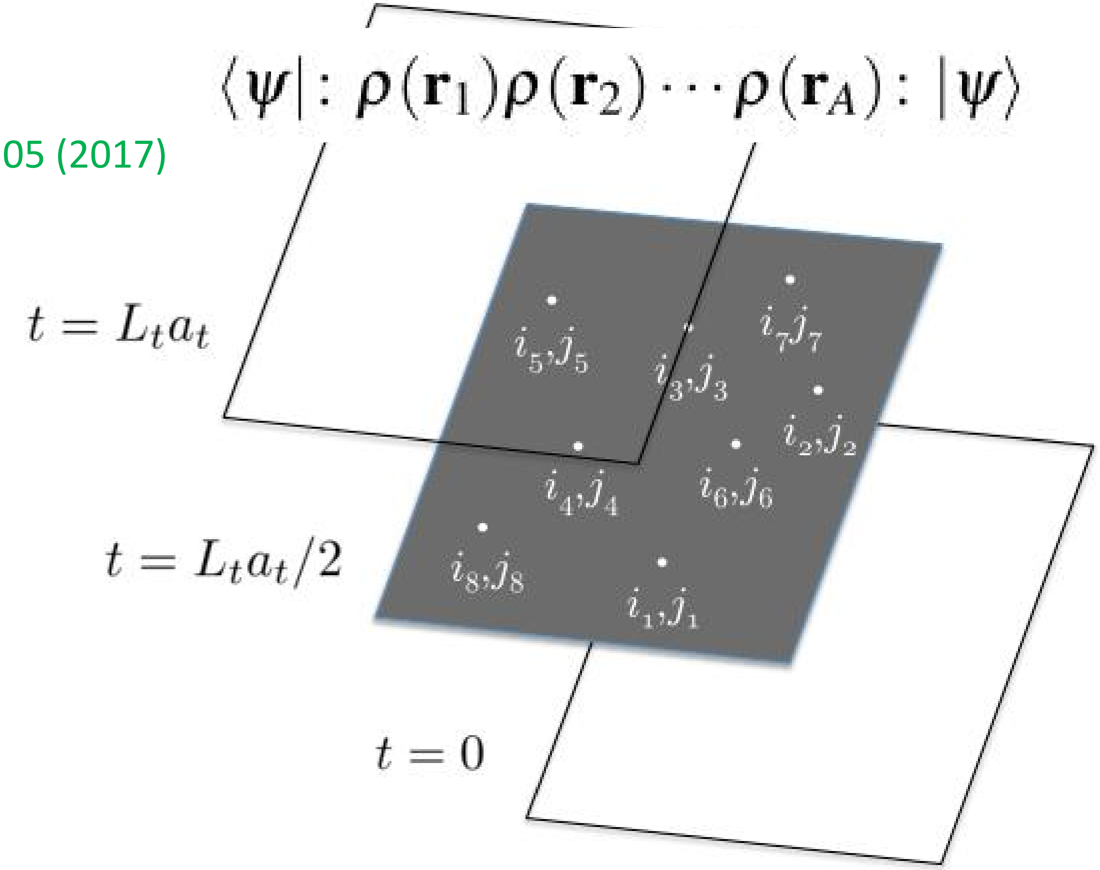
$$|\Phi_{s_i,L_t}\rangle = M_{s_i}^{L_t}|\Phi_0\rangle = \mathscr{A}\left[\phi_{s_i,1}(\mathbf{r}_1)\phi_{s_i,2}(\mathbf{r}_2)\ldots\phi_{s_i,A}(\mathbf{r}_A)\right]$$

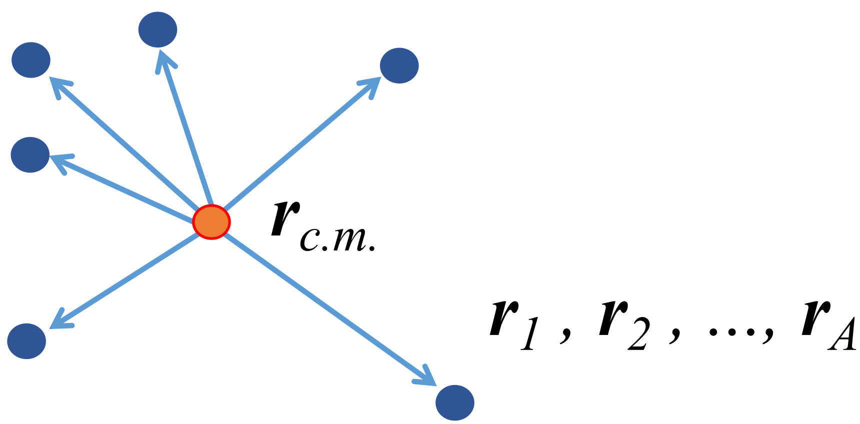
Theoretical Framework

- 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.





Those millions of A-body positions might be useful to describe the shape and geometry of nuclei

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

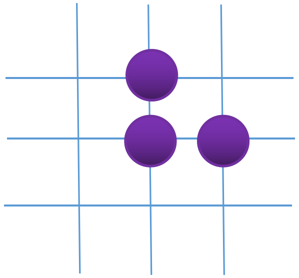
C_2 [MeV^{-2}]	C_3 [MeV^{-5}]	s_L	s_{NL}
-2.15×10^{-5}	6.17×10^{-12}	0.08	0.05

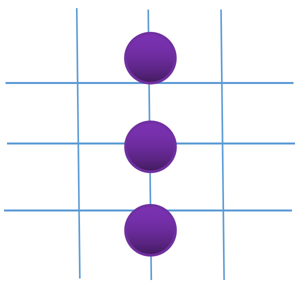
	NLEFT	Exp.
E(^{4}He) [MeV]	-28.1 (1)	-28.3
E(^{12}C) [MeV]	-91.6 (1)	-92.2
r_c(^{12}C) [fm]	2.52 (1)	2.47 (2)

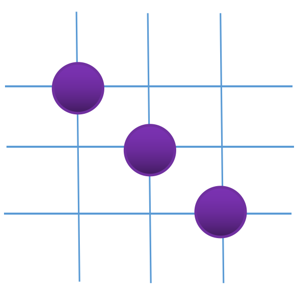
S. Shen, T. A. Lähde, D. Lee, U.-G. Meißner, arXiv:2202.13596

Calculation of the Hoyle State

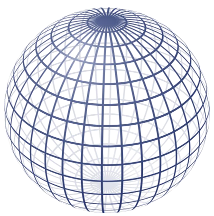
- Hoyle state

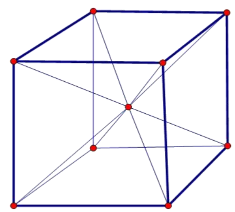






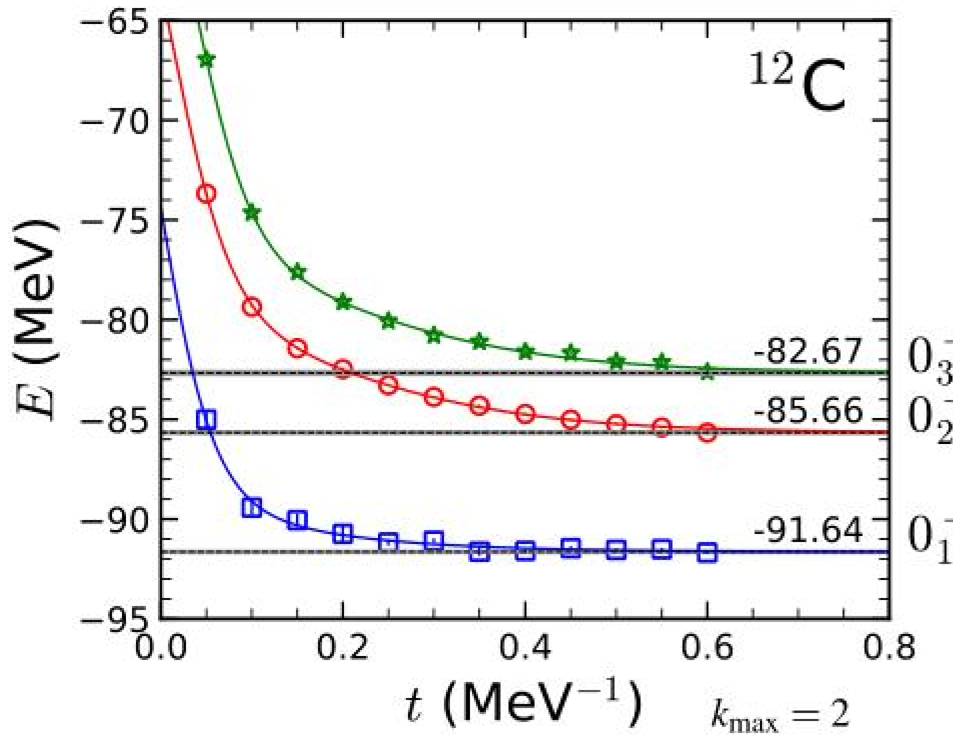
Angular momentum projection: SO(3) group reducted to cubic group O





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

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

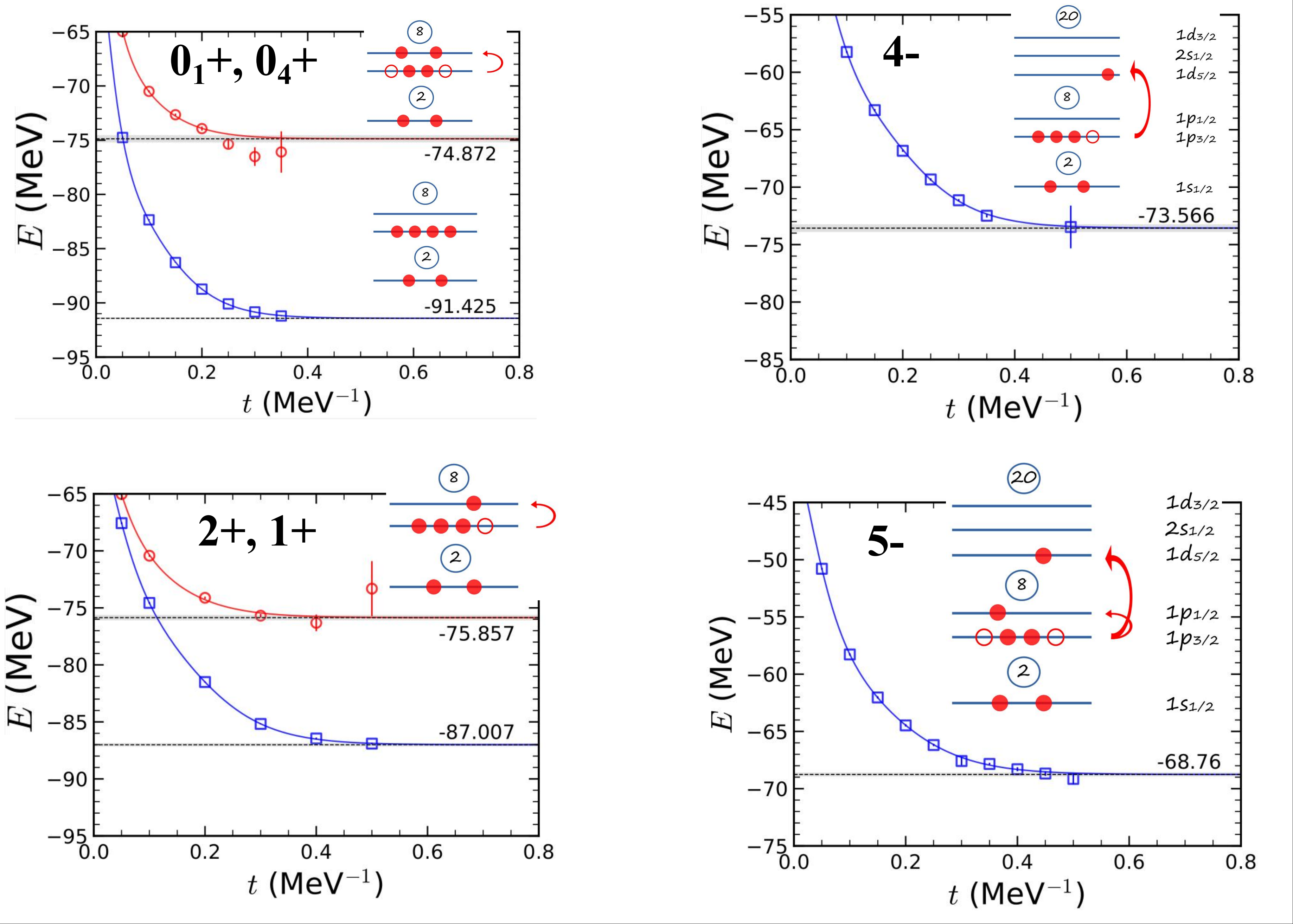


$$E_i(t) = \frac{E_i + \sum_{k=1}^{k_{\max}} (E_i + \Delta E_{i,k}) c_{i,k} e^{-\Delta E_{i,k} t}}{1 + \sum_{k=1}^{k_{\max}} c_{i,k} e^{-\Delta E_{i,k} t}}$$

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

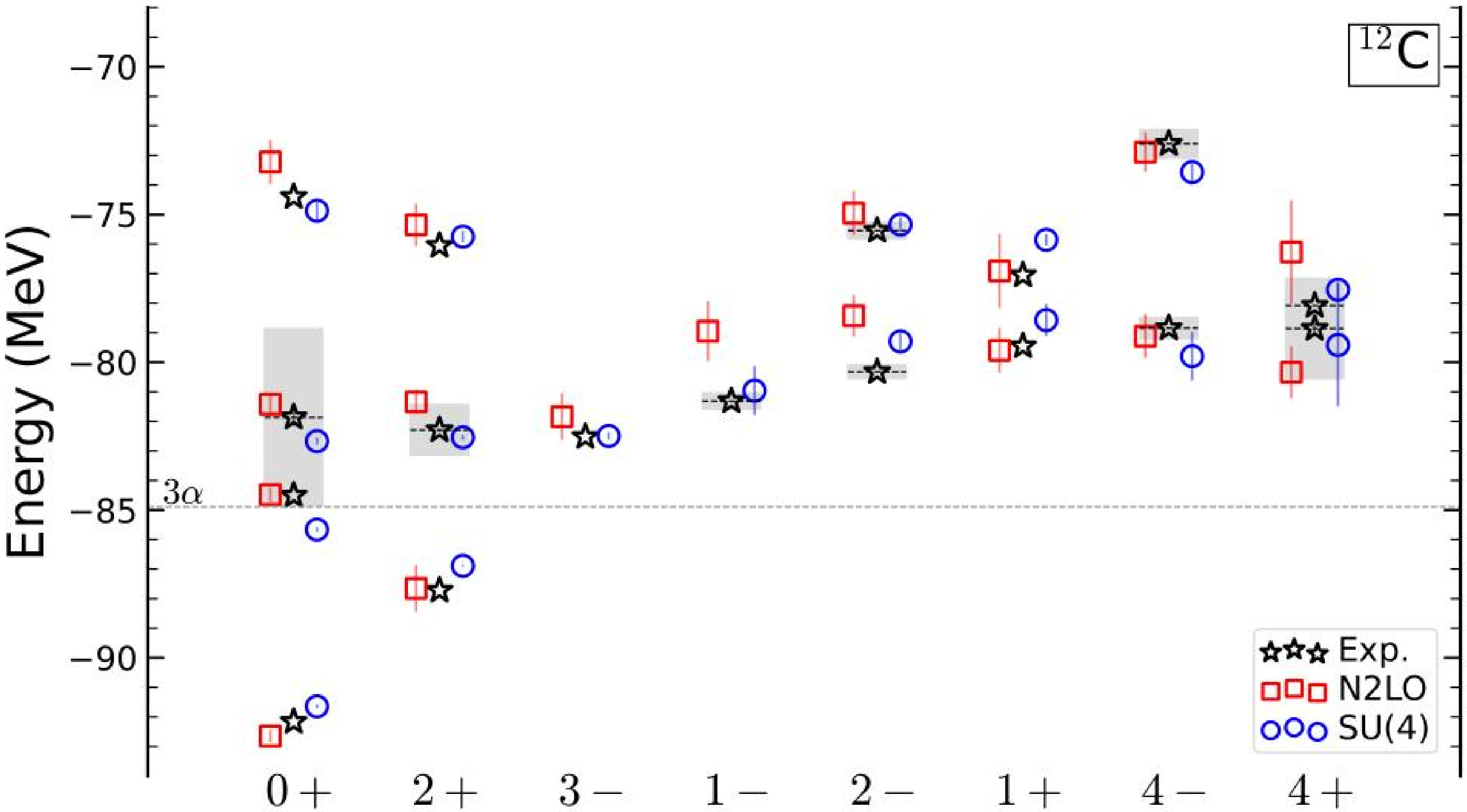
Web figures from: https://en.wikipedia.org/wiki/Sphere
https://math.ucr.edu/home/baez/icosidodecahedron/7.html

Shell-Model States Used as Initial Wave



Low-lying Spectrum

- Spectrum of ^{12}C calculated by NLEFT using N2LO and SU(4) interaction in comparison with experimental data.



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

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 fm^2 and for $B(E2)$ e^2 fm^4.

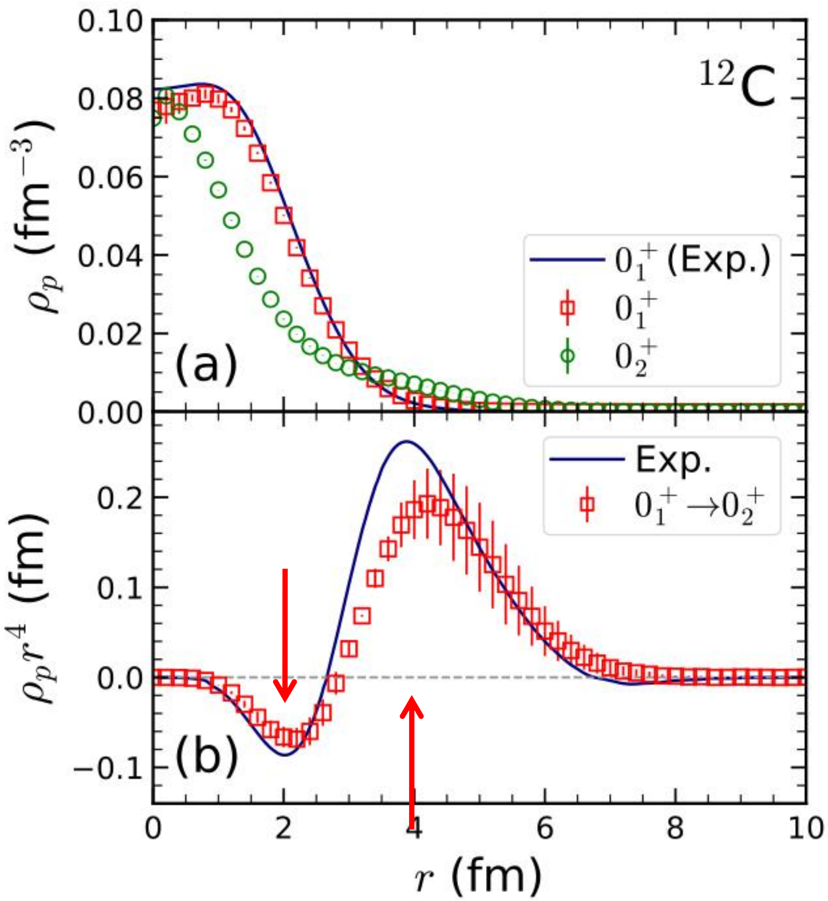
	NLEFT	FMD	α cluster	NCSM	GCM	Exp.
$Q(2_1^+)$	6.8(3)(1.2)	–	–	6.3(3)	–	8.1(2.3)
$Q(2_2^+)$	−35(1)(1)	–	–	–	–	–
$M(E0, 0_1^+ \to 0_2^+)$	4.8(3)	6.5	6.5	–	6.2	5.4(2)
$M(E0, 0_1^+ \to 0_3^+)$	0.4(3)	–	–	–	3.6	–
$M(E0, 0_2^+ \to 0_3^+)$	7.4(4)	–	–	–	47.0	–
$B(E2, 2_1^+ \to 0_1^+)$	11.4(1)(4.3)	8.7	9.2	8.7(9)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

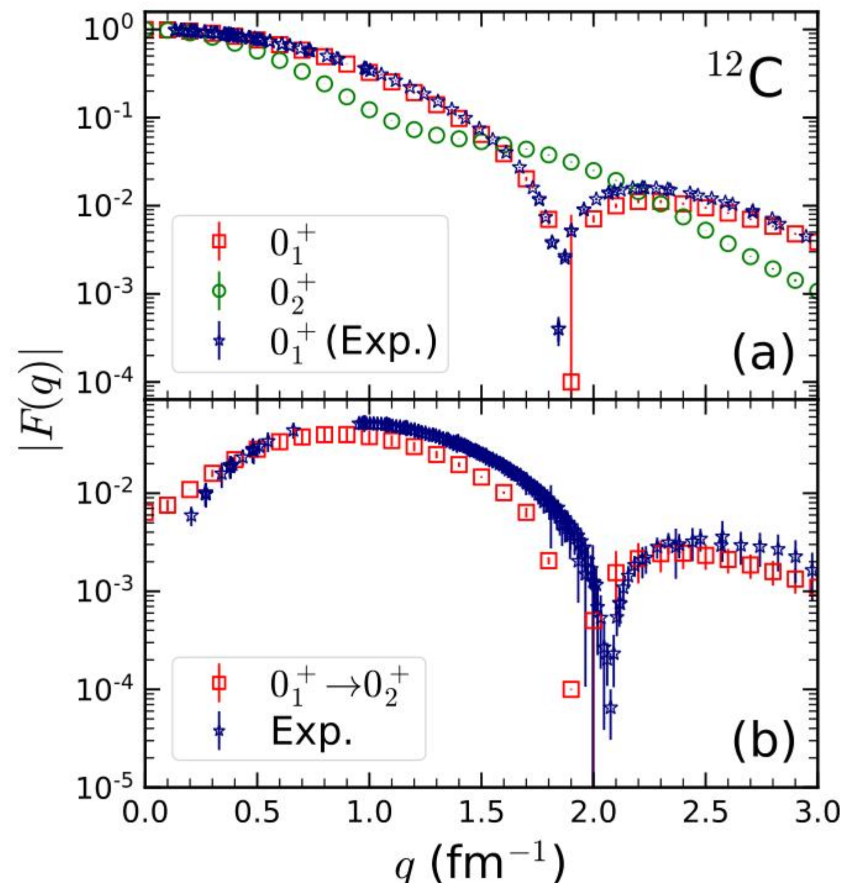
fermion molecular dynamics (FMD) M. Chernykh et al., PRL 98, 032501 (2007)
α cluster M. Chernykh et al., PRL 98, 032501 (2007)
BEC Y. Funaki et al., PRC 67, 051306 (2003); EPJA 24, 321 (2005)
in-medium no-core shell model (NCSM) A. D'Alessio et al., PRC 102, 011302 (2020)
generator coordinate method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



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



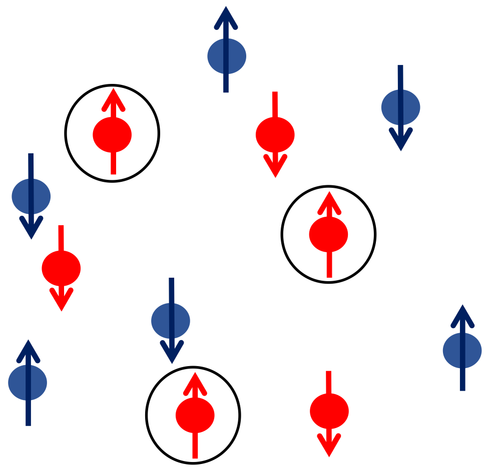
Exp. M. Chernykh et al., PRL 105, 022501 (2010)

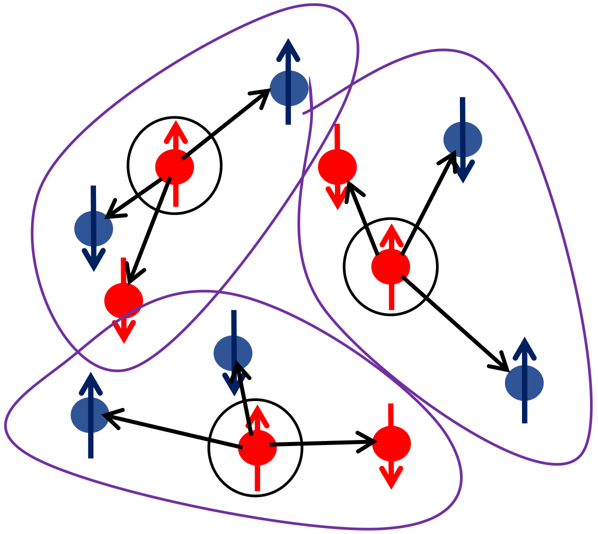
I. Sick and J. S. Mccarthy, NPA 150, 631 (1970)

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

Investigation of the Geometry

- Define (α) clusters
  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.

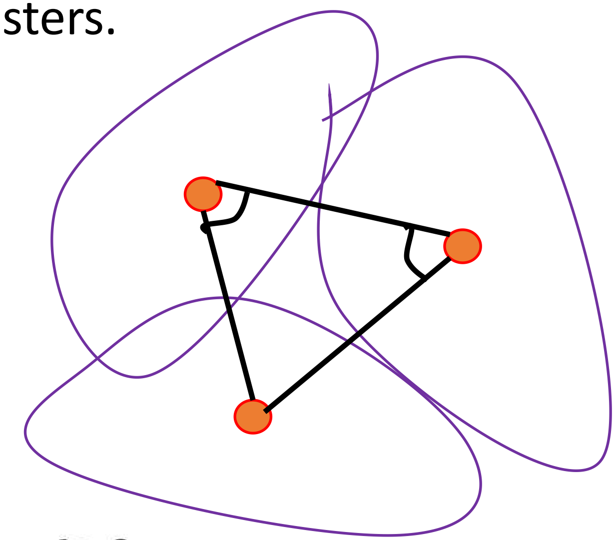


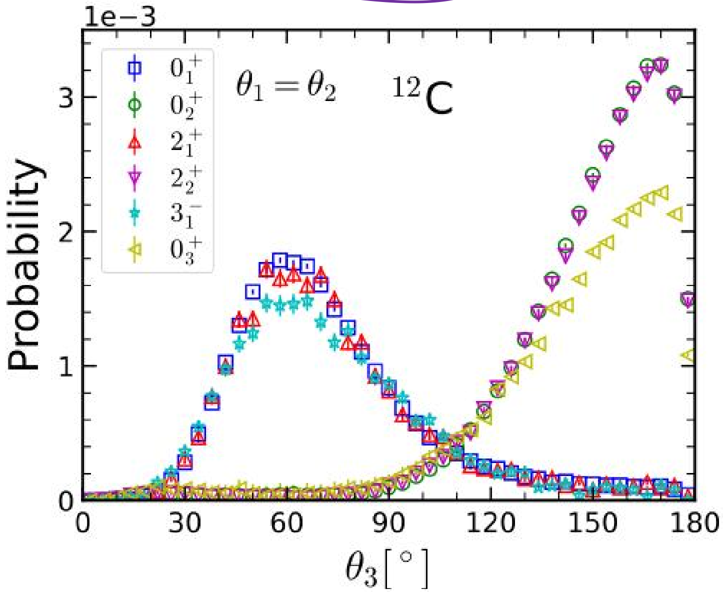


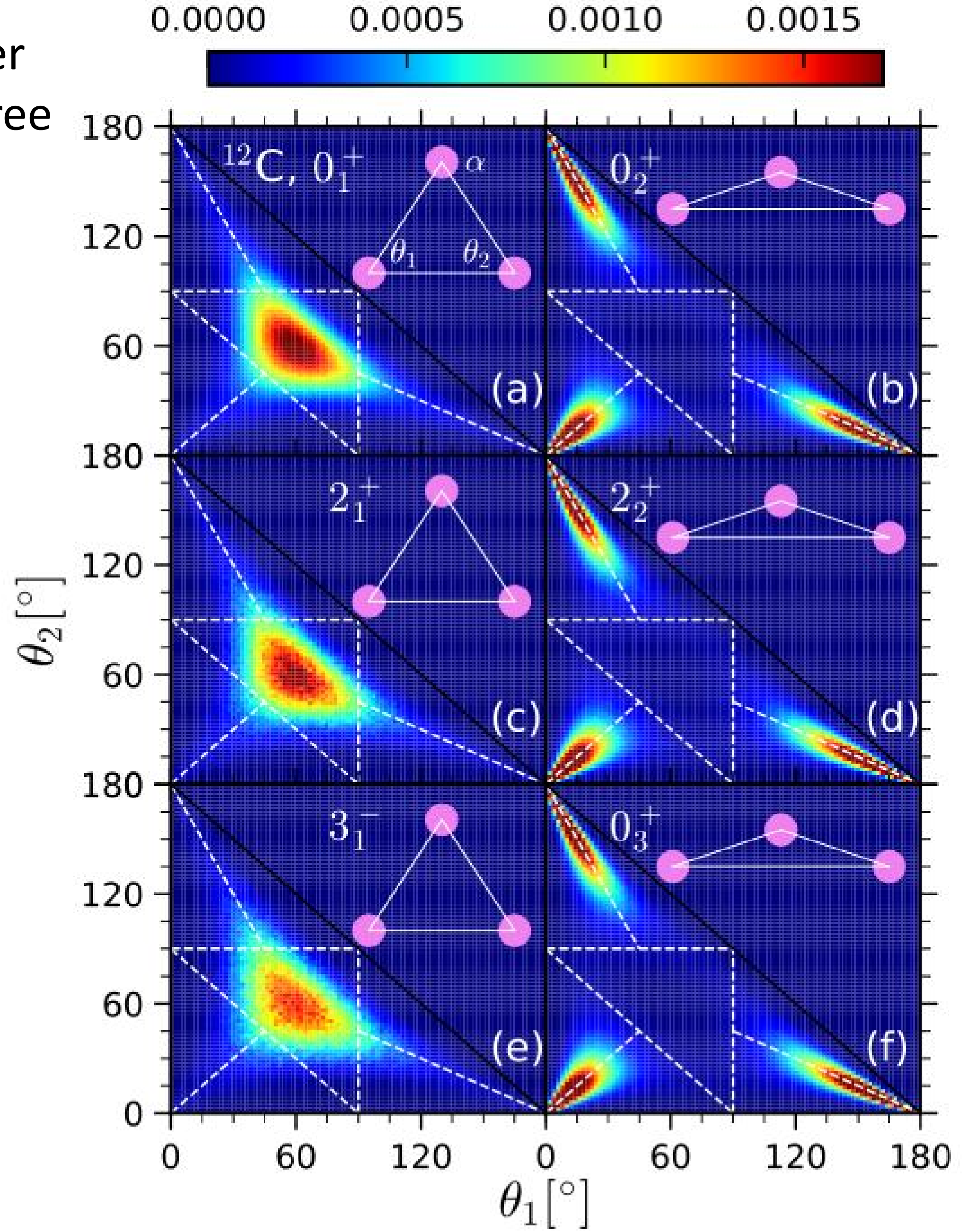
	12C, 0_1+	12C, 0_2+	4He
rms α cluster [fm]	1.65	1.71	1.63

Distribution of Angles

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







Density Distribution

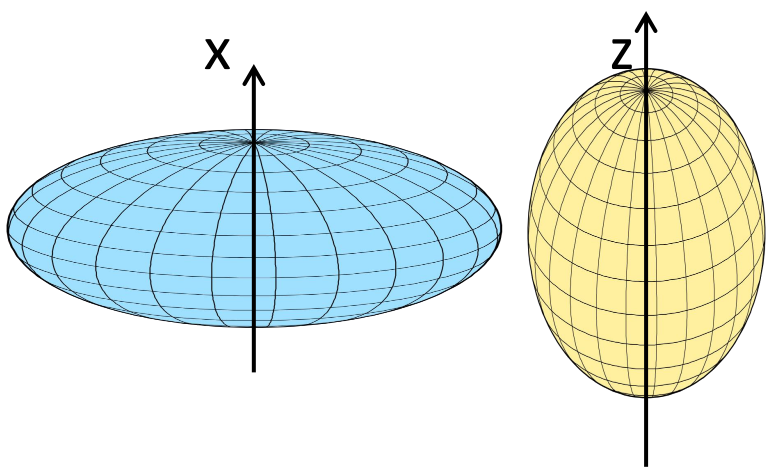
➢ Alignment of configurations:

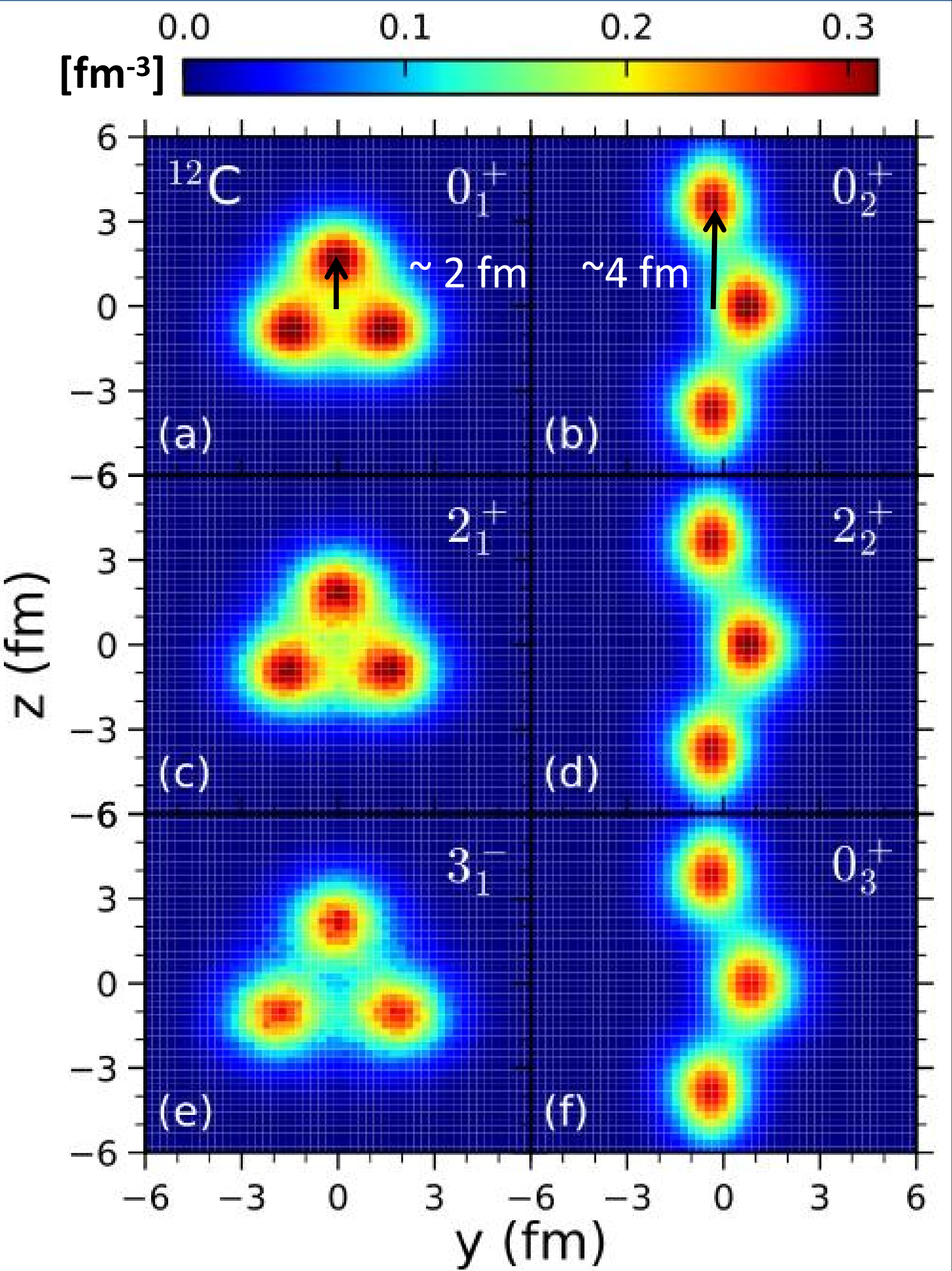
For equilateral triangle type:

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).

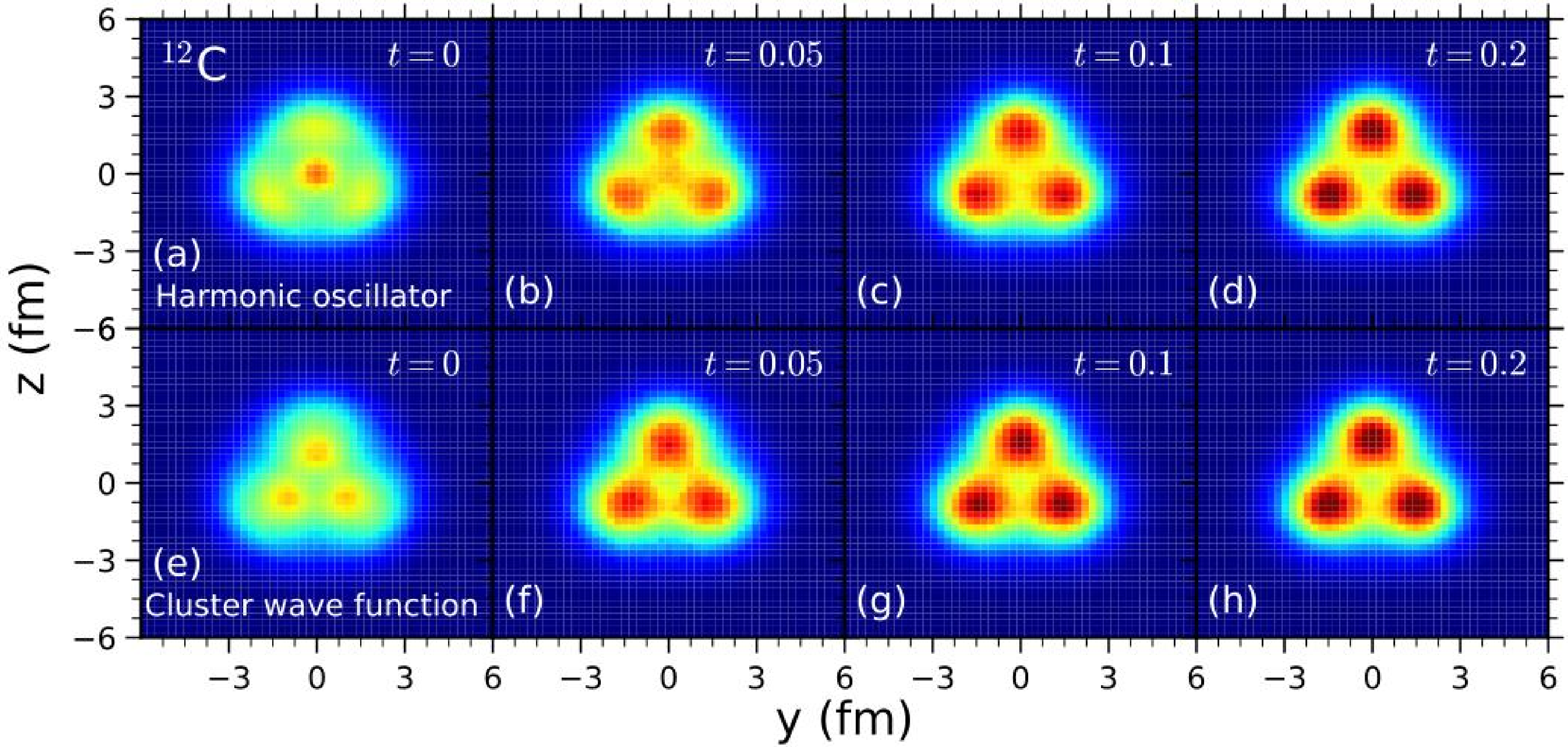




Web figure from: https://en.wikipedia.org/wiki/Spheroid

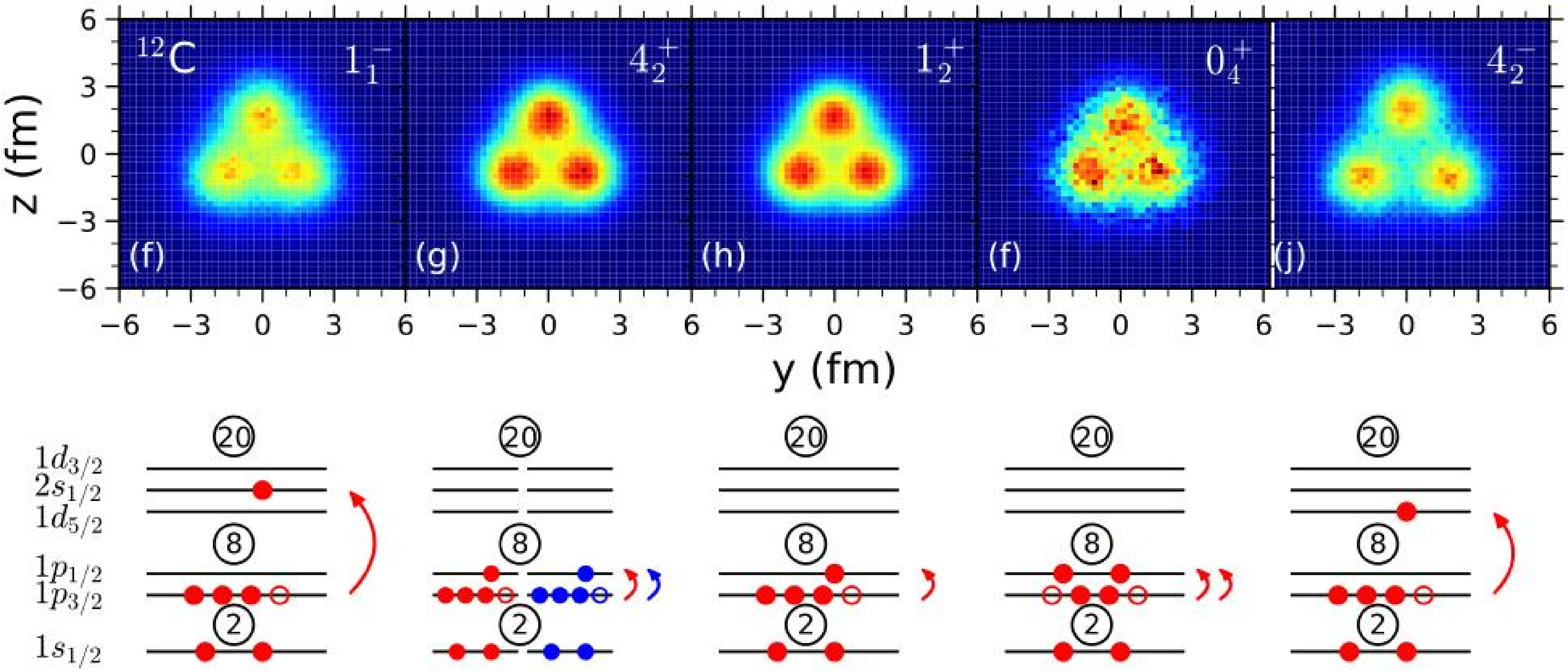
Cluster Formation

- 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}.



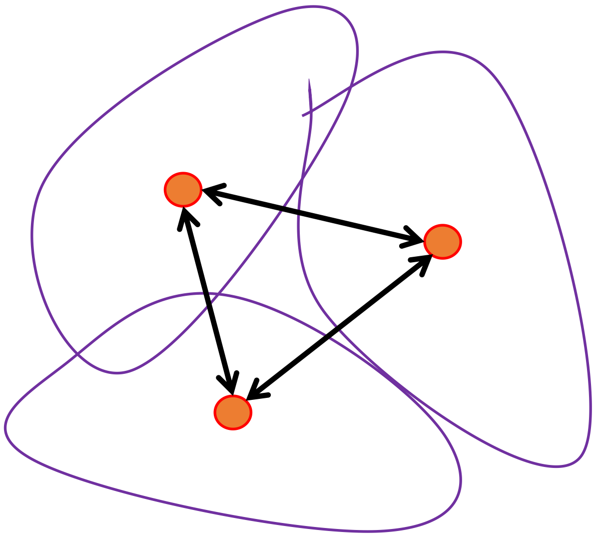
confirms the finding in Ref. E. Epelbaum et al., PRL 109, 252501 (2012)

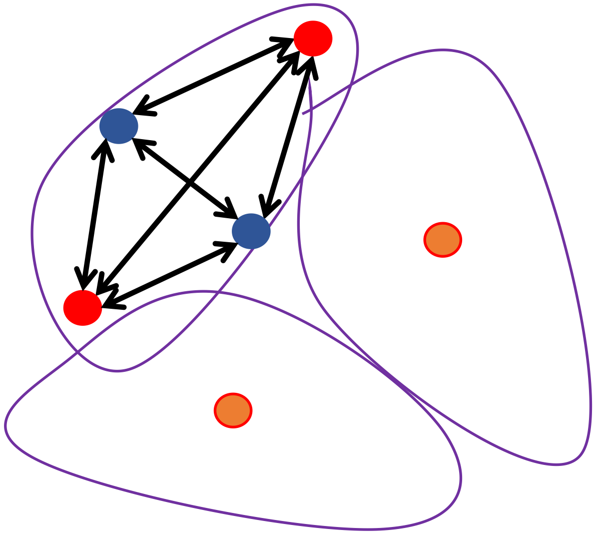
Shell-Model States as Initial Wave

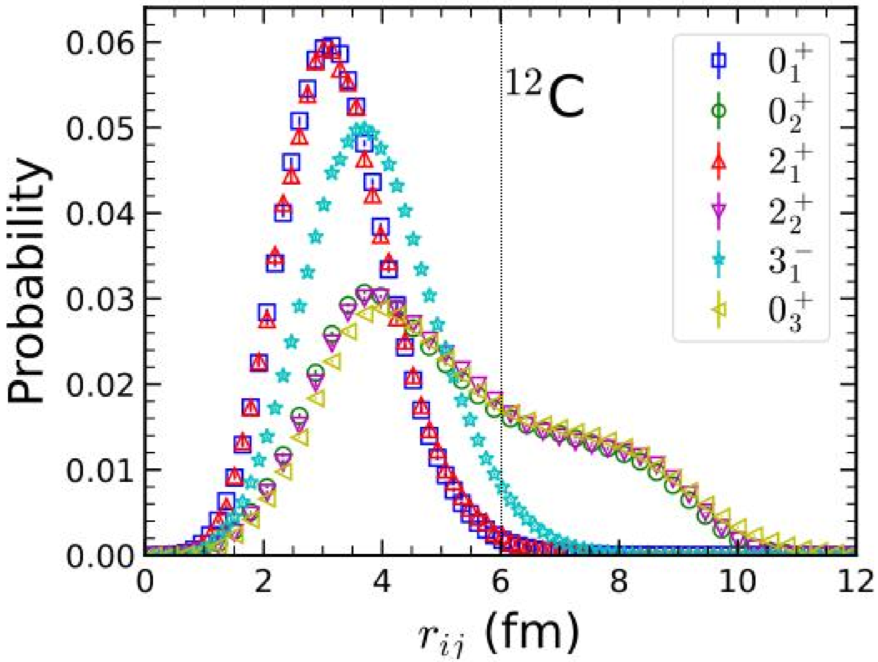


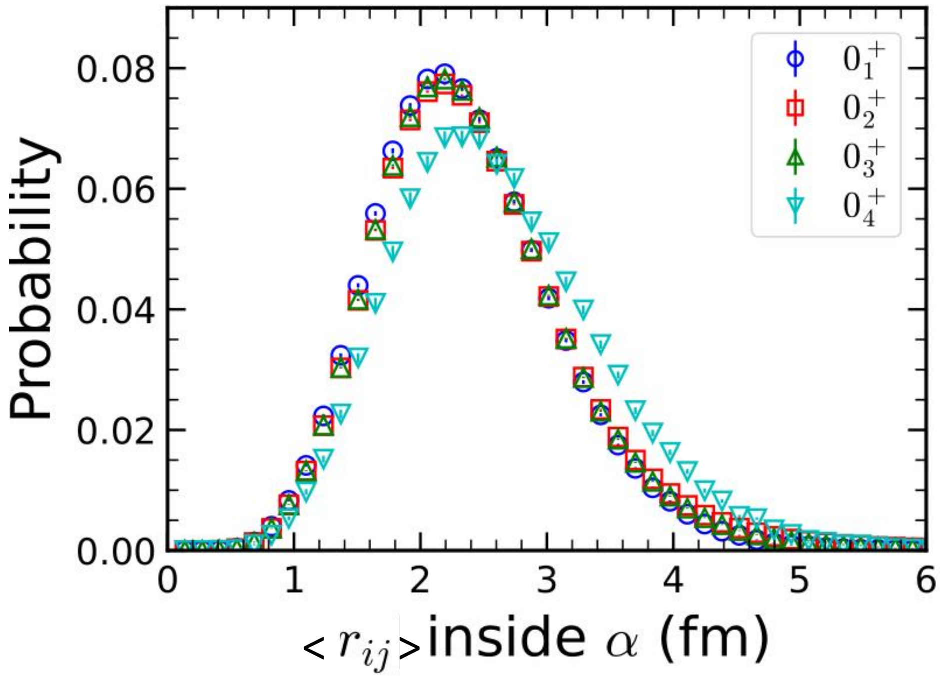
- α cluster structure is less clear due to single-particle excitation, especially when excited to the next shell.

Cluster Excitation? Single-Particle Excitation?



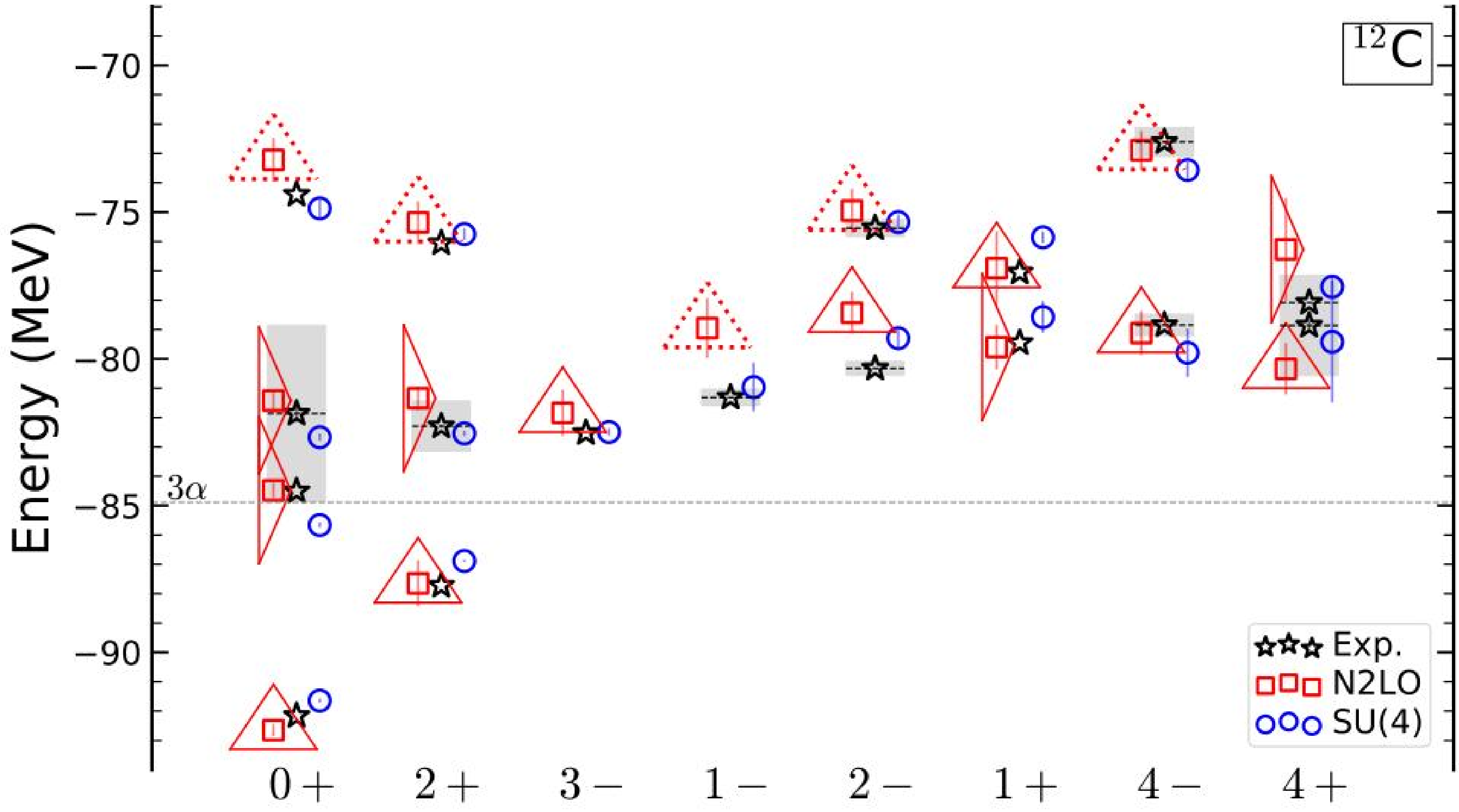






Geometry Information in the Low-Lying Spectrum

- 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

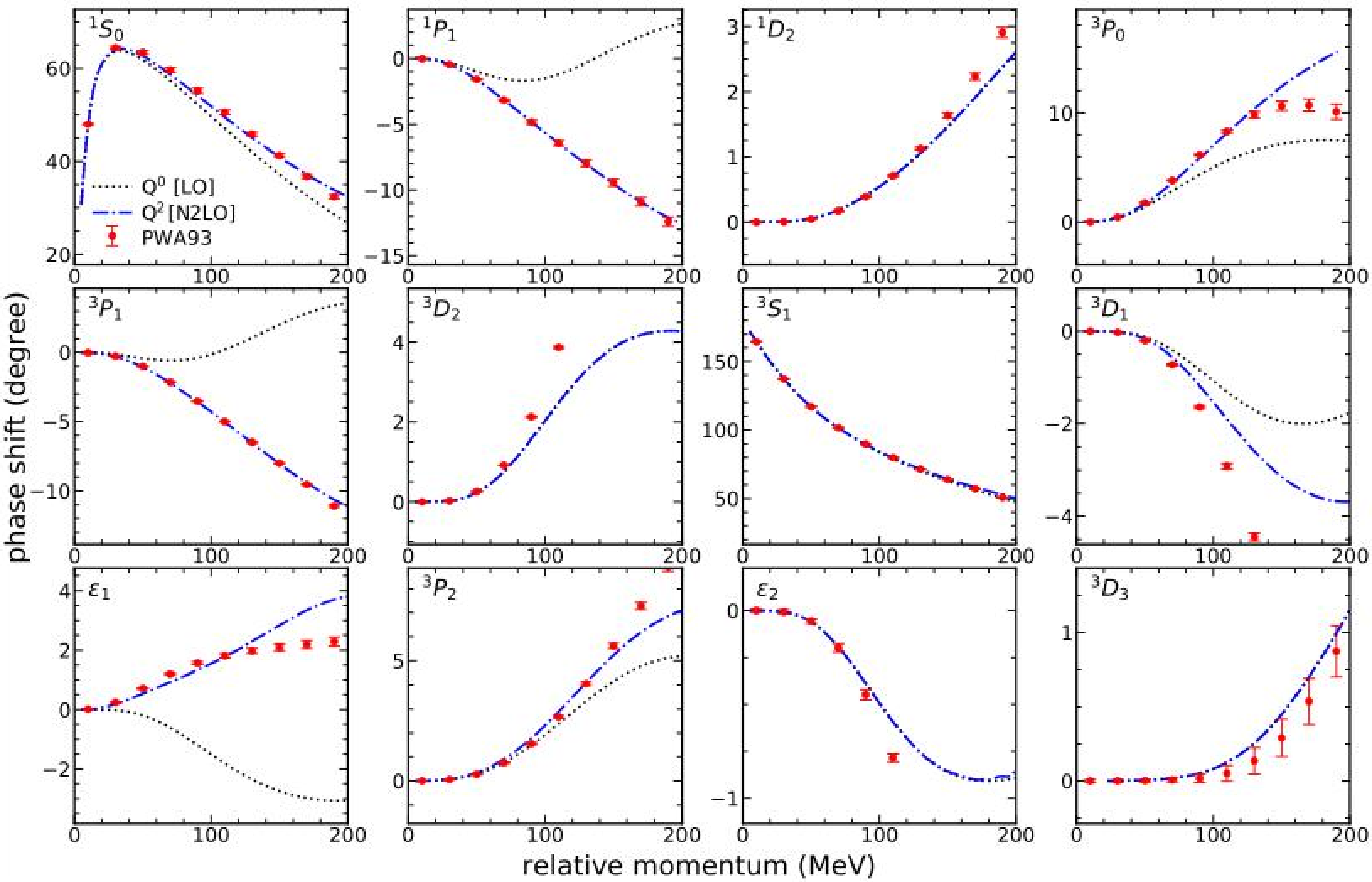
- ^{16}O
- full N3LO interaction   Elhatisari et al., arXiv:2210.17488
- ... ...

THANK YOU!

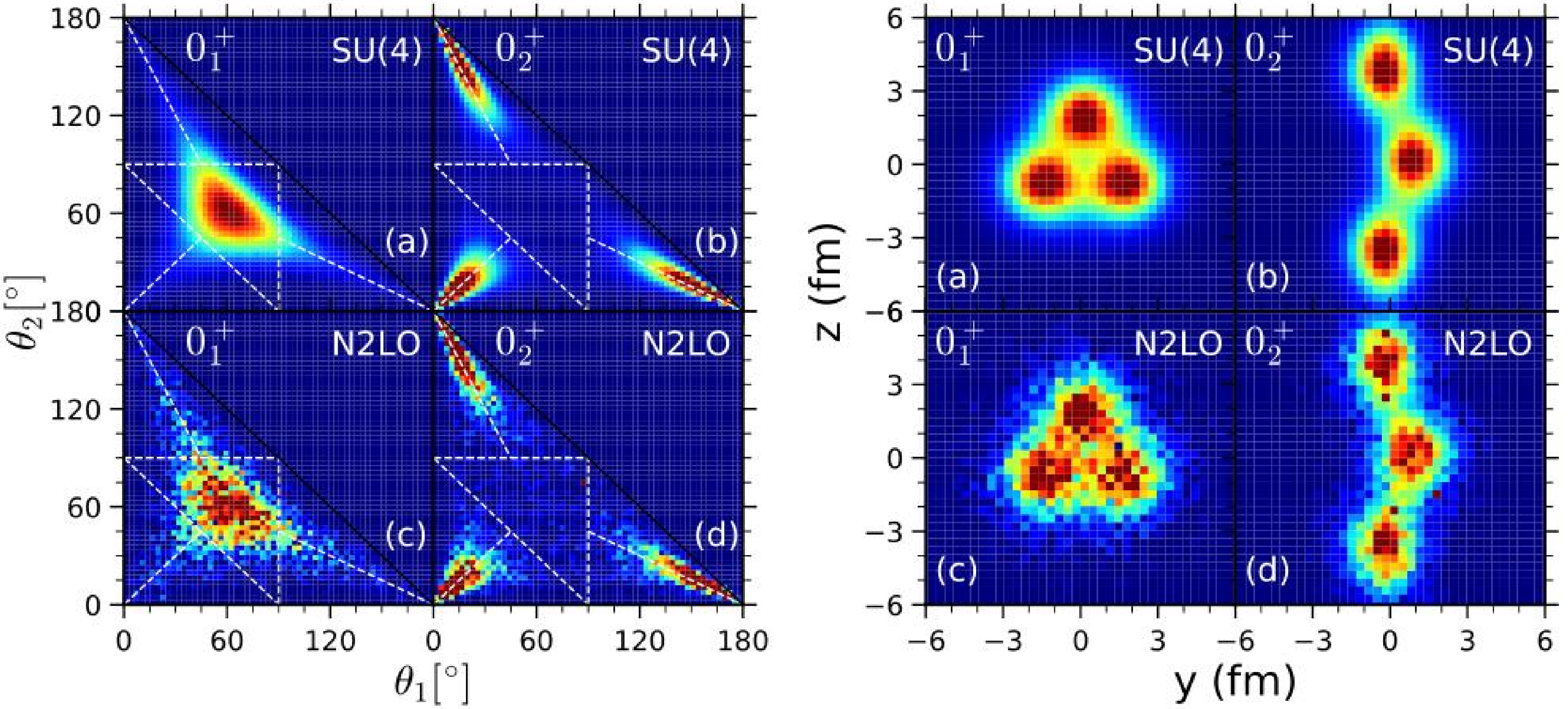
	C_0	$C_{\mathrm{GIR},0}$	$C_{\mathrm{GIR},1}$	$C_{\mathrm{GIR},2}$	s_{NL}	s_{L}
SU(4)	−0.17395	−0.07001	0.01417	−0.00125	0.1	0.06

	C_0	$C_{\mathrm{GIR},0}$	$C_{\mathrm{GIR},1}$	$C_{\mathrm{GIR},2}$
$Q^0,\ {}^1S_0$	0.44365	0.07410	−0.00980	−0.00128
$Q^0,\ {}^3S_1$	−0.25149	−0.04505	0.01092	−0.00170
$Q^2,\ {}^1S_0$	0.55249	0.02521	0.01665	−0.01042
$Q^2,\ {}^3S_1$	−0.01090	1.15209	−0.64469	0.22634
$Q^2,\ {}^1S_0^{0,1}$	0.03241	−0.03062	0.00780	−0.00135
$Q^2,\ {}^3S_1^{0,1}$	0.02738	0.18172	−0.09556	0.03264
$Q^2,\ {}^3S_1-{}^3D_1$	−0.49342	0.09280	0.03828	−0.02687
$Q^2,\ {}^1P_1$	0.96569	0.95481	−0.21826	0.02956
$Q^2,\ {}^3P_0$	−0.19448	−0.07901	0.01729	−0.00206
$Q^2,\ {}^3P_1$	0.92671	0.91735	−0.20962	0.02836
$Q^2,\ {}^3P_2$	−0.04801	−0.03012	0.00730	−0.00114

	c_D	c_E	s_{L}
3N	−0.77527	0.67901	0.2

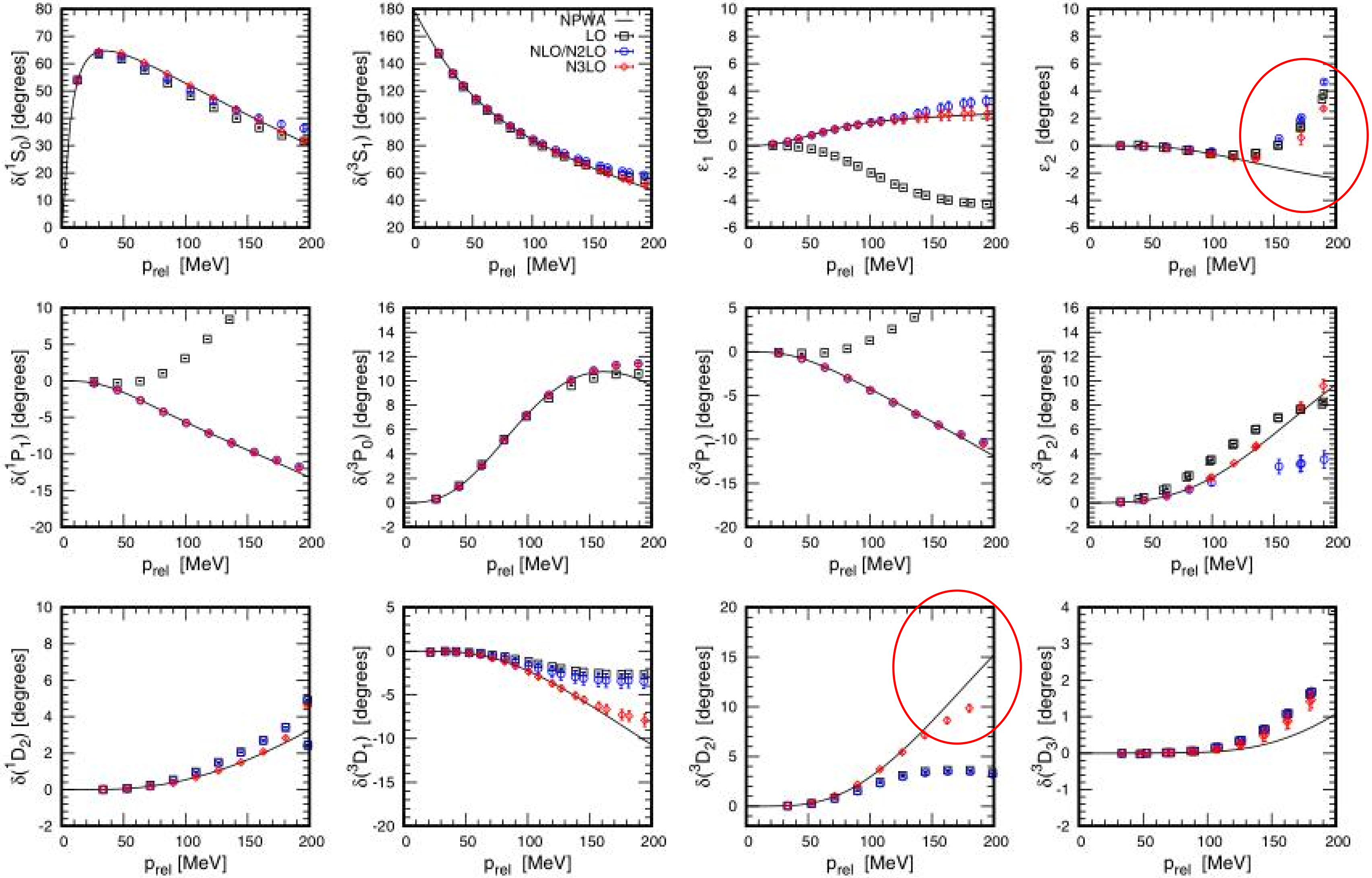


phase shift (degree)
relative momentum (MeV)
$^1S_0$
$^1P_1$
$^1D_2$
$^3P_0$
$^3P_1$
$^3D_2$
$^3S_1$
$^3D_1$
ε_1
$^3P_2$
ε_2
$^3D_3$
Q^0 [LO]
Q^2 [N2LO]
PWA93

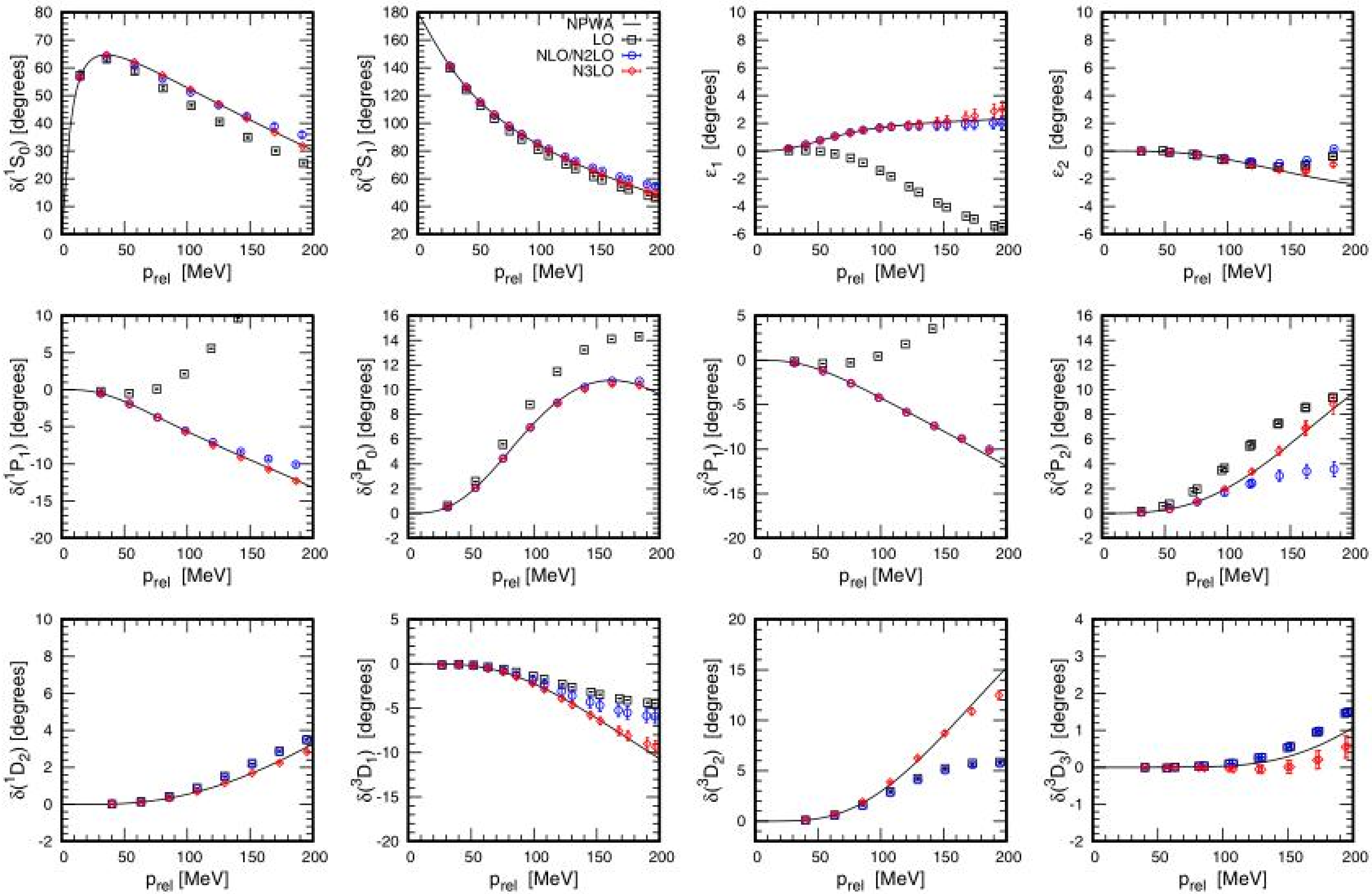


0_1^+ SU(4) (a)
0_2^+ SU(4) (b)
0_1^+ N2LO (c)
0_2^+ N2LO (d)
$\theta_2[^\circ]$
$\theta_1[^\circ]$
z (fm)
y (fm)

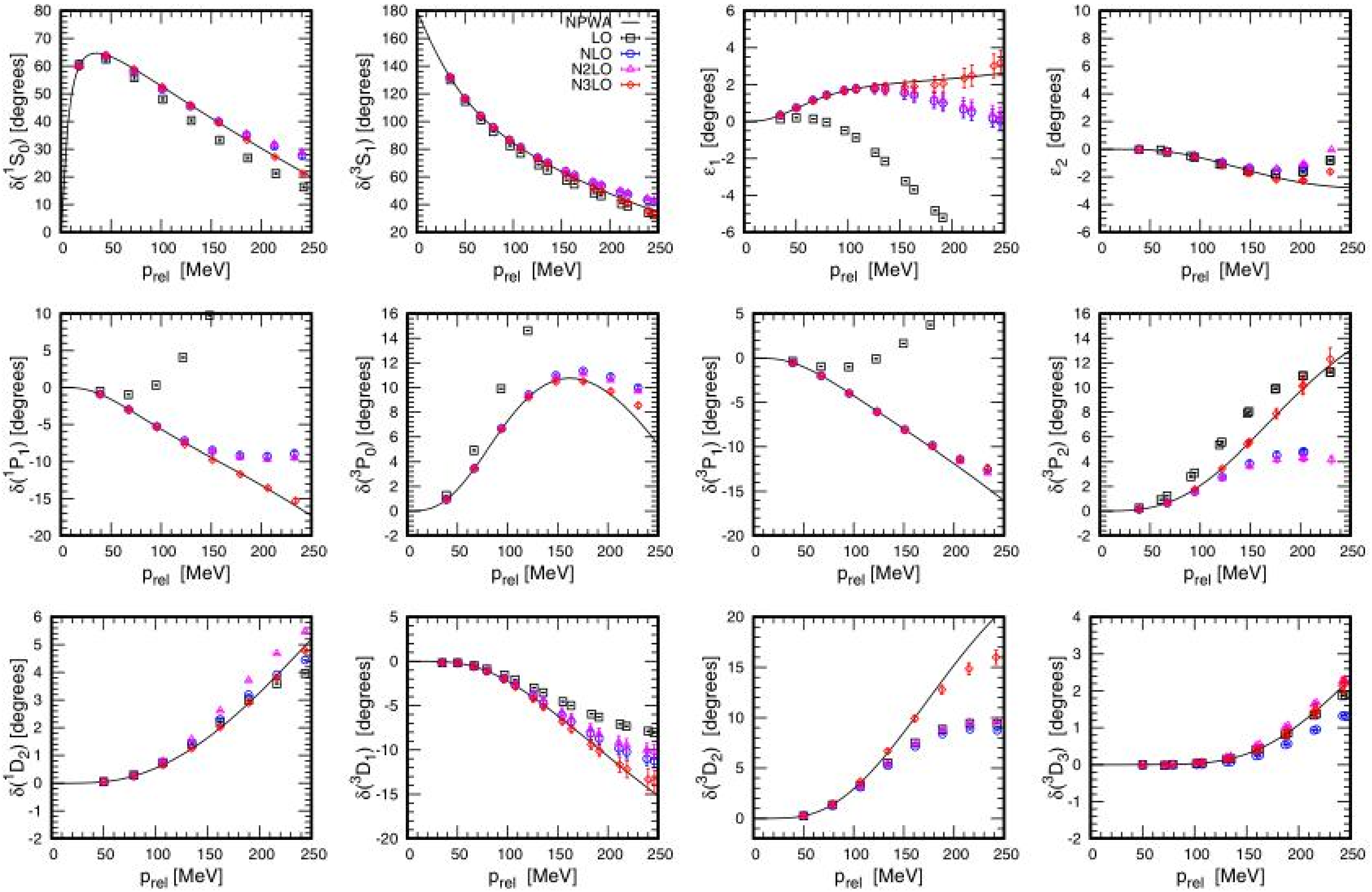
$a = 1.97$ fm $\quad \pi/a \sim 314$ MeV



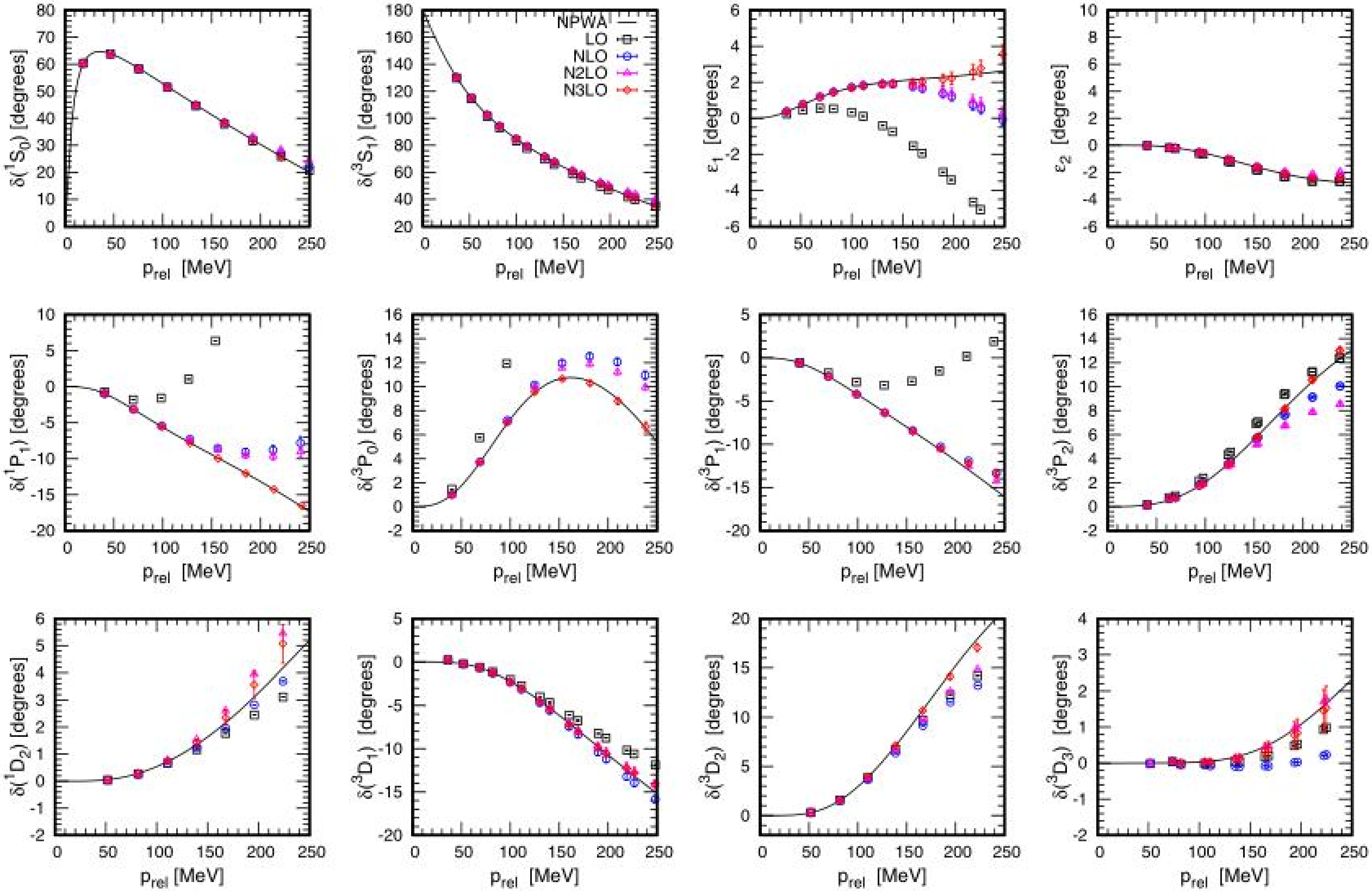
$a = 1.64$ fm $\pi/a \sim 378$ MeV

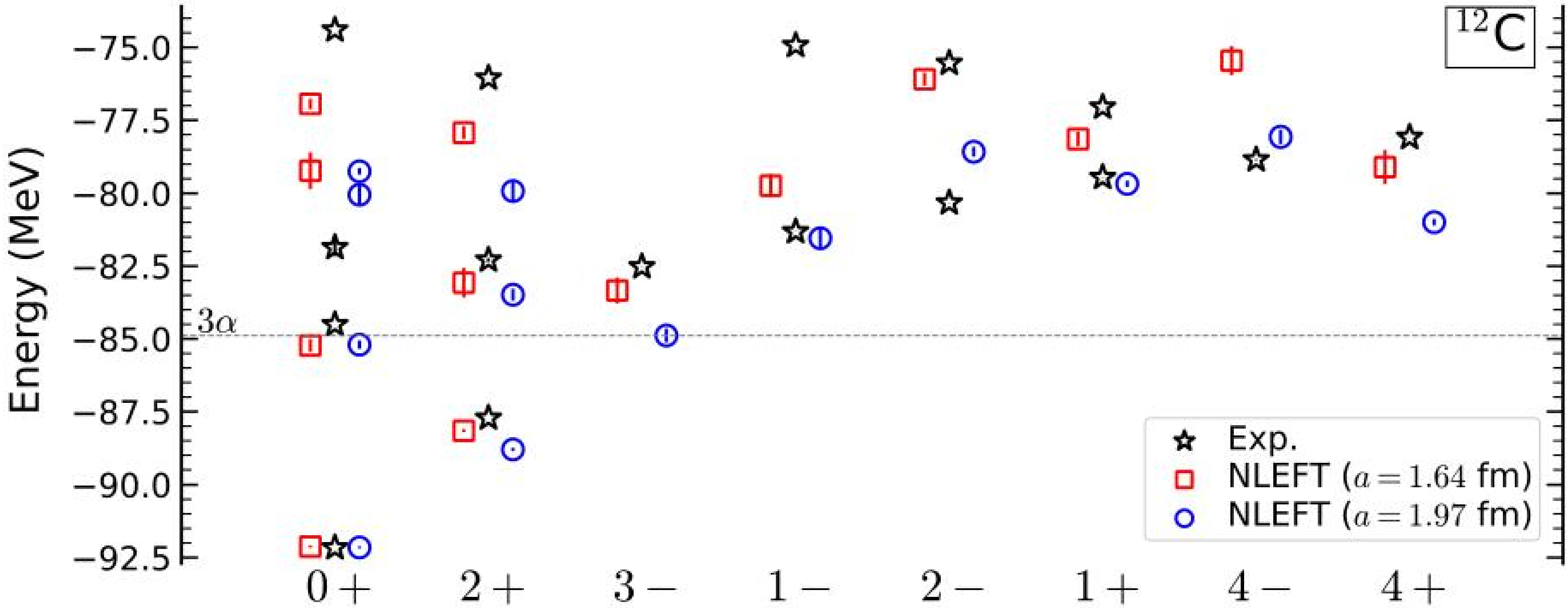


$a = 1.32$ fm $\quad \pi/a \sim 469$ MeV



$a = 0.99$ fm $\quad \pi/a \sim 626$ MeV

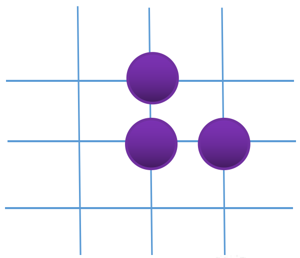


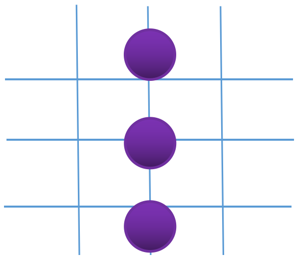


S. Shen, T. A. Lähde, D. Lee, U.-G. Meißner, EPJA 57, 276 (2021)

Decomposition of Hoyle State

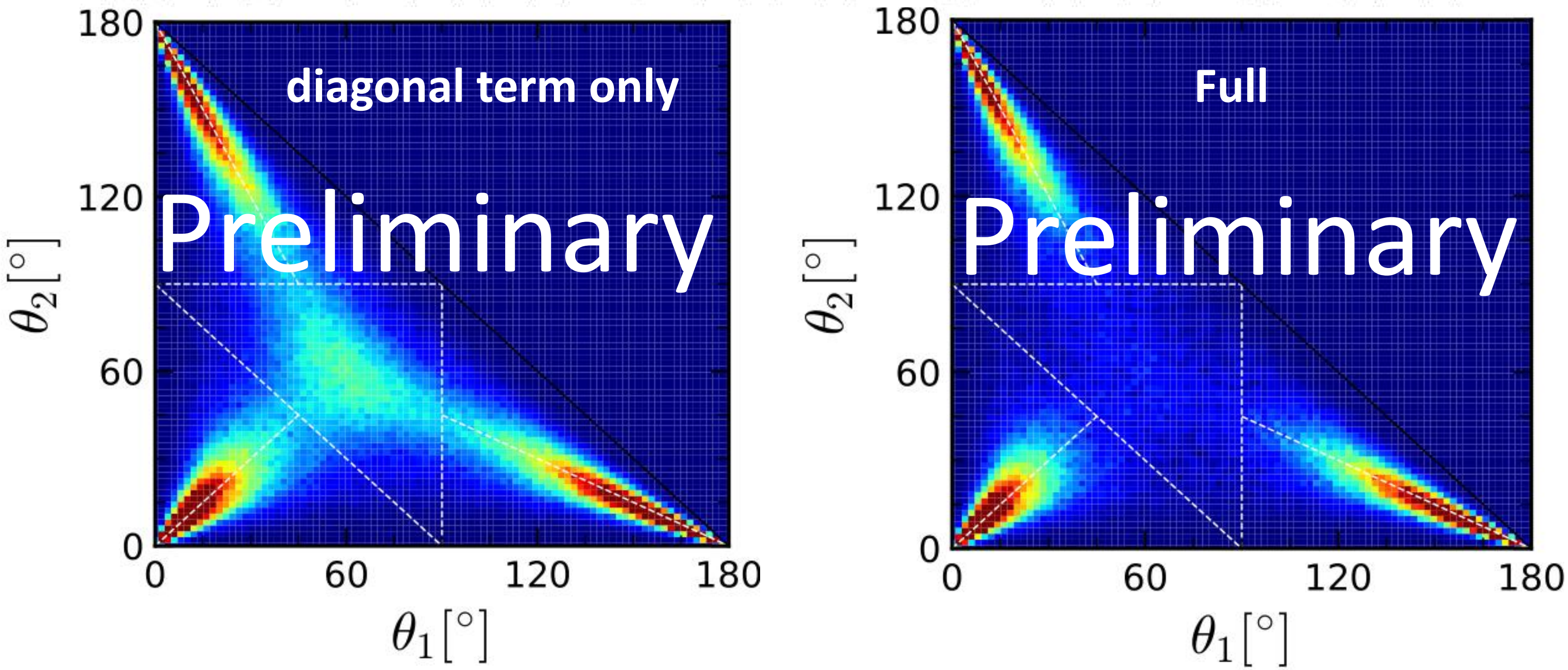
$$|0_1^+\rangle = c_{11}|1\rangle + c_{12}|2\rangle$$
$$|0_2^+\rangle = c_{21}|1\rangle + c_{22}|2\rangle$$





c_{ij}	1	2
0_1+	164.8	8.7
0_2+	-79.0	301.8

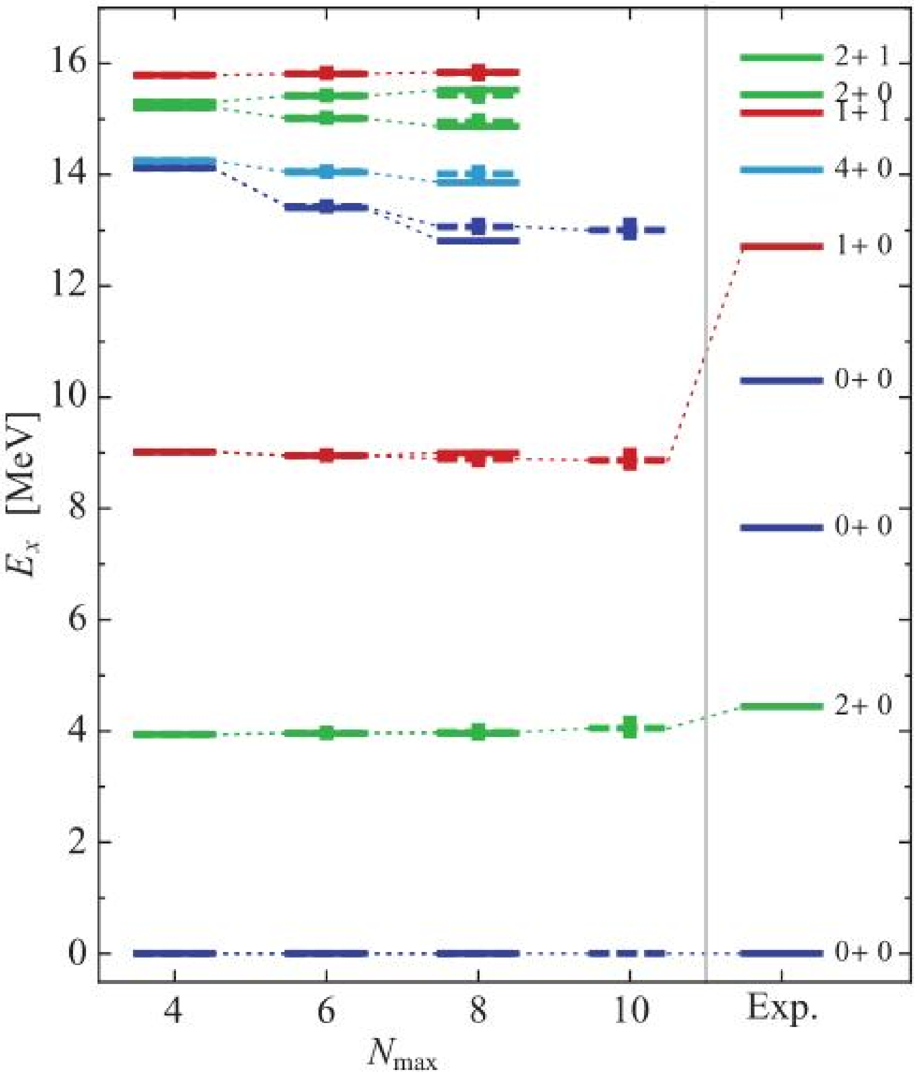
$$\langle 0_2^+|O|0_2^+\rangle = |c_{21}|^2\langle 1|O|1\rangle + |c_{22}|^2\langle 2|O|2\rangle + c_{21}^* c_{22}\langle 1|O|2\rangle + c_{22}^* c_{21}\langle 2|O|1\rangle$$



three α-like clusters with the probability 2/3, and 1/3 in a modestly ellipsoidal shape of β_2 ~ 0.3

T. Otsuka et al., Nature Commu. (2022) 13:2234

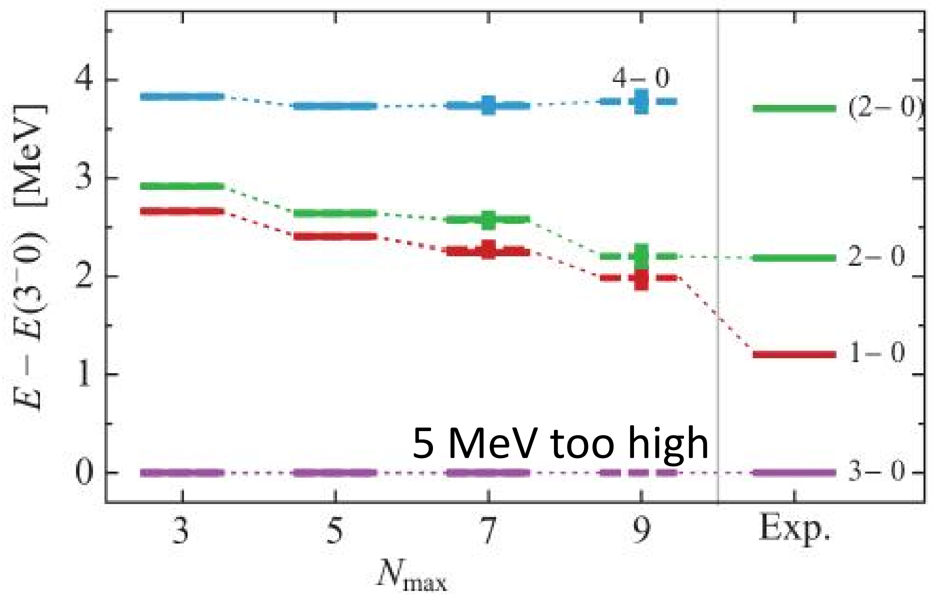
Maris P, Vary JP, Calci A, Langhammer J, Binder S, Roth R., Phys Rev C. (2014) 90:014314
D. R. Entem and R. Machleidt, Phys. Rev. C 68, 041001 (2003)



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,¶]



Cluster Formation

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \frac{m}{2}(\omega_x x^2 + \omega_y y^2 + \omega_z z^2)$$

$$\omega_\rho^2 = \omega_x^2 = \omega_y^2 = \omega_0^2\left(1+\frac{2}{3}\delta^2\right)^2\left(1+\frac{2}{3}\delta\right),$$
$$\omega_z^2 = \omega_0^2\left(1+\frac{2}{3}\delta^2\right)^2\left(1-\frac{4}{3}\delta\right).$$