Int. Symp. Clustering as a Window on the Hierarchical Structures of Quantum Systems (CLUSHIQ2022)
Sendai
Nov. 2 (Oct. 31-Nov. 3), 2022

Untold story of the Hoyle state
- first *ab initio* calculation of ^{12}C -

Takaharu Otsuka

Clusters & Hierarchies

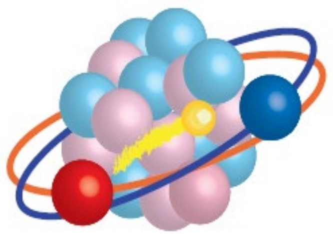
"Clustering as a window on the hierarchical structure of quantum matter" (2018-2022)
Grant-in-Aid for Science Research on Innovative Areas（新学術領域 MEXT Kakenhi 18H05400)

JICFuS
東京大学 THE UNIVERSITY OF TOKYO
RIKEN NISHINA CENTER
JAEA

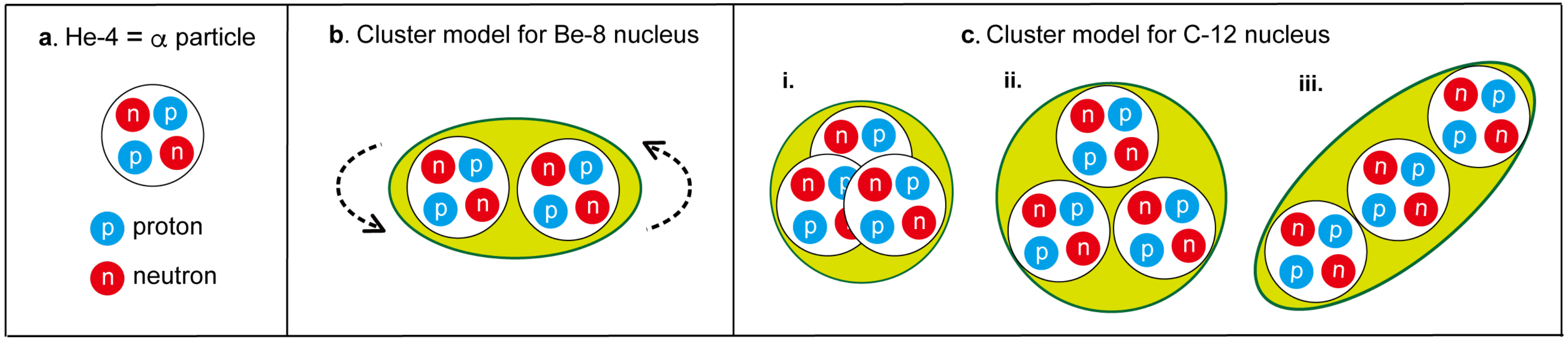
This work was supported also by MEXT as "Program for Promoting Researches on the Supercomputer Fugaku" (Simulation for basic science: from fundamental laws of particles to creation of nuclei) and "Priority Issue on post-K computer" (Elucidation of the Fundamental Laws and Evolution of the Universe), and by JICFuS.

normal nuclear matter

quantum liquid with a uniform density of nucleons



α cluster formation - clusters close or apart -



Pioneers (before 1960)

bond coupling

Wefelmeier, W. Von, Ein geometrisches Modell des Atomkerns. Z. Phys. Hadrons Nucl. 107, 332 (1937).

Wheeler J. A., Molecular Viewpoints in Nuclear Structure, Phys. Rev. **52**, 1083 (1937).

Morinaga, H., Interpretation of some of the excited states of 4n self-conjugate nuclei, Phys. Rev. C **101**, 254 (1956).

linear formation

Brink, D., Alpha-Particle Model of Light Nuclei. The Proc. Intl. School of Physics Enrico Fermi, Course, 36 (1966), p. 247.

Ikeda, K., Takigawa, N. and Horiuchi, H., The systematic structure-change into the molecule-like structures in the self-conjugate 4n nuclei. Prog. Thoer. Phys. Suppl., **E68**, 464 (1968).

Arima, A., Horiuchi, H., Kubodera, K. and Takigawa, N., Clustering in Light Nuclei, in *Advances in Nuclear Physics*, ed. by Baranger M. and Vogt E., (Springer, Boston, MA., 1973), **5**, 345.

Freer, M., Horiuchi, H., Kanada-En'yo, Y., Lee, D. and Meißner, U.-G., Microscopic clustering in light nuclei. Rev. Mod. Phys. **90**, 035004 (2018).

Alpha formation near the threshold energy

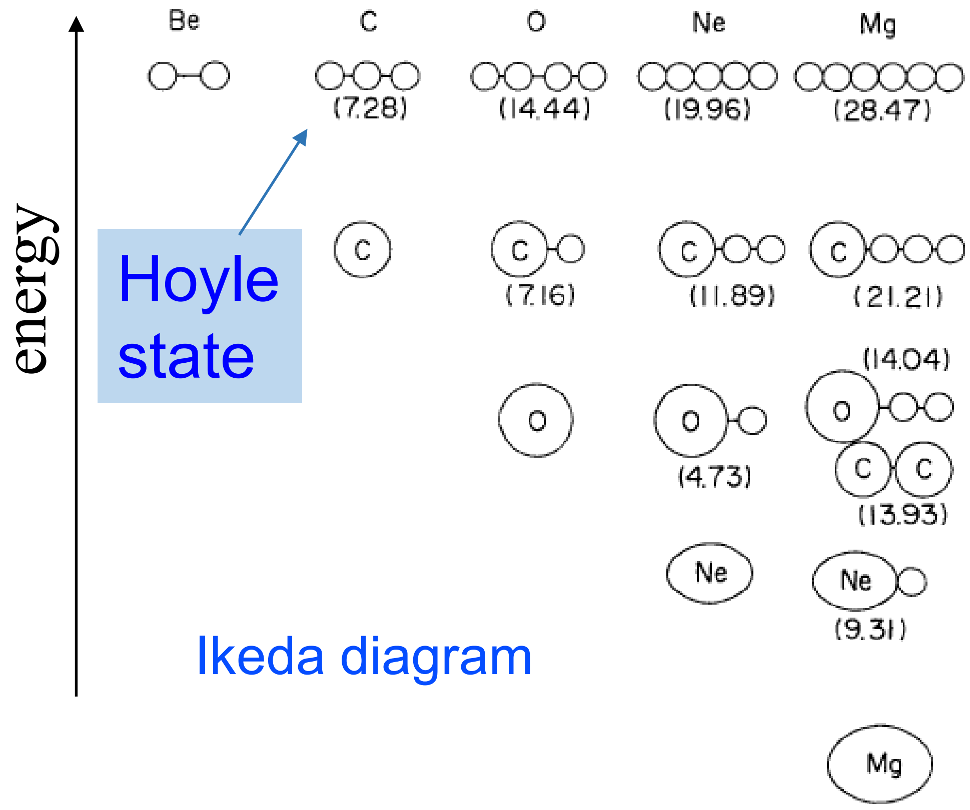


Fig. 1. Threshold energy for each decay mode. In the figure, the threshold energy for each decay mode is given in MeV. The systematics suggests the possible molecular nature around each energy. Some of the molecular states are already found and are represented in Fig. 2.

Supplement of the Progress of Theoretical Physics, Extra Number, 1968

The Systematic Structure-Change into the Molecule-like Structures in the Self-Conjugate 4*n* Nuclei

Kiyomi IKEDA,*) Noboru TAKIGAWA and Hisashi HORIUCHI

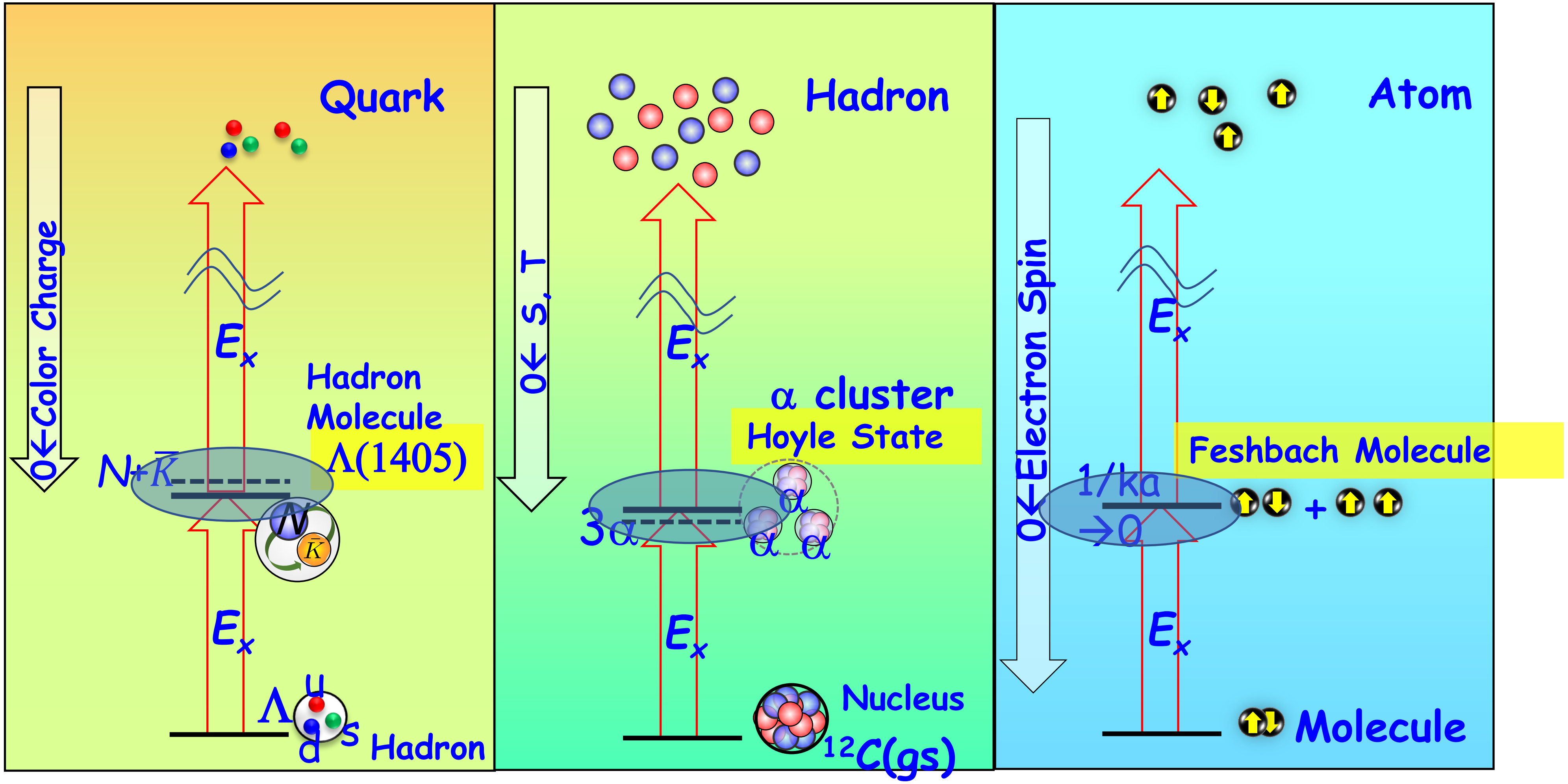
The alpha clustering in atomic nuclei was considered to occur near the threshold energy. This sounds a nice idea.

This picture has been a strong guiding principle for half a century.

Nevertheless, we re-visit it.

Semi-Hierarchy: Clustering and Hierarchy of Matter

from Nakamura's talk

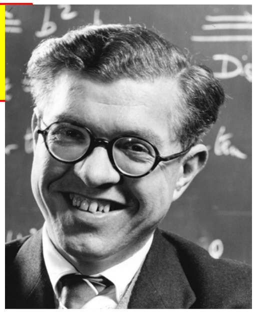


✓ Threshold: **Clustering near Threshold → Semi-Hierarchy**

This talk ➔ α clustering in nuclei may not need threshold effects

The preformed α particle(=cluster) can come out if the energy is above the threshold.

Hoyle state of ^{12}C Ex = 7.65 MeV



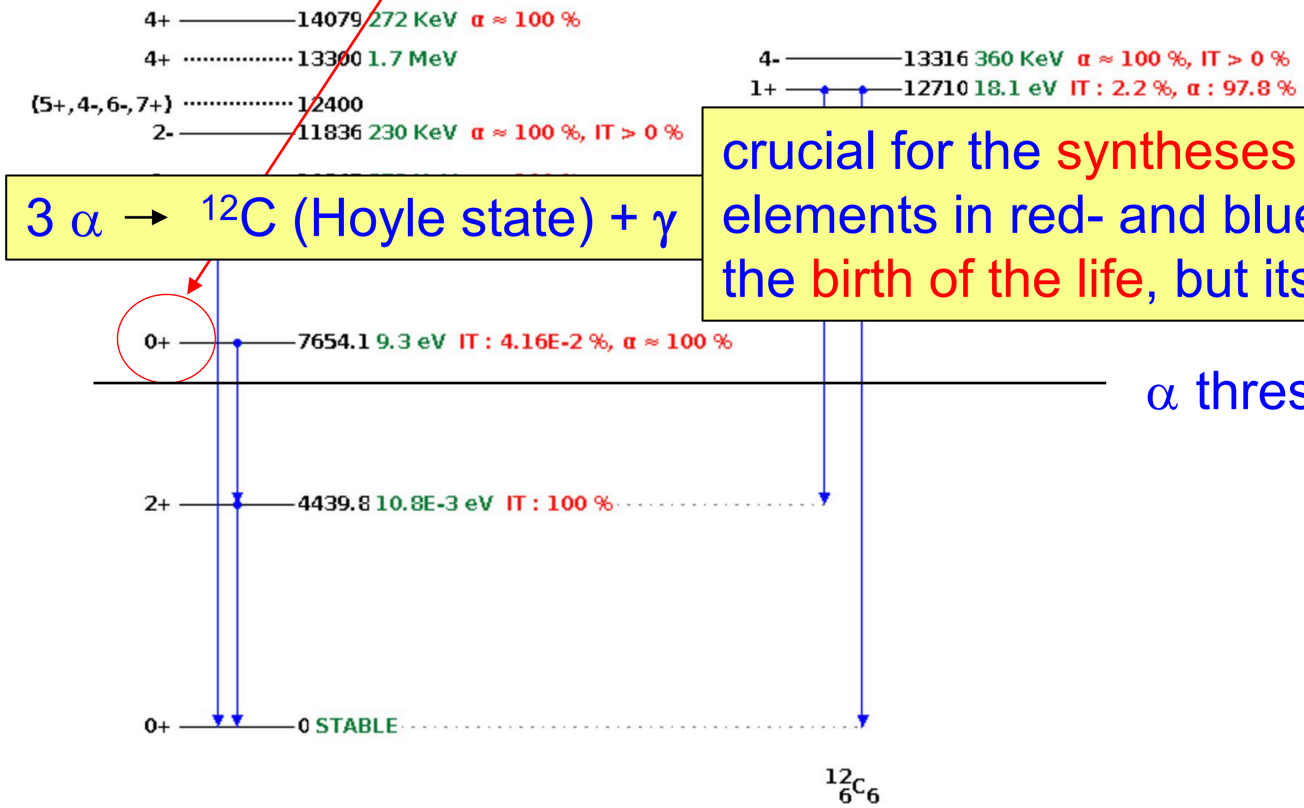
ON NUCLEAR REACTIONS OCCURRING IN VERY HOT STARS. I. THE SYNTHESIS OF ELEMENTS FROM CARBON TO NICKEL

F. Hoyle*

Mount Wilson and Palomar Observatories
Carnegie Institution of Washington
California Institute of Technology

Received December 22, 1953

$A_0 = 4$, $Z_0 = 2$, and $A_1 = 8$, $Z_1 = 4$, in the formulae of the previous section. The important energy level of the C^{12} nucleus in the present problem is one very recently identified by Dunbar, Pixley, Wenzel, and Whaling (1953). This level occurs at about 7.68 mev above ground level, which corresponds to a value of E_R of about 0.31 mev. (It will



3 α → ^{12}C (Hoyle state) + γ

crucial for the syntheses of carbon and other heavier elements in red- and blue-giant stars and further for the birth of the life, but its structure remains unknown

α threshold

The clustering is one of the fundamental problems in physics, as is in this project.

Foundation from sound underlying bases

Its contemporary versions

***Ab initio* calculations on clustering aspects**

- ~~[Green's Function Monte Carlo (GFMC)]~~

  Variational Monte Carlo (VMC)

  [Wiringa et al. 2000]

- No Core Full Configuration (NCFC) :

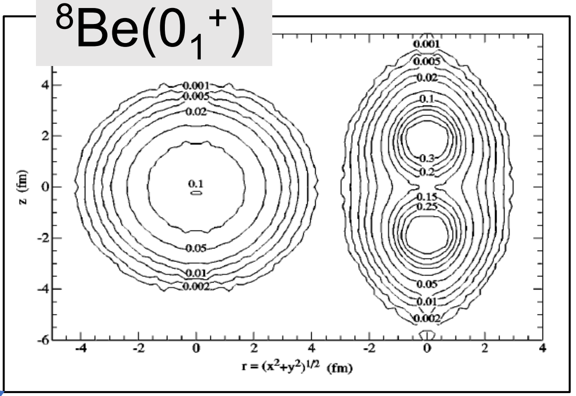
  [Cockrel et al. 2012] *Not clustering*

- Lattice EFT : Hoyle state [Epelbaum et al. 2012]

  Initial setup

- Besides many microscopic models/formulations, such as FMD, AMD, DFT/MF approaches.

^{8}Be(0_1^+)



^{8}Li(2_1^+) lab. frame density

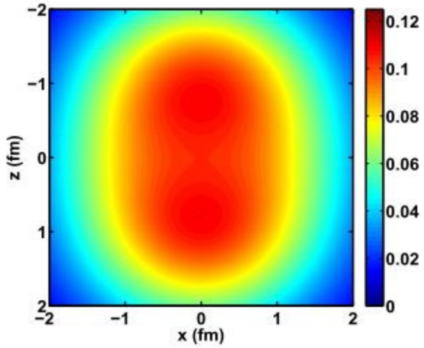
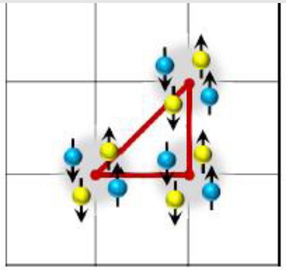


FIG. 12: (Color online) The $y = 0$ slice of the translationally-inv
density for the same state is on the right. These densities were

^{12}C (0_1^+, 2_1^+)



How to calculate ?

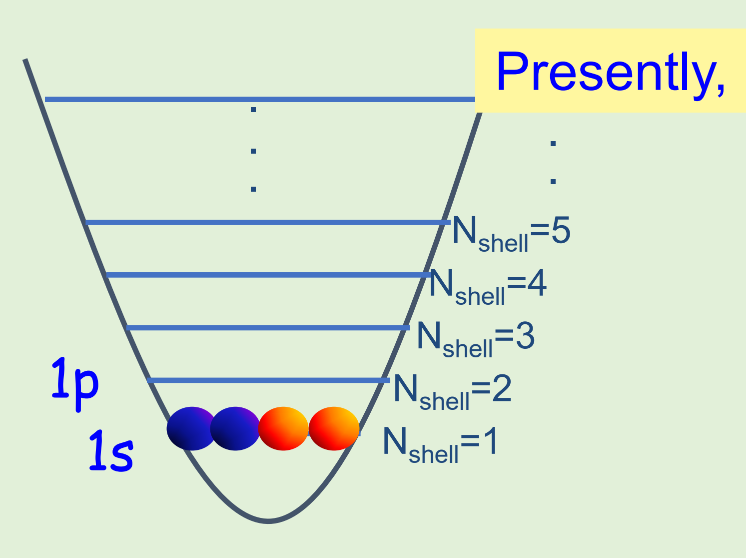
ab initio No-Core Monte Carlo Shell Model (MCSM)

advanced CI method on supercomputers

No inert core, *or* all nucleons are activated

Nucleon-nucleon interactions are fixed prior to this study, based on fundamental approaches such as the chiral Effective Field Theory of QCD.

Single-particle states included



Presently, a model space up to Nshell =7 (6 hw) is adopted

Solve the Schrodinger equation

$$H\,\Psi = E\,\Psi$$

E : eigenenergy

Ψ : eigenstate

Nucleon-Nucleon interaction

+ kinetic energy

Be : JISP16 fitted to *NN* scattering + fine tuning

Shirokov, A. M., Vary, J. P., Mazur, A. I. and Weber, T. A., Realistic nuclear Hamiltonian: Ab exitu approach. Phys. Lett. B **644**, 33 (2007).

C : Daejeon16 based on chiral EFT with SRG + fine tuning

Shirokov, A. M., Shin, I. J., Kim, Y., Sosonkina, M., Maris P. and Vary, J. P., N3LO *NN* interaction adjusted to light nuclei in *ab exitu* approach. Phys. Lett. B **761**, 87 (2016).

Machleidt, R. & Entem, D. R., Chiral effective field theory and nuclear forces, Phys. Rep. **503**, 1 (2011).

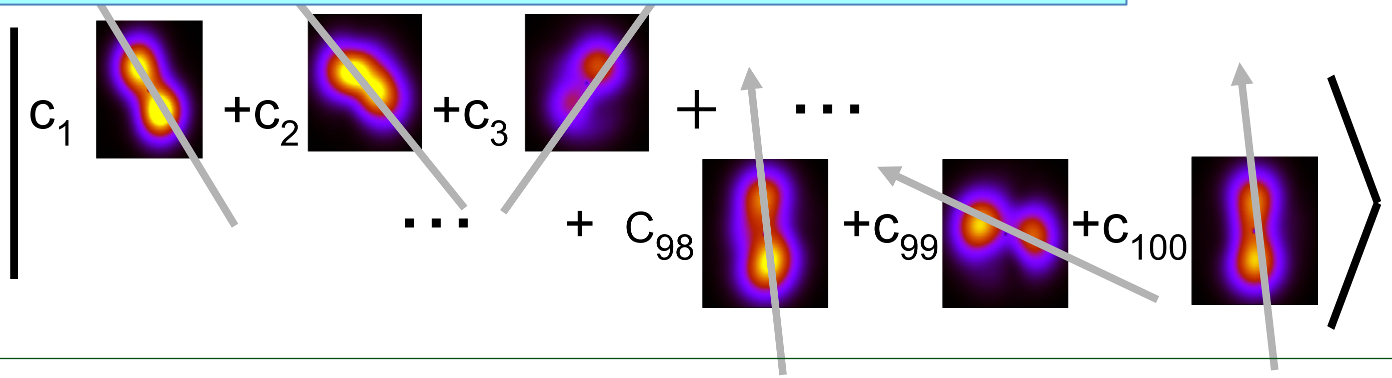
The interactions are fixed prior to the present calculation.

MCSM eigenstate : $\left|\Psi(D)\right\rangle = \sum_{n=1}^{N_B} c_i P^{J,\Pi} \boxed{\left|\phi(D^{(n)})\right\rangle}$

Deformed Slater determinant with three axes of ellipsoid

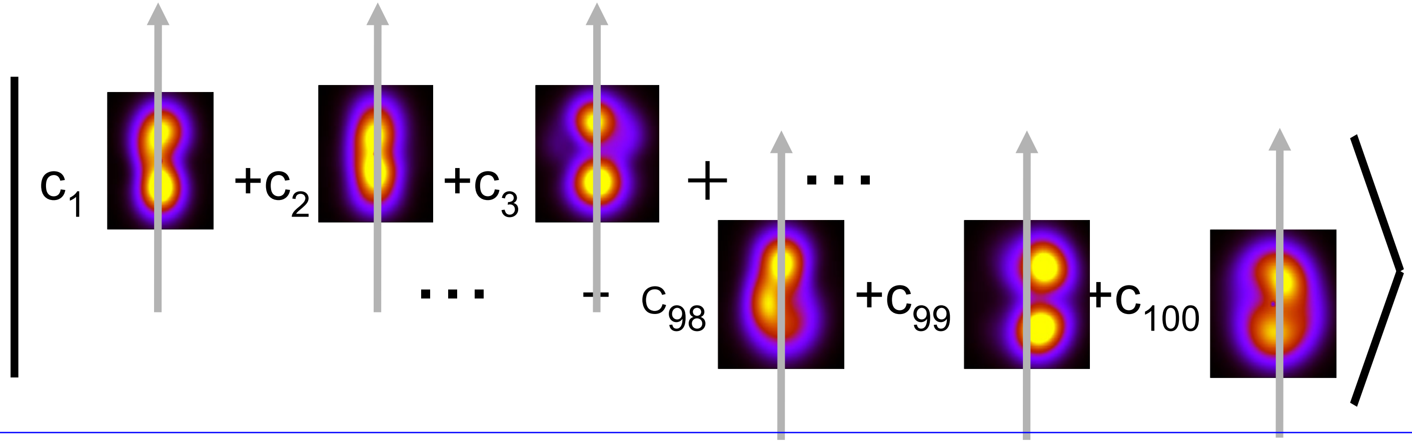
For J^{π} projected states, individual orientations are not relevant.

$\left|\Psi_{\text{lab.}}(D)\right\rangle =$



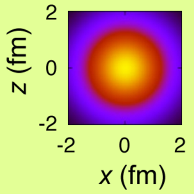
In order to obtain the **snap shot** (or intrinsic density profile), all basis vectors are aligned.
CI-calculation values of observables are not changed.

$\left|\Psi_{\textbf{intr.}}(D)\right\rangle =$



Snapshot of density profile

^{4}He

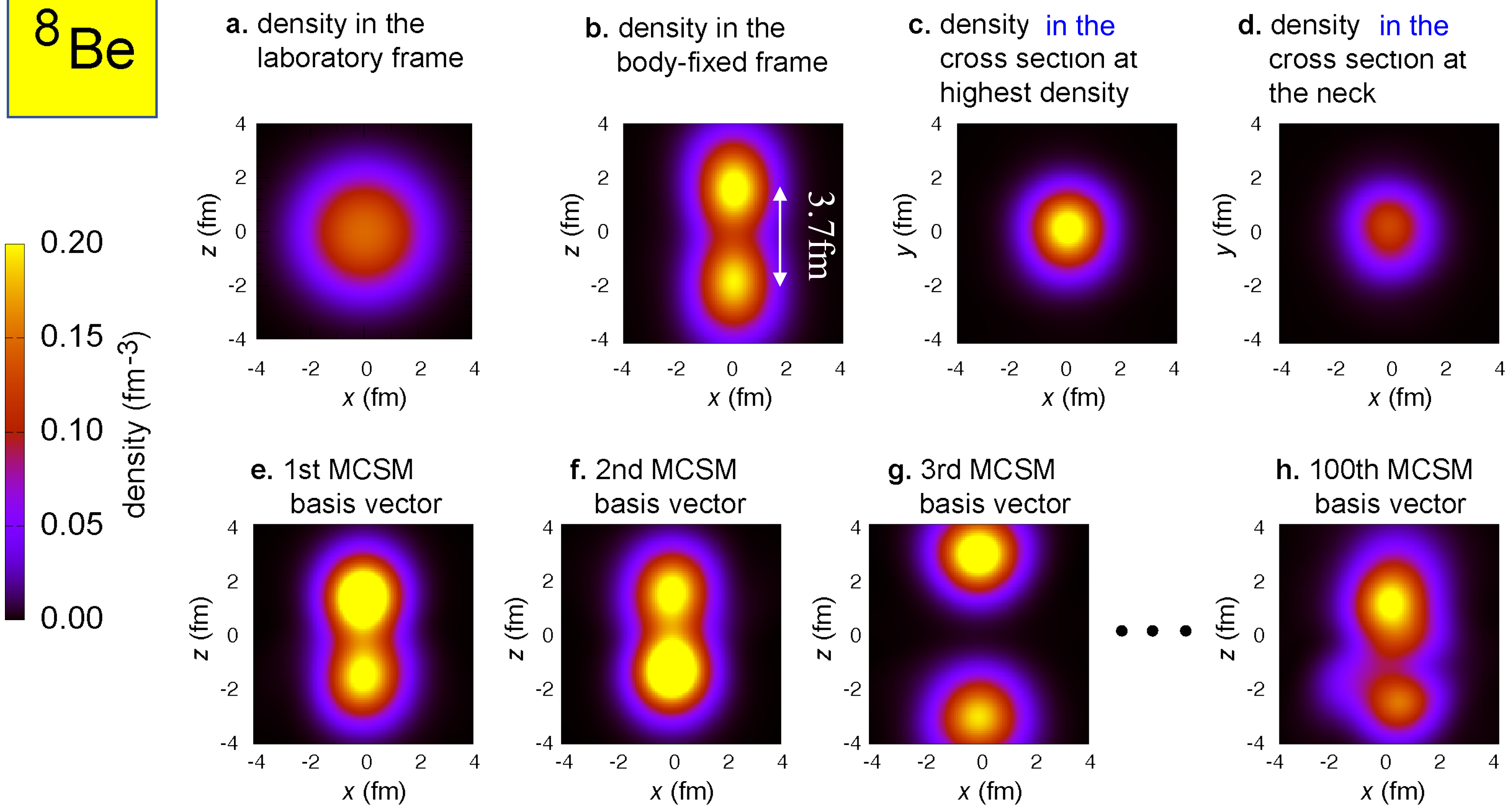


Laboratory-frame

Body-fixed (intrinsic) frame

Q aligned superposed state

^{8}Be



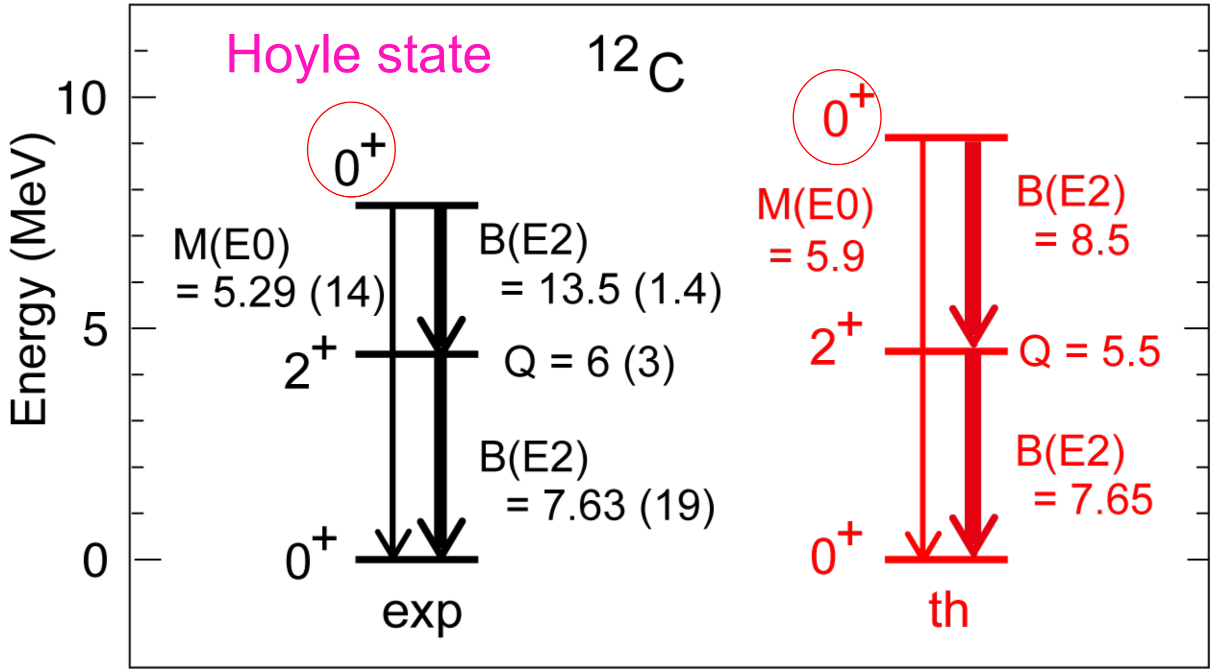
Alignment of MCSM basis vectors (Q aligned)

Energy level & transition strength of ^{12}C

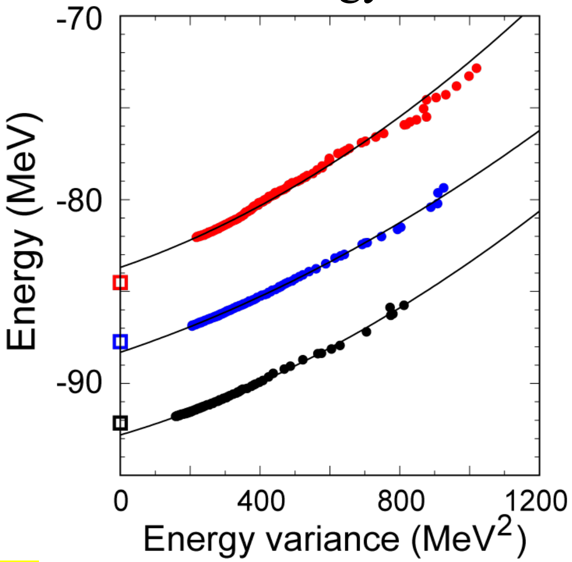
ab initio no-core MCSM + Daejeon 16 interaction (Shirokov et al.)
based on chiral EFT (Machleidt-Entem, 2011)

charges protons 1e
neutrons 0e

correlation effects are explicitly treated
(no medium correction needed)



convergence pattern as
functions of energy variance

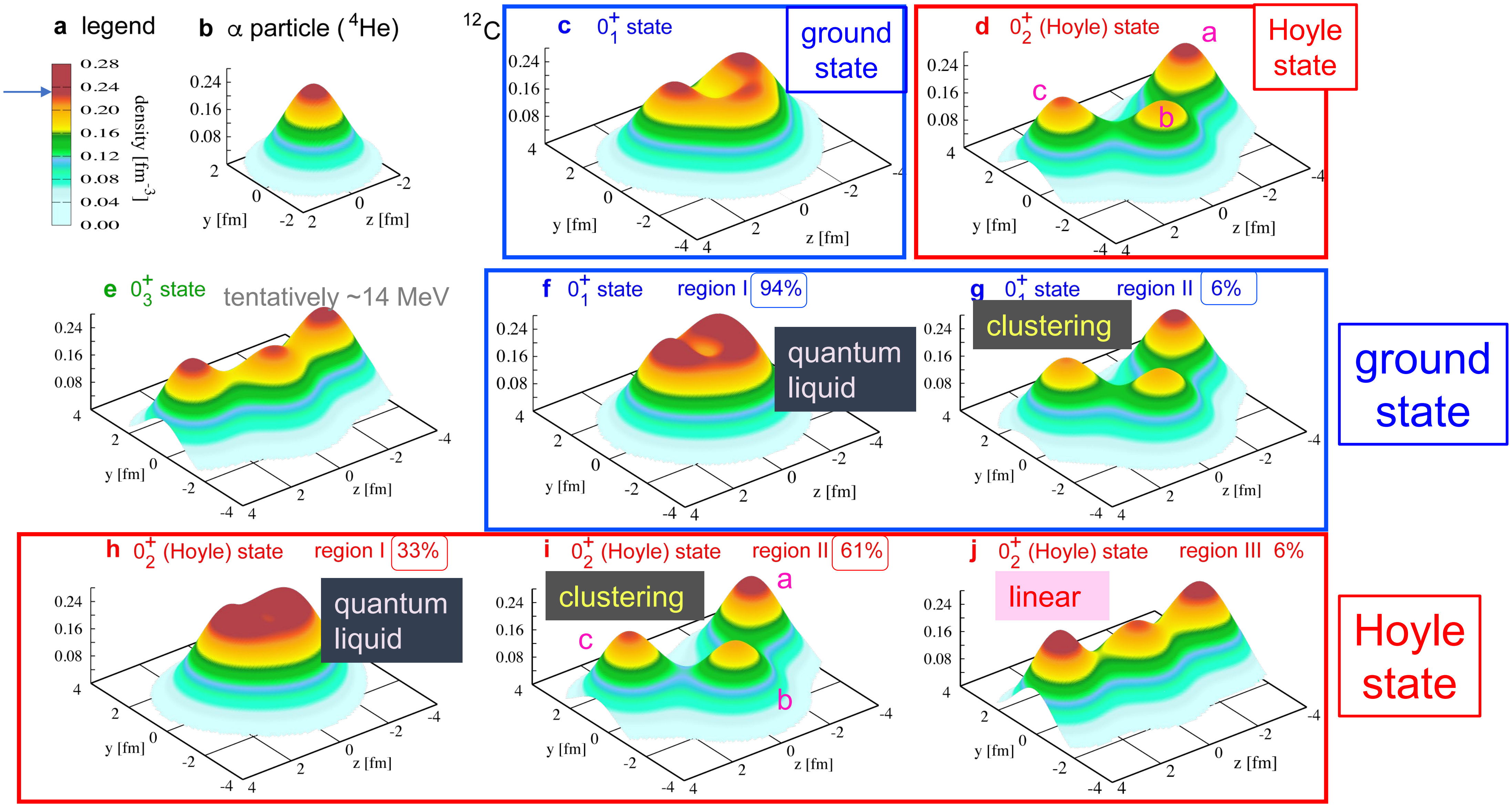


Strong deformation (β_2~0.6, oblate) in the 0^+_1 and 2^+_1 states can now be described from *first principles*.

Stringent test for the Daejeon 16 interaction and the present No-Core MCSM.

Total and decomposed nucleon-densities in body-fixed frame

with proper orthogonalization



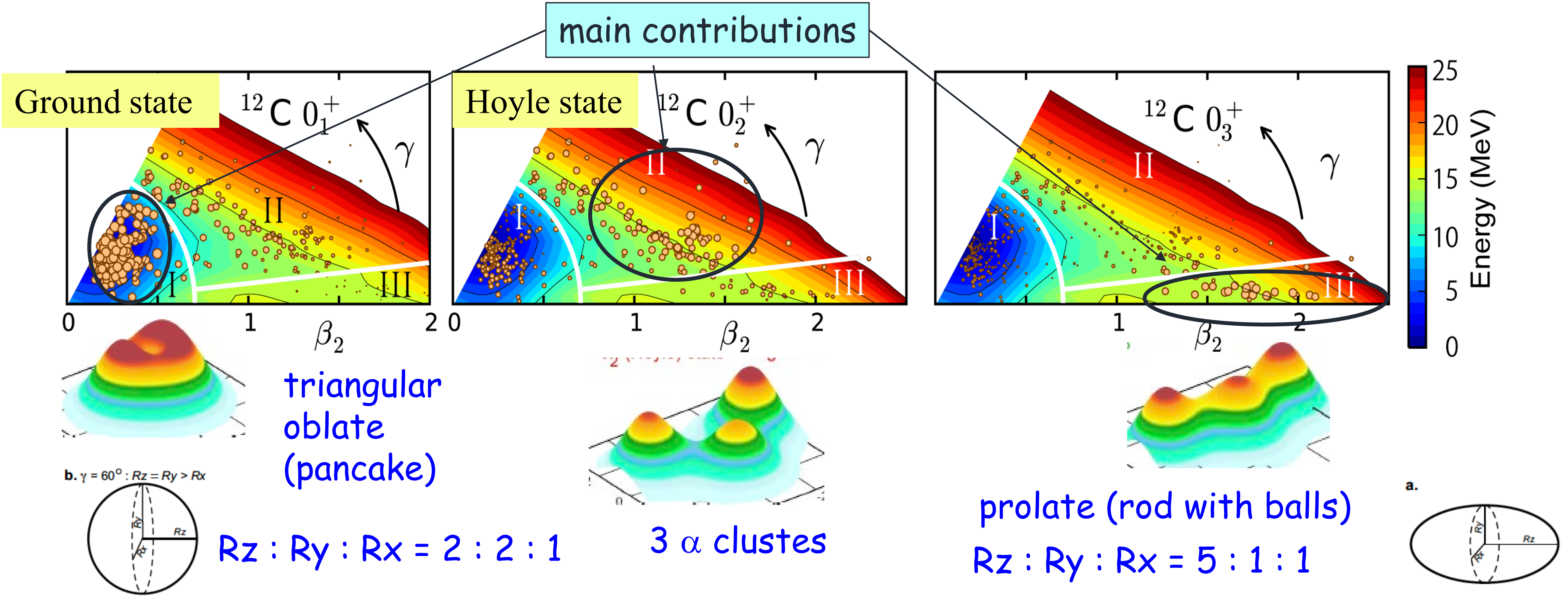
MCSM eigenstates are expanded by basis vectors (deformed Slater determinants) classified by quadrupole moments (*T plot* by *Tsunoda*)

Basis vectors are divided into three groups

I $\beta_2 < 0.7$

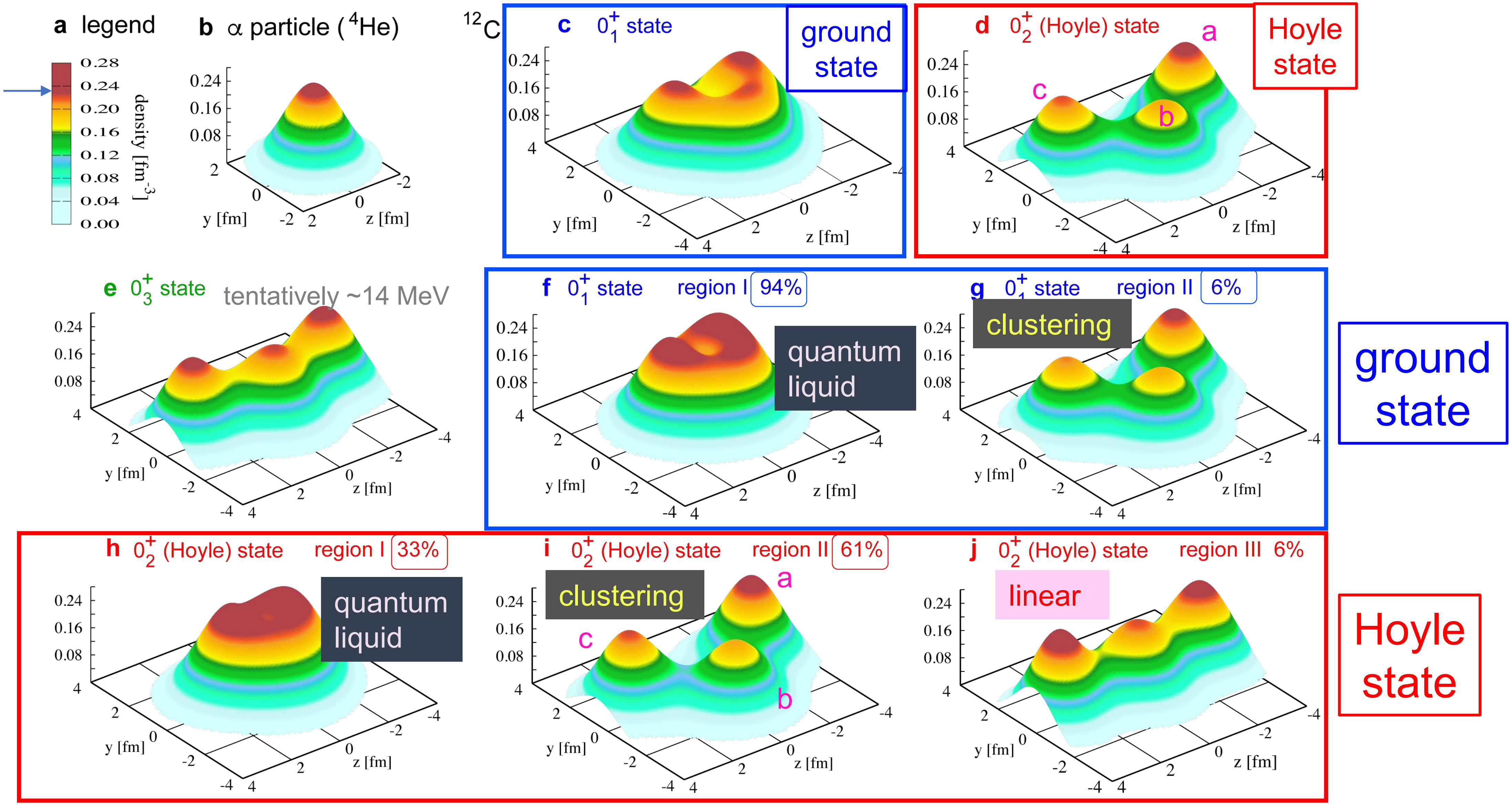
II triaxial

III very prolate

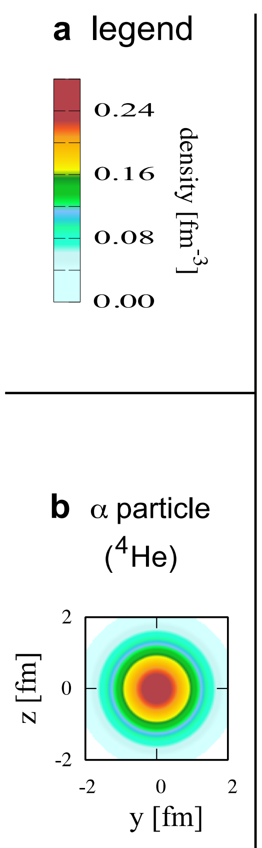


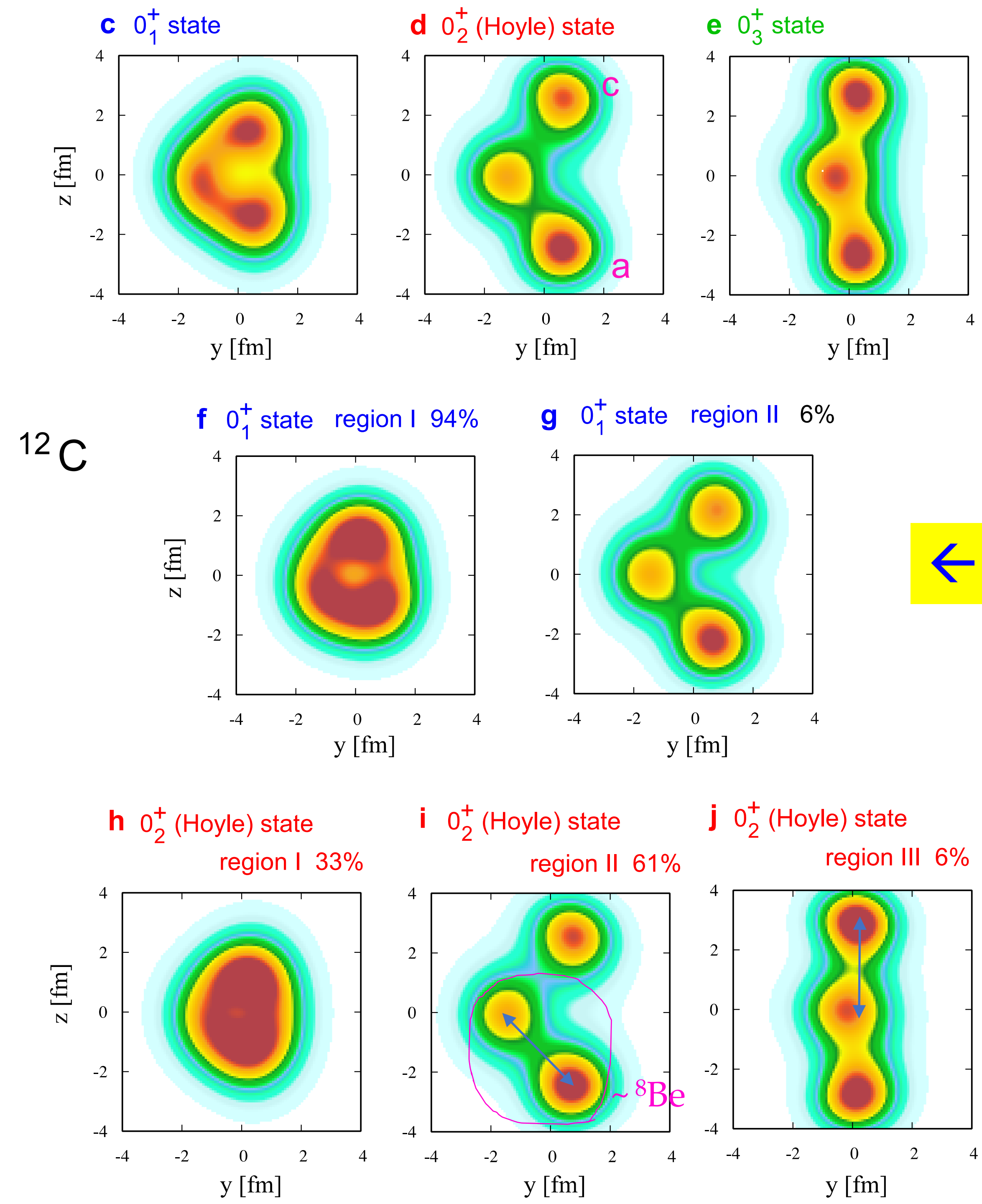
Total and decomposed nucleon-densities in body-fixed frame

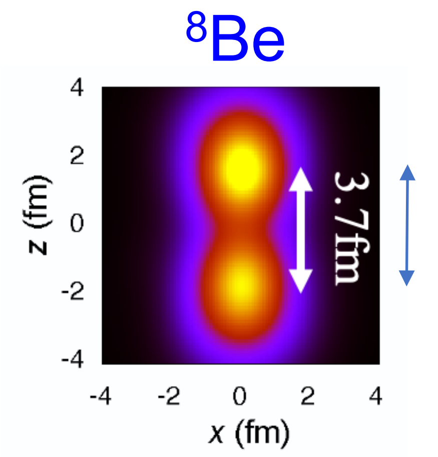
with proper orthogonalization



2-dimensional presentation



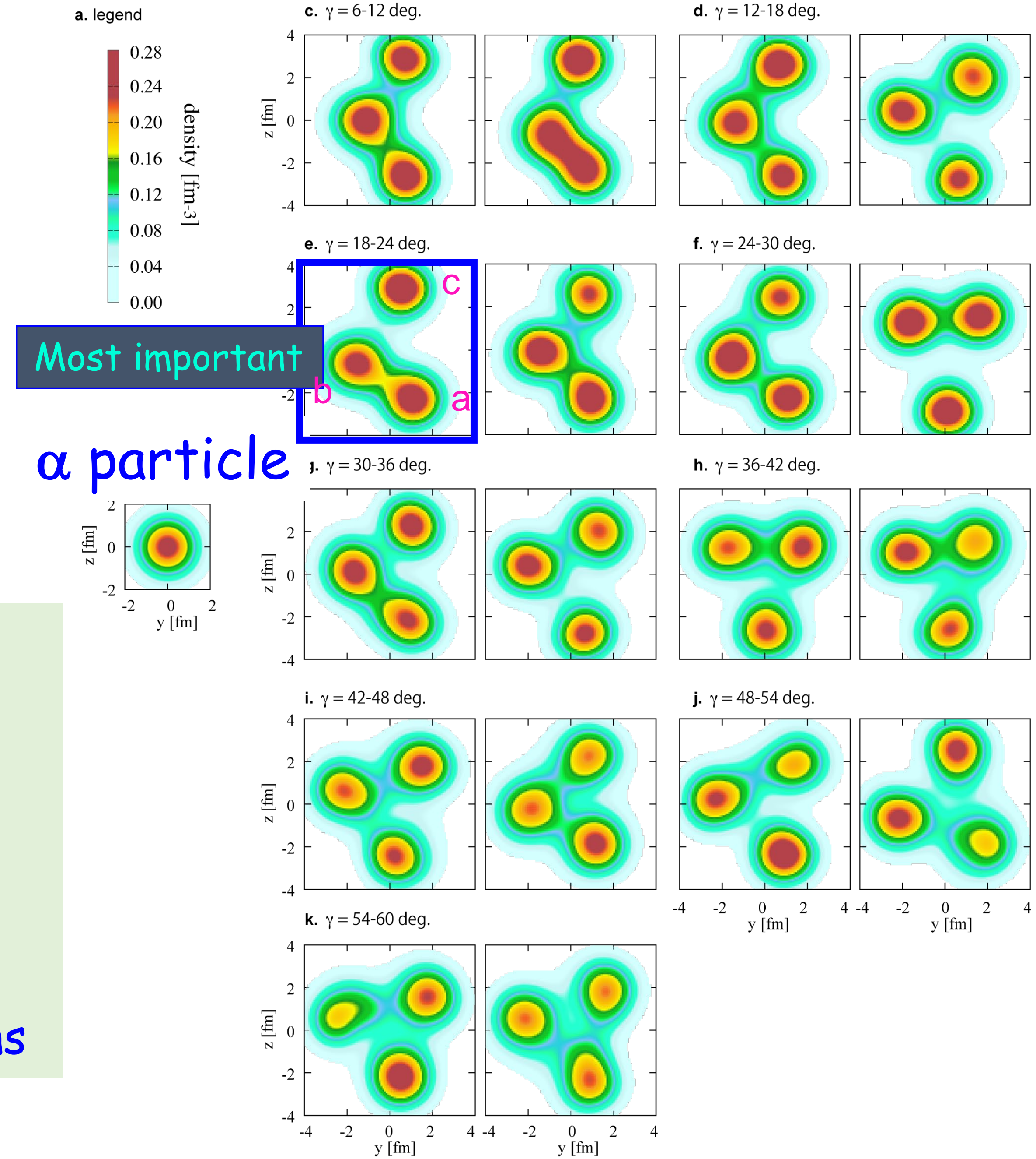




← ground state

← Hoyle state

density profiles of major MCSM basis vectors (Slater determinants) in region II for the Hoyle state.



Triangle configurations with three α clusters are favored by nuclear forces

Fluctuations emerge within such configurations

A completely different analysis (no physics, data science)

classification of MCSM basis vectors by the cluster analysis of through unsupervised statistical learning

distance : $D(i,j) = 1 - |(\phi_i, \phi_j)|^2$ for basis vectors ϕ_i and ϕ_j

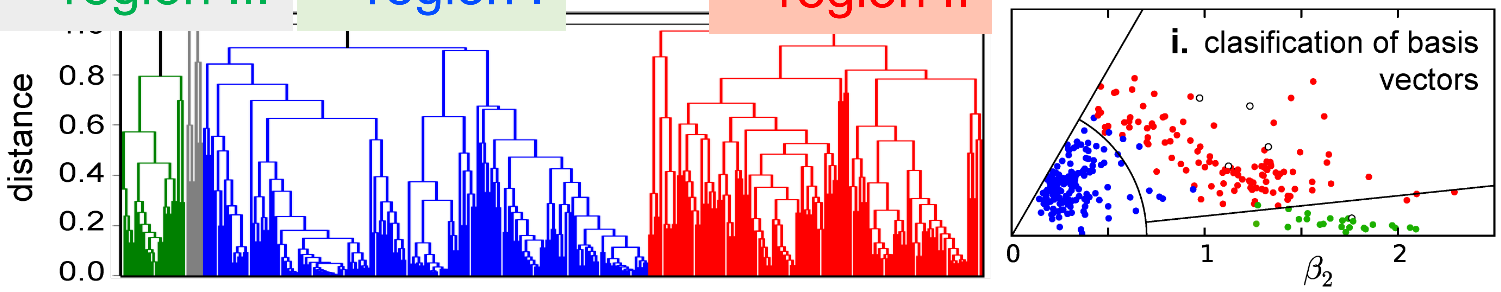
where parenthesis means a scalar product (overlap integral) with the $J^\pi = 0^+$ projection

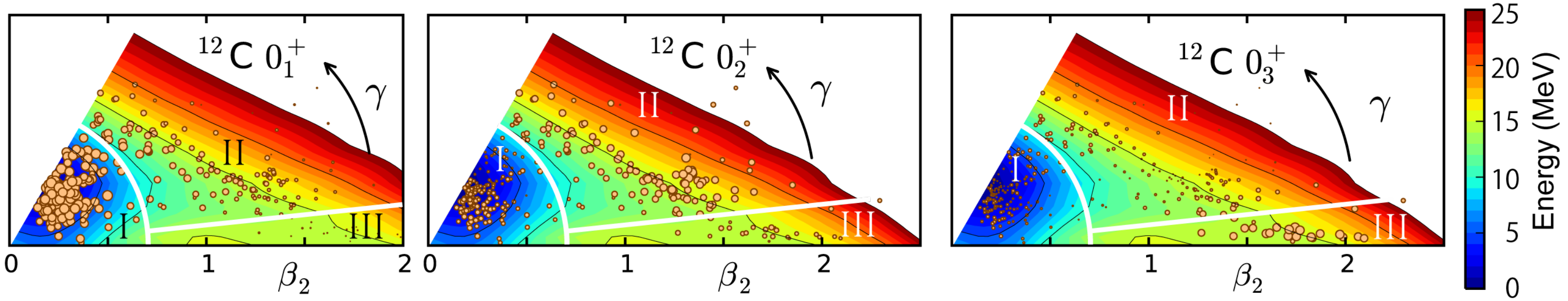
connect basis vectors from the shortest distance to longer up to the threshold

➔ leads to almost the same decomposition scheme (the heart of the present picture)

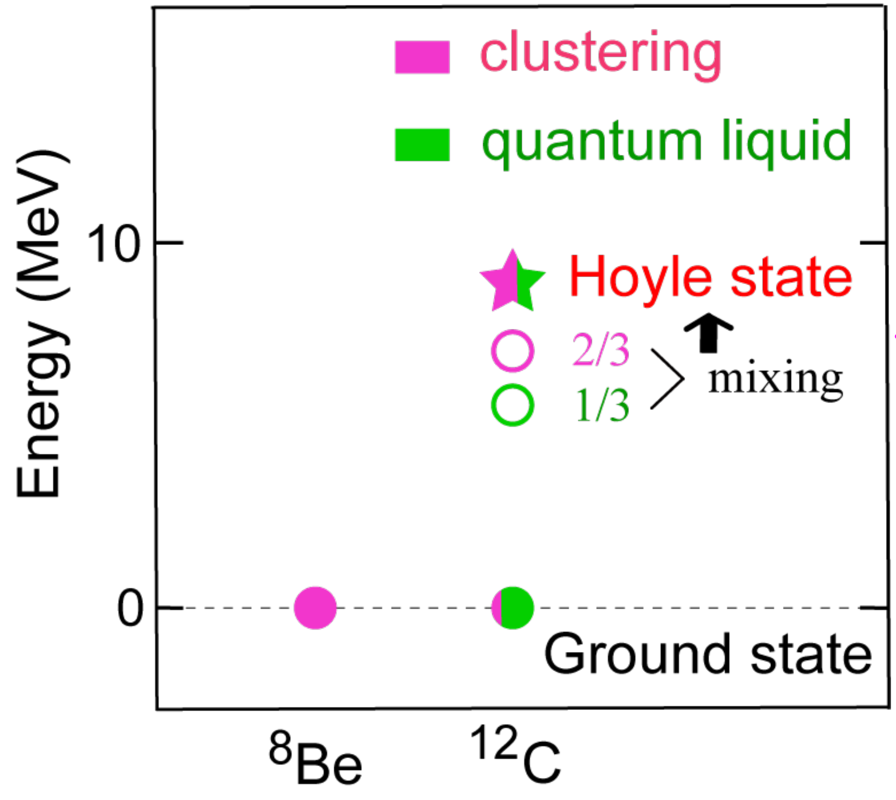
~region III ~region I ~region II

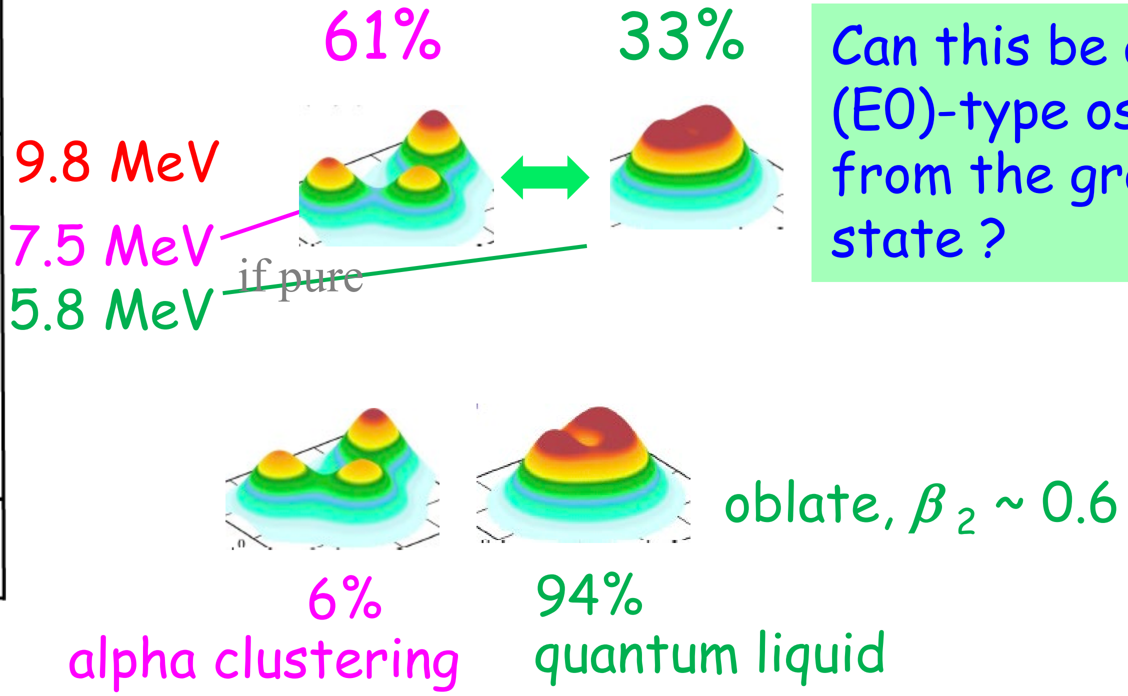
h. Dendrogram for ^{12}C (cluster analysis through unsupervised statistical learning)





Transition from ^{8}Be to ^{12}C, and the crossover in the ground & Hoyle states of ^{12}C





Can this be a radial (E0)-type oscillation from the ground state ?

Ground state :

the mixing matrix element is ~ -3 MeV (attractive effect) with 6% (ampl. ~ 0.24) alpha clustering.

→alpha decay, alpha knockout

Hoyle state

The mixing occurs also due to the orthogonality to the ground state.

The mixing pushes the Hoyle state upwards by ~3 MeV (repulsive effect).

Point-proton radius of the ground state

TABLE II: Computed point-proton radii of light nuclei with JISP16 and Daejeon16 NN interactions in comparison with results extracted from experiments [78]. Note that, in the case

Nuclide	$\hbar\omega$ (MeV)	$\sqrt{\langle \hat{r}^2 \rangle_{pp}}$ (fm) MCSM $N_{shell} = 7$	$N_{shell} \to \infty$	Expt.
		Daejeon16		
^{4}He	20	1.511	1.510(2)	1.467
^{8}Be	10	2.619	2.59(3)	2.519 (^{7}Be) 2.385 (^{9}Be)
^{12}C	15	2.292	2.31(3)	2.334
^{16}O	15	2.381	2.40(2)	2.575
^{20}Ne	15	2.572	2.59(3)	2.931

Matter radius of the Hoyle state

0.36 fm larger than the ground-state value

diff. ~ 0.5 fm in experiment by the Ogloblin group

diff. = 1.1 ~ 1.9 fm in other theories

Danilov, A. N., Belyaeva, T. L., Demyanova, A. S., Goncharov, S. A. & A Ogloblin, A. Determination of nuclear radii for unstable states in ^{12}C with diffraction inelastic scattering. *Phys. Rev. C.* **80**, 054603 (2009).

PHYSICAL REVIEW C **104**, 054315 (2021)

Abe *et al.*, systematic calculations of ground-state properties

Ground-state properties of light 4*n* self-conjugate nuclei in *ab initio* no-core Monte Carlo shell model calculations with nonlocal *NN* interactions

T. Abe,[1,2] P. Maris,[3] T. Otsuka,[4,1,5] N. Shimizu,[2] Y. Utsuno,[5,2] and J. P. Vary[3]
[1]*RIKEN Nishina Center, Wako, Saitama 351-0198, Japan*
[2]*Center for Nuclear Study, the University of Tokyo, Hongo, Tokyo 113-0033, Japan*
[3]*Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA*
[4]*Department of Physics, the University of Tokyo, Hongo, Tokyo 113-0033, Japan*
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Summary

α clustering from first principles without any assumption for ^{8,10,12}Be and ^{12}C

Perfect *ab initio* realization of the oblate rotational band in ^{12}C (energy & E2)

Hoyle state shows a novel structure: superposition of quantum liquid and tri-α clusters

It might be interpreted as an "radial" oscillation between compact and cluster structures ?
Some analogue in molecular (trimer) structure ?

Nuclear forces favor both quantum liquid and α clustering, with more binding for the former.
The transition between them is not a phase transition but a crossover involving mixing.

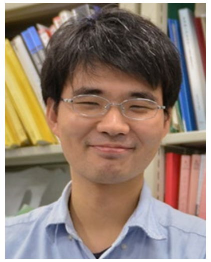
α cluster emerges even in the well-bound ground state, *α decay, α knockout, etc.*

"Threshold" is not needed. Soft interactions may not suffice to reproduce this feature.

nature COMMUNICATIONS 13, 2234 (2022) *open access*

α-Clustering in atomic nuclei from first principles with statistical learning and the Hoyle state character

T. Otsuka[1,2,3], T. Abe[2,4], T. Yoshida[4,5], Y. Tsunoda[4], N. Shimizu[4], N. Itagaki[6], Y. Utsuno[3,4], J. Vary[7], P. Maris[7] & H. Ueno[2]



Collaborators

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Tooru Yoshida (RIST, CNS, U. Tokyo)

Yusuke Tsunoda (CNS, U. Tokyo→Tsukuba)

N. Shimizu (CNS, U. Tokyo→Tsukuba)

N. Itagaki (Kyoto→Osaka Metropolitan)

Y. Utsuno (JAERI)

H. Ueno (RIKEN)

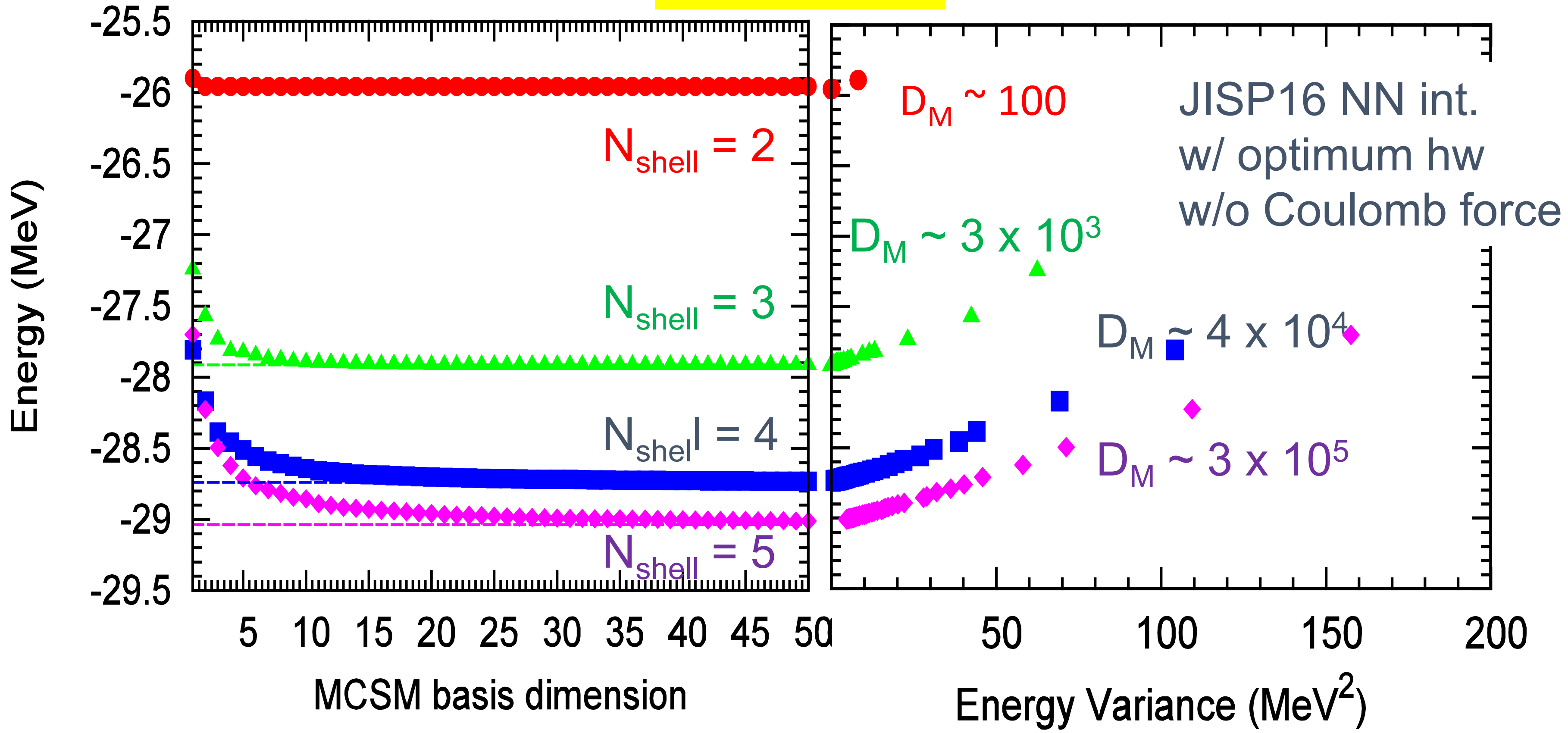
James Vary (Iowa State U.)

Pieter Maris (Iowa State U.)

END

Thank you for your attention

^{4}He(0$^+$;gs)



Extrapolation by the variance

$$\langle \Delta H^2 \rangle = \langle H^2 \rangle - \langle H \rangle^2$$

$$\langle H \rangle = E_0 + E_1 \langle \Delta H^2 \rangle + E_2 \langle \Delta H^2 \rangle^2 + \cdots$$

N. Shimizu *et al.*, Phys. Rev. C82, 061305 (2010)

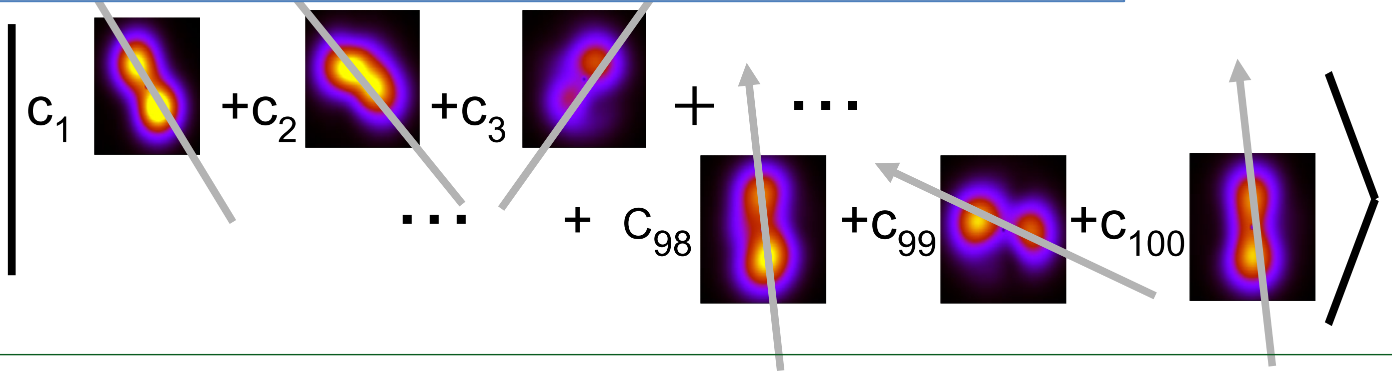
based on T. Mizusaki & M. Imada, Phys. Rev. C65, 064319 (2002)

MCSM eigenstate : $\left|\Psi(D)\right\rangle = \sum_{n=1}^{N_B} c_i P^{J,\Pi} \boxed{\left|\phi(D^{(n)})\right\rangle}$

Deformed Slater determinant with three axes of ellipsoid

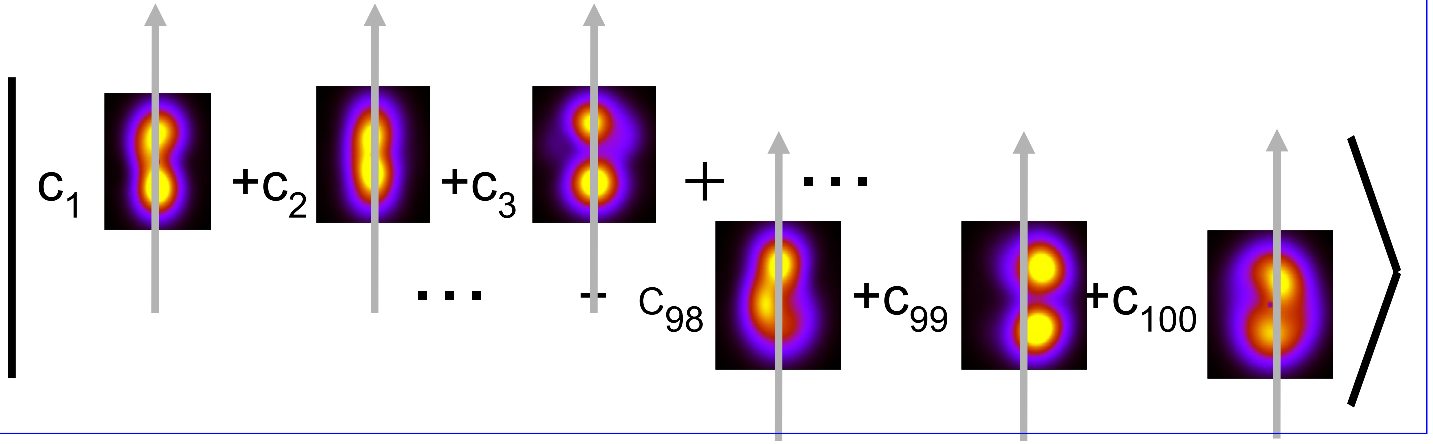
For J^π projected states, individual orientations are not relevant.

$\left|\Psi_{B.A.}(D)\right\rangle =$

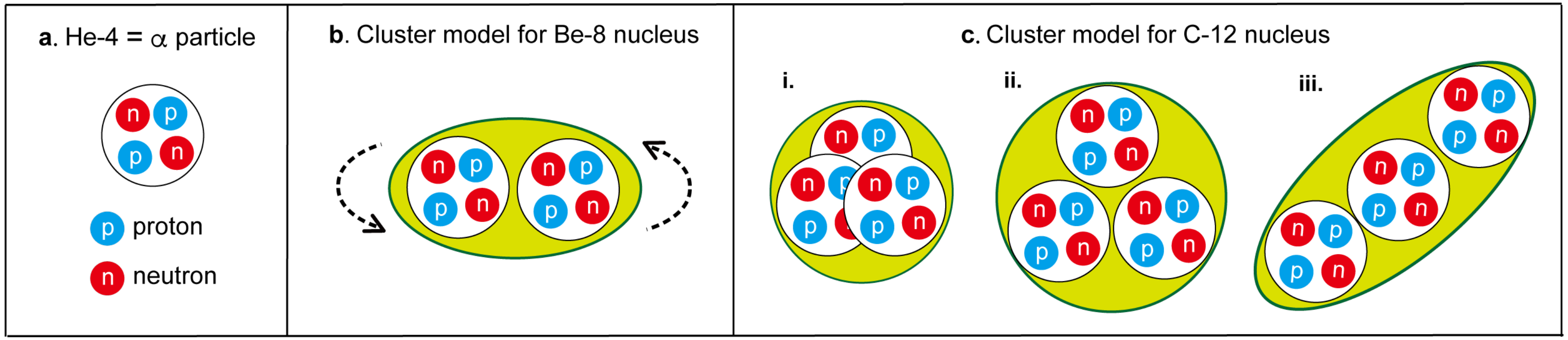


For "intrinsic state", all basis states are aligned so that three axes of the ellipsoid are placed on the given directions, e.g. the longest one on the z axis.

$\left|\Psi_{\mathbf{intr.}}(D)\right\rangle =$



α cluster formation - intuitive image -



Pioneers (before 1960)

bond coupling

Wefelmeier, W. Von, Ein geometrisches Modell des Atomkerns. Z. Phys. Hadrons Nucl. 107, 332 (1937).
Wheeler J. A., Molecular Viewpoints in Nuclear Structure, Phys. Rev. **52**, 1083 (1937).
Morinaga, H., Interpretation of some of the excited states of 4n self-conjugate nuclei, Phys. Rev. C **101**, 254 (1956).

linear formation

Brink, D., Alpha-Particle Model of Light Nuclei. The Proc. Intl. School of Physics Enrico Fermi, Course, 36 (1966), p. 247.
Ikeda, K., Takigawa, N. and Horiuchi, H., The systematic structure-change into the molecule-like structures in the self-conjugate 4n nuclei. Prog. Thoer. Phys. Suppl., **E68**, 464 (1968).
Arima, A., Horiuchi, H., Kubodera, K. and Takigawa, N., Clustering in Light Nuclei, in *Advances in Nuclear Physics*, ed. by Baranger M. and Vogt E., (Springer, Boston, MA., 1973), **5**, 345.
Freer, M., Horiuchi, H., Kanada-En'yo, Y., Lee, D. and Meißner, U.-G., Microscopic clustering in light nuclei. Rev. Mod. Phys. **90**, 035004 (2018).

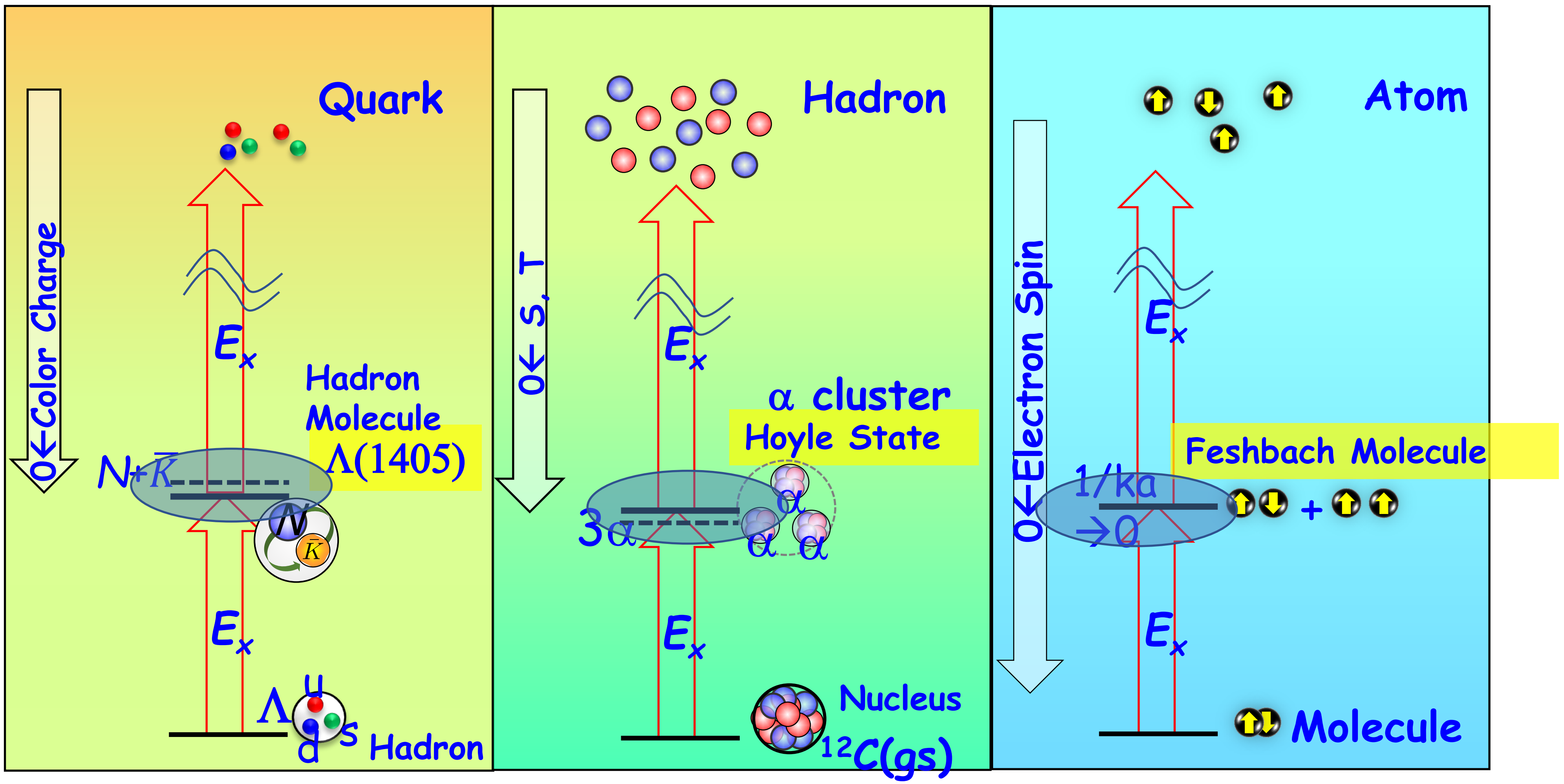
The snapshot state in the body-fixed frame is needed,
as this snapshot state gives the snapshot of density profile.

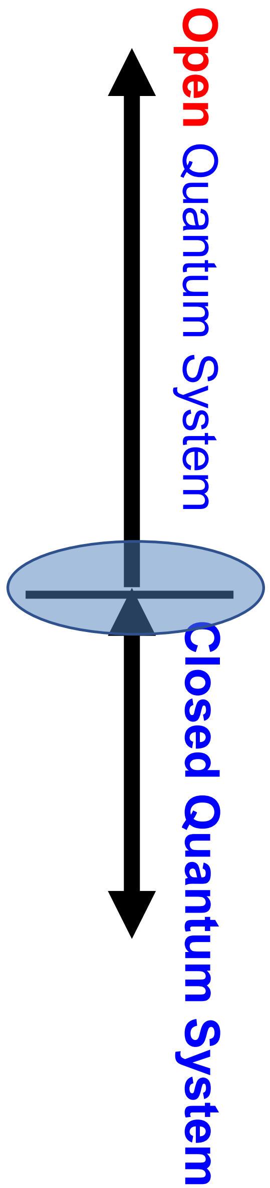
(*The snapshot state is nothing but the intrinsic state in most literatures.*)

(The corresponding states in the lab. frame are obtained by rotating it.)

It is difficult (or impossible) to observe it experimentally.

Semi-Hierarchy: Clustering and Hierarchy of Matter





- ✓ Threshold: **Clustering near Threshold → Semi-Hierarchy**
- ✓ Degree of Freedom : **Neutralization of Charge, Spin(S), Isospin(T)**

T-plot : visualization of MCSM eigenvector on Potential Energy Surface

eigenstate $\Psi = \sum_i c_i P[J^\pi] \Phi_i$

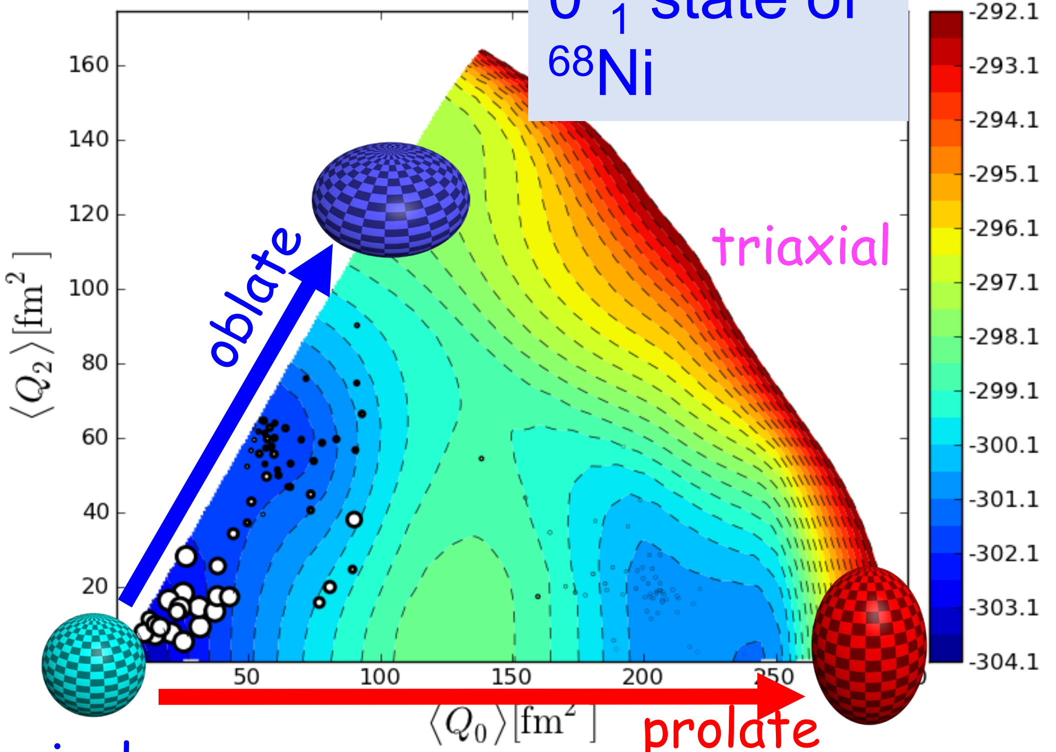
stochastically deformed Slater determinant
→ intrinsic shape

amplitude

projection onto J^π

- PES is calculated by CHF for the shell-model Hamiltonian
- Location of circle : quadrupole deformation of unprojected MCSM basis vectors
- Area of circle : overlap probability between each projected basis and eigen wave function

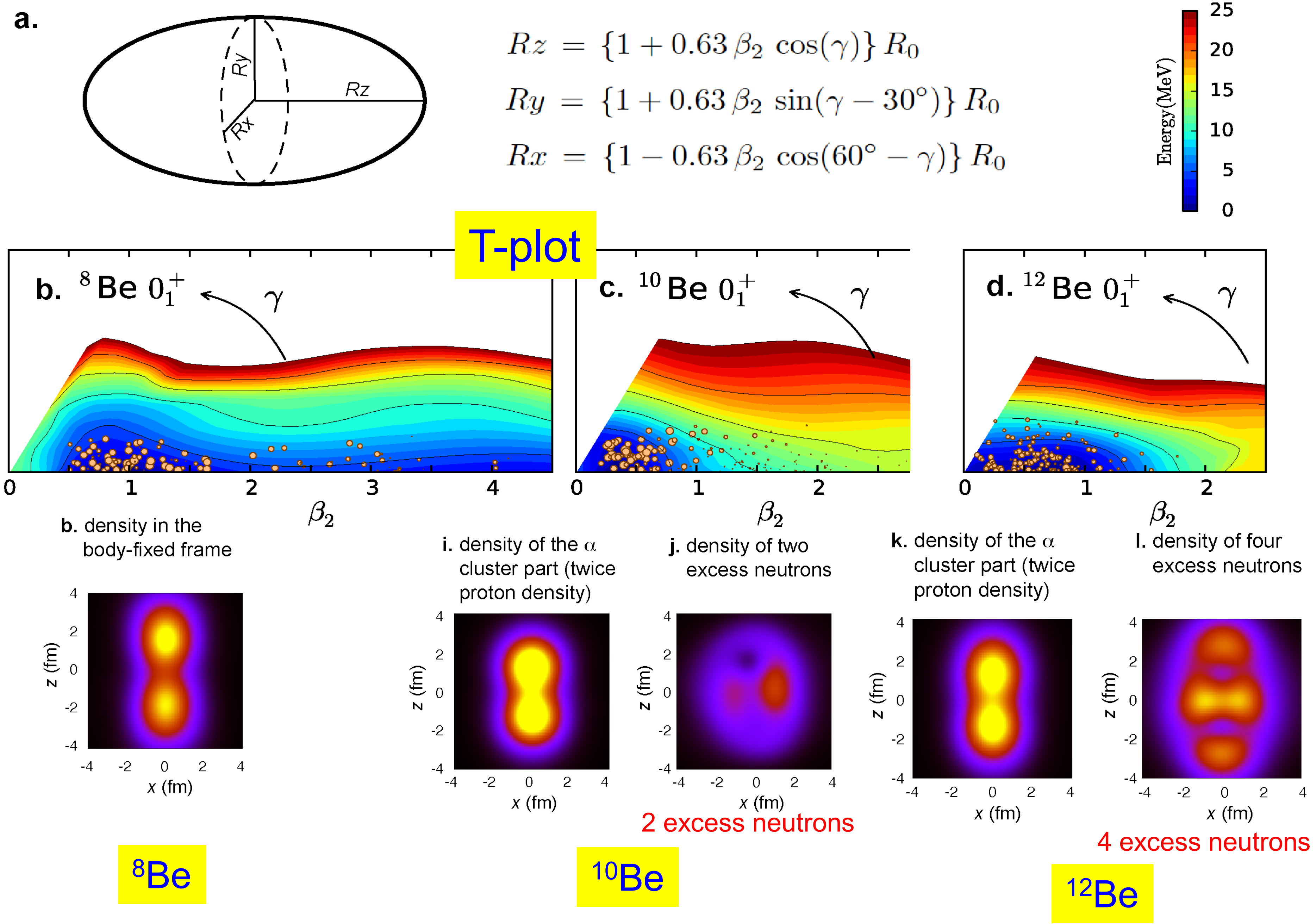
0^+_1 state of ^{68}Ni



Y. Tsunoda, *et al.*
PRC 89, 031301 (R) (2014)

Y. Tsunoda

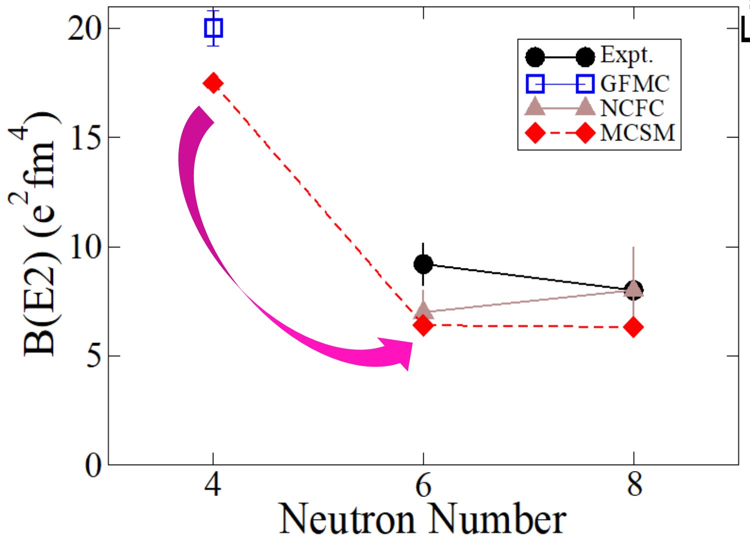
T-plot analysis of 0+ states applied to Be isotopes

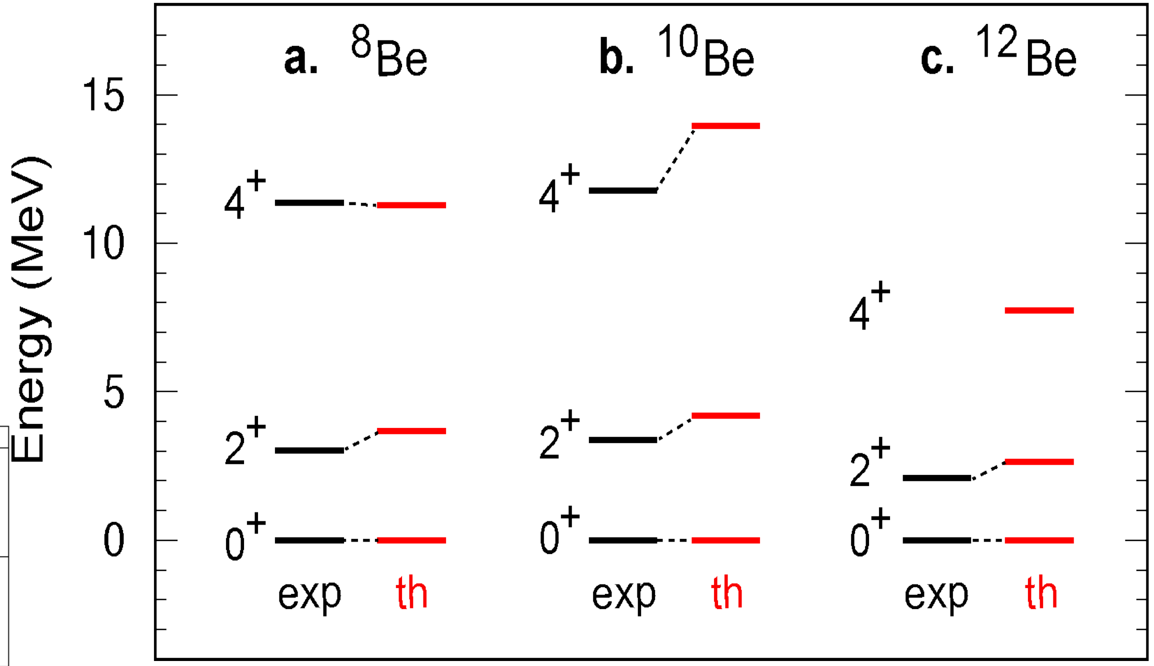


Levels and B(E2)'s of Be isotopes

calculated with
hw=15MeV, Nshell=6
With JISP16 interaction

B(E2) Exp:
^{8}Be Datar *et al.* 2013 + estimate
by GFMC
^{10}Be McCutchan *et al.* 2009
^{12}Be Imai *et al.* 2009





excitation level patterns indicate the occurance of the rotational motion of a deformed "object"

→ nucleus seen in the body-fixed (intrinsic) frame