Workshop on Multineutron Clusters in Nuclei and in Stars
ICTP-SAIFR
São Paulo, Brazil
June 4 (2-6), 2025

Emerging cluster and molecular structures of exotic Be isotopes in the ab initio no-core MCSM

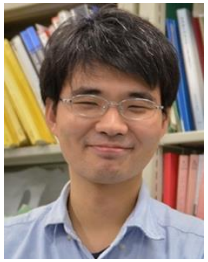
Takaharu Otsuka

Supported by "Program for promoting research on the supercomputer Fugaku", MEXT, Japan (JPMXP1020230411)

1. No-core *ab initio* Monte Carlo Shell Model

2. C isotopes brief reminder

3. Be isotopes - clusters + excess neutrons -

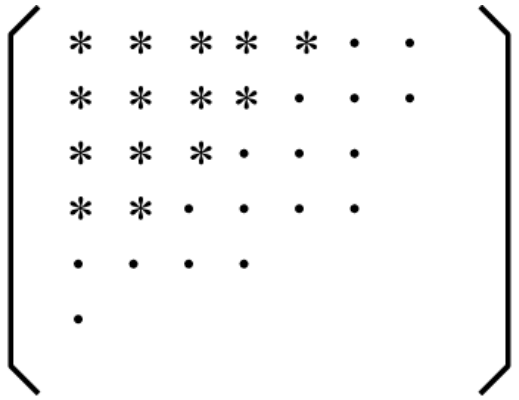


Collaborators

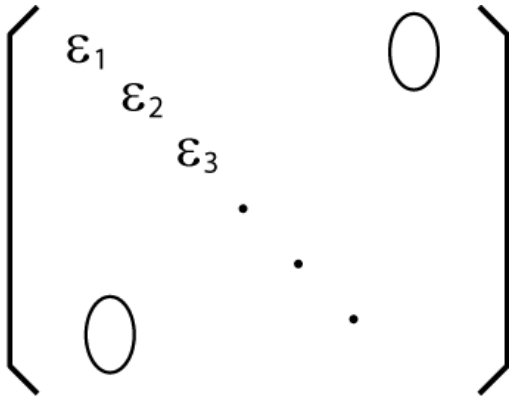
Toru Yoshida (RIST)
Takashi Abe (Keio U.)
Yusuke Tsunoda and N. Shimizu (U. Tsukuba)
N. Itagaki (Osaka Metropolitan U.),
Y. Utsuno (JAERI), H. Ueno (RIKEN)
James Vary & Pieter Maris (Iowa State U.)

Two types of shell-model calculations

dim. <~ 10^{10}

$H =$ 

diagonalization

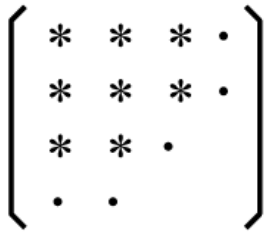


Conventional Shell Model

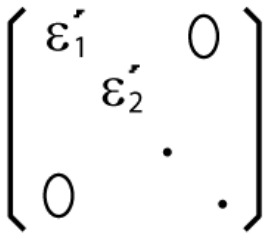
all Slater determinants

Direct diagonalization

For bigger problems

$H \approx$ 

diagonalization



~100 dim.

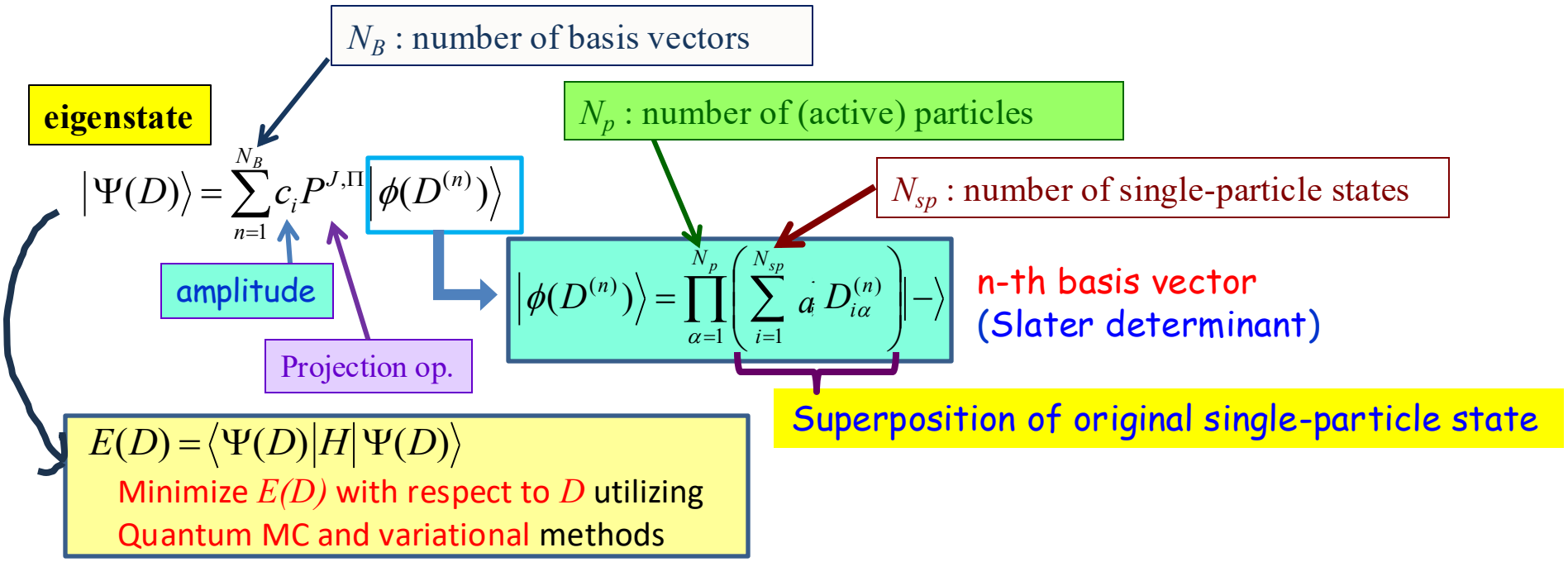
Monte Carlo Shell Model

bases important for a specific eigenstate

Selected

important basis vectors

Basic formulation of Monte Carlo Shell Model



Step 1 : Shift randomly matrix matrix D. (The initial guess can be taken from Hartree-Fock.)
Select the one producing the lowest $E(D)$ (rate < 0.1 %)

Step 2 : Polish D by means of the conjugate gradient (CG) method variationally.

More steps : Repeat steps 1 & 2 for additional basis vectors.

Eur. Phys. J. A (2025) 61:82
https://doi.org/10.1140/epja/s10050-025-01545-1

THE EUROPEAN PHYSICAL JOURNAL A

Review

History of the concept of nuclear shape

David Verney[a]

Université Paris-Saclay, CNRS/IN2P3, IJCLab, 91405 Orsay, France

"If I had a great calculating machine, I would perhaps apply it to the Schrödinger equation of each metal and obtain its cohesive energy, its lattice constant, etc. It is not clear, however, that I would gain a great deal by this. Presumably, all the results would agree with the experimental values and not much would be learned from the calculation. What would be preferable, instead, would be a vivid picture of the behavior of the wave function"

E. P. Wigner quoted by E. Guth at the Conference on Bases for Nuclear Spin-Parity Assignments,
Gatlinburg, Tennesse (1965) [1]

T-plot of
Monte Carlo Shell Model

direct visualization of fully correlated wave functions

Use β_2 and γ as partial labelling of many-body basis vectors

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

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

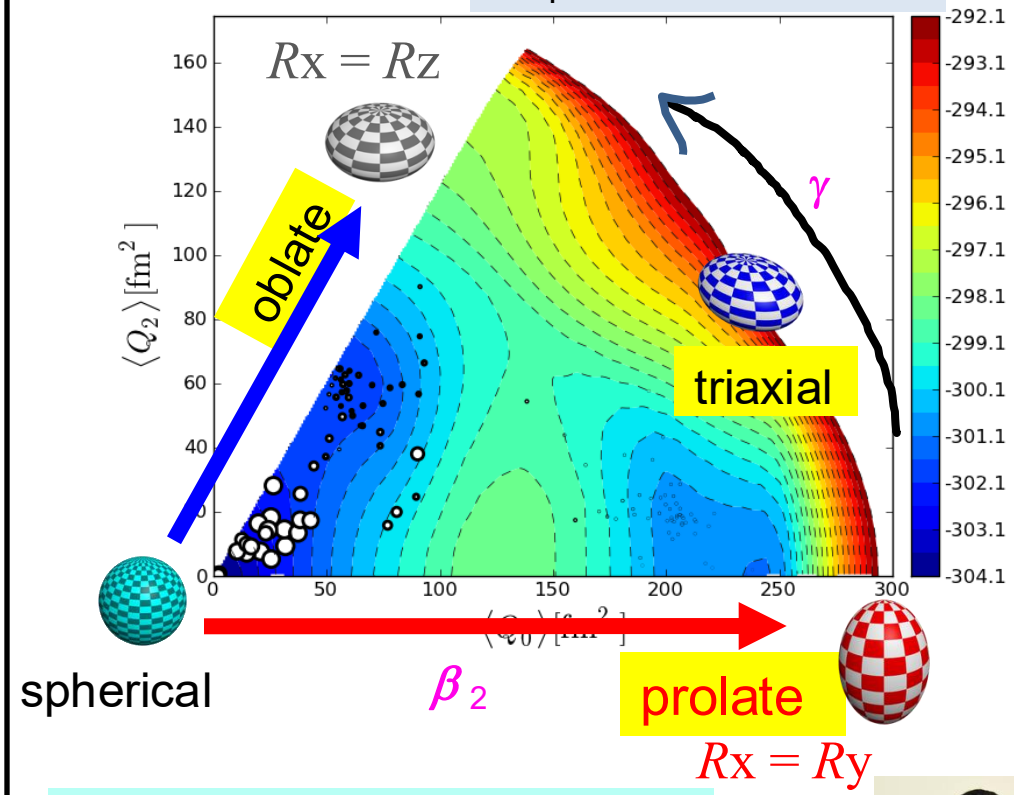
stochastically deformed Slater determinant
→ intrinsic shape

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)

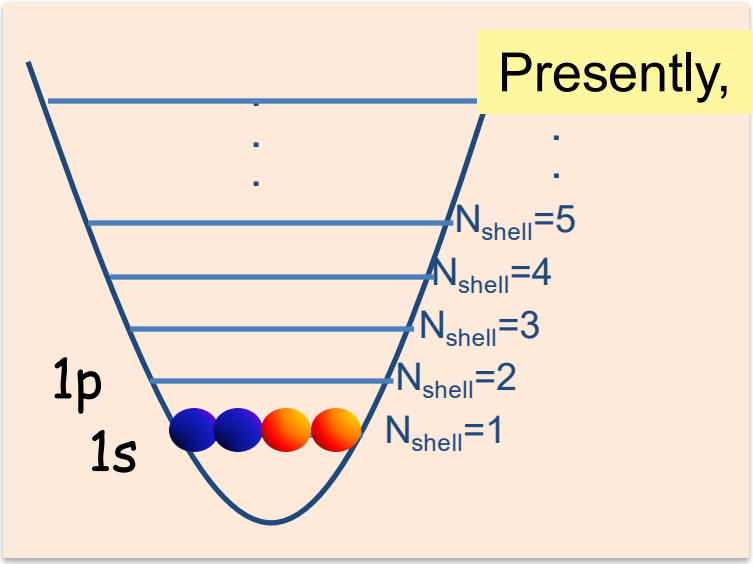
ab initio No-Core Monte Carlo Shell Model

(MCSM)

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, up to Nshell =7 (6 hw)

Solve the Schrödinger 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).

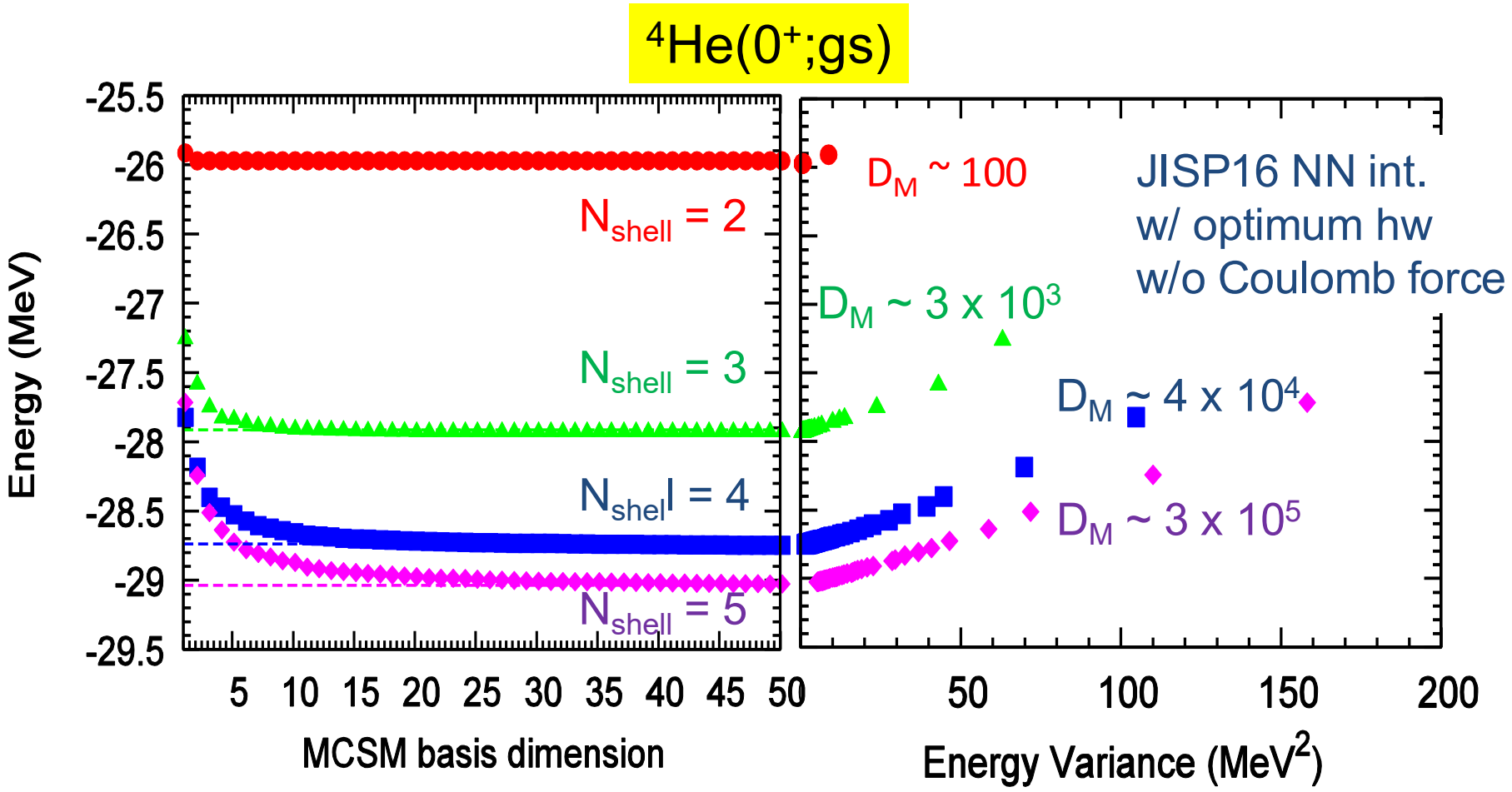
Daejeon in Korea

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.



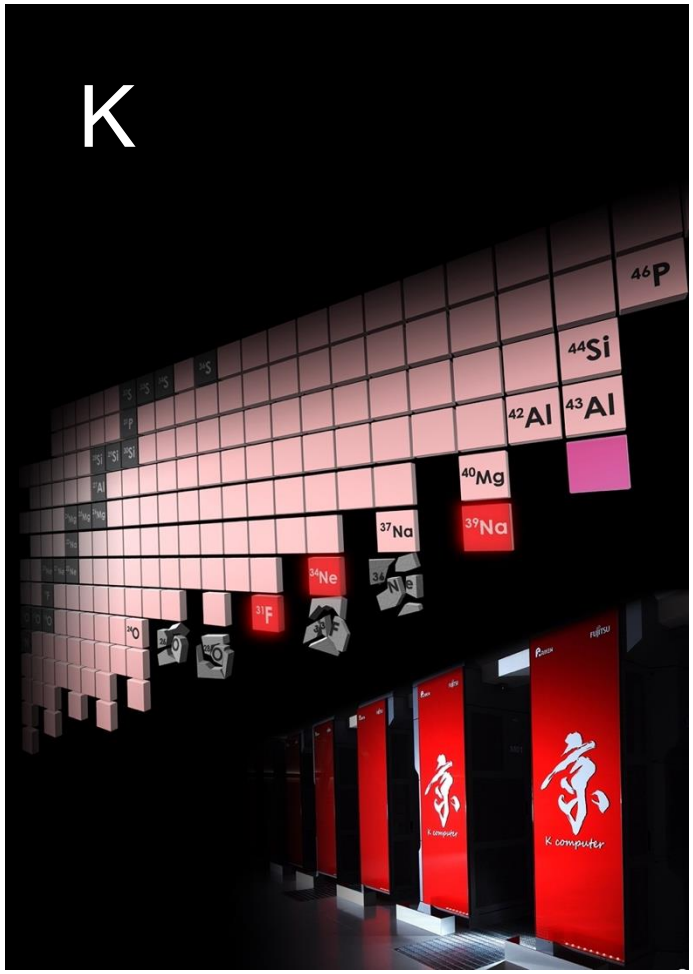
Extrapolation by the energy variance $\langle \Delta H^2 \rangle = \langle H^2 \rangle - \langle H \rangle^2$

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

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

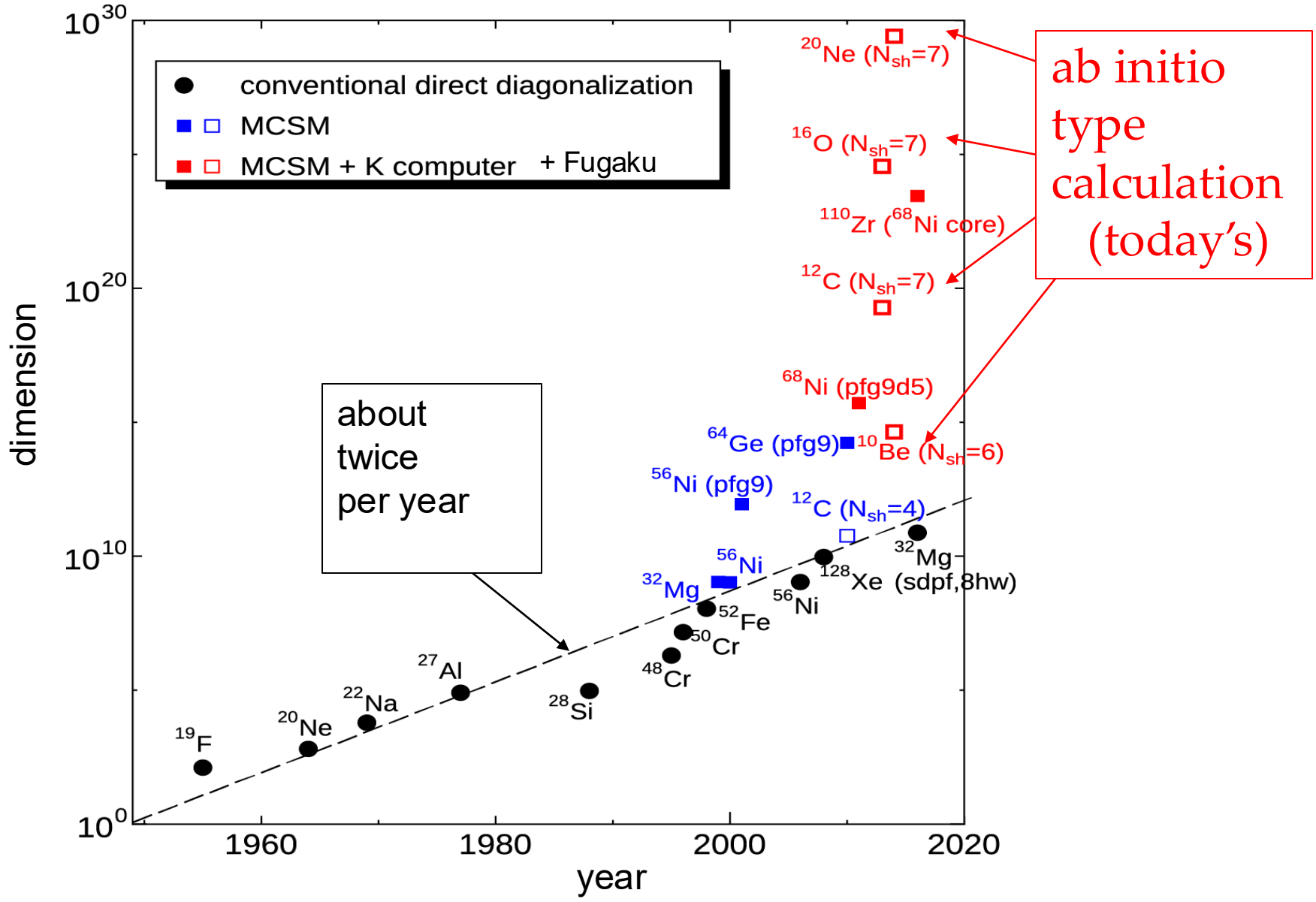
based on T. Mizusaki & M. Imada, Phys. Rev. C65, 064319 (2002)

Supercomputers contributing to this study



写真下部:理化学研究所提供

Dimension of the shell-model many-body Hilbert space (ab initio)



A paper dedicated to *ab initio* no-core Monte Carlo Shell Model calculation

on 4n self-conjugate nuclei (e.g., ^{4}He, ^{8}Be, ^{12}C, ^{16}O, etc.)

Not exactly this work

PHYSICAL REVIEW C **00**, 004300 (2021)

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] N. Shimizu,[2] Y. Utsuno,[5] 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*

[5]*Advanced Science Research Center, Japan Atomic Energy Agency, Tokai, Ibaraki 319-1195, Japan*

(Received 29 June 2021; accepted 5 October 2021; published xxxxxxxxxx)

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nature COMMUNICATIONS

NATURE COMMUNICATIONS | (2022) 13:2234 |
https://doi.org/10.1038/s41467-022-29582-0 |

ARTICLE

https://doi.org/10.1038/s41467-022-29582-0 OPEN

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

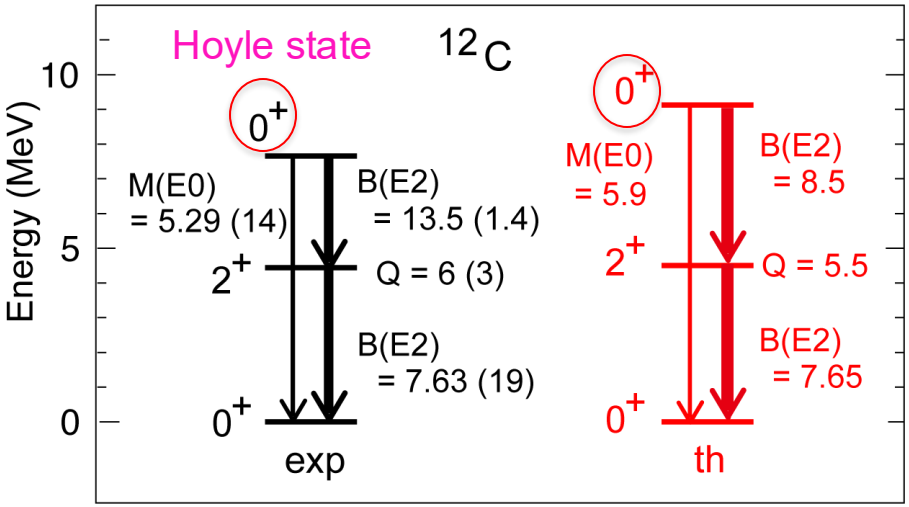
T. Otsuka[1,2,3✉], T. Abe[2,4], T. Yoshida[4,5], Y. Tsunoda[4], N. Shimizu[4], N. Itagaki[6], Y. Utsuno[3,4], J. Vary[7], P. Maris[7] & H. Ueno[2]

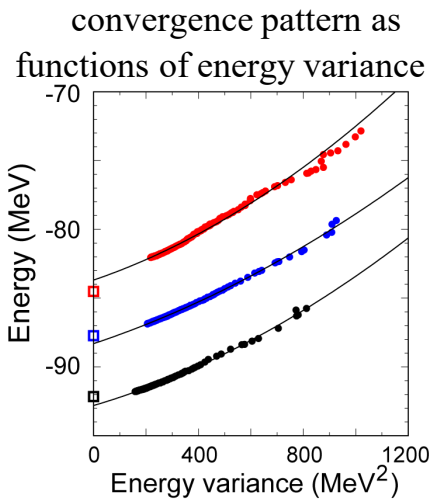
Energy level & transition strength of ^{12}C

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)



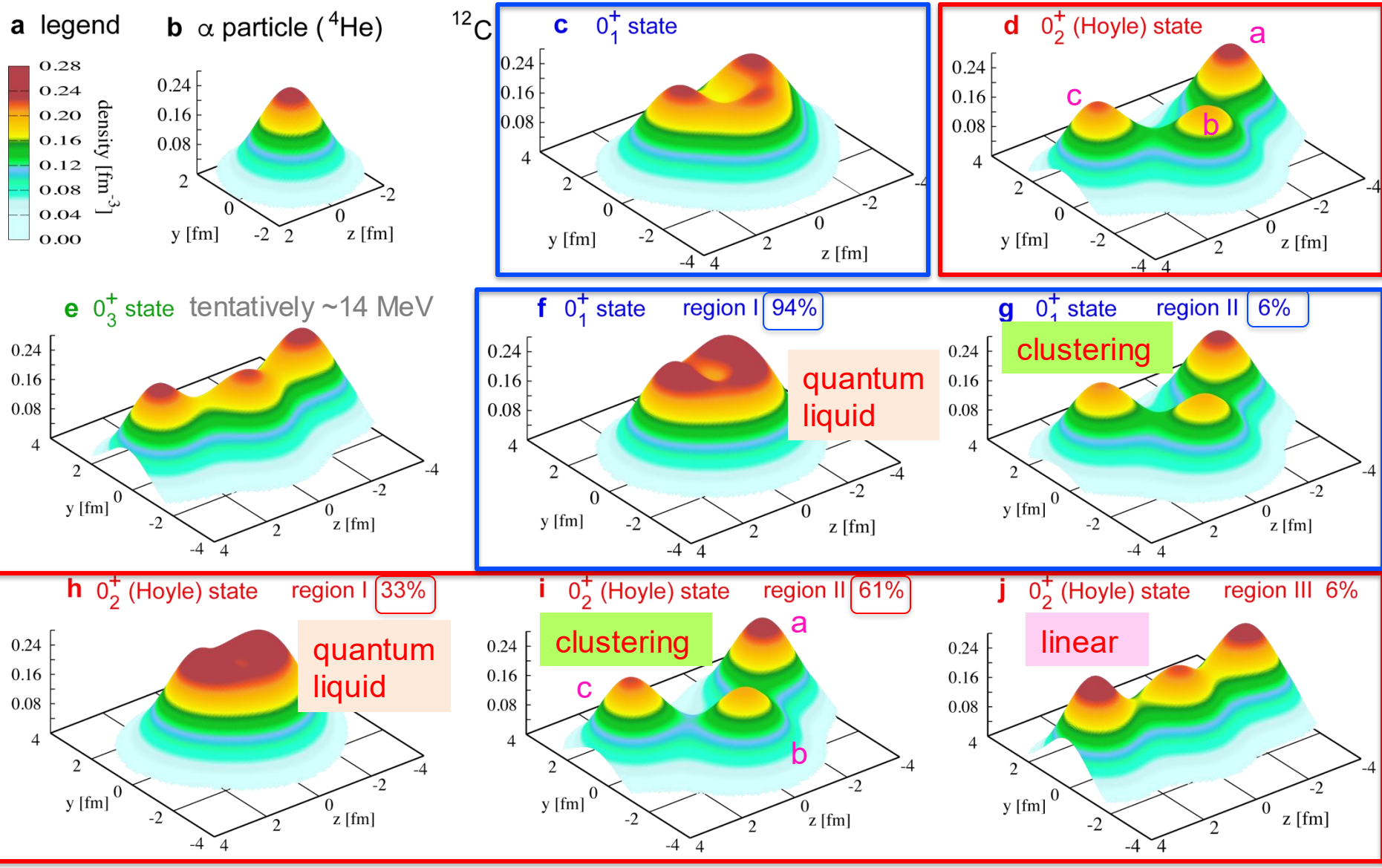


Strong deformation (β_2~0.6, oblate) in the 0^+_1 and 2^+_1 states can now be described from *first principles*.

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

Nucleon densities in the body-fixed frame

after proper orthogonalization



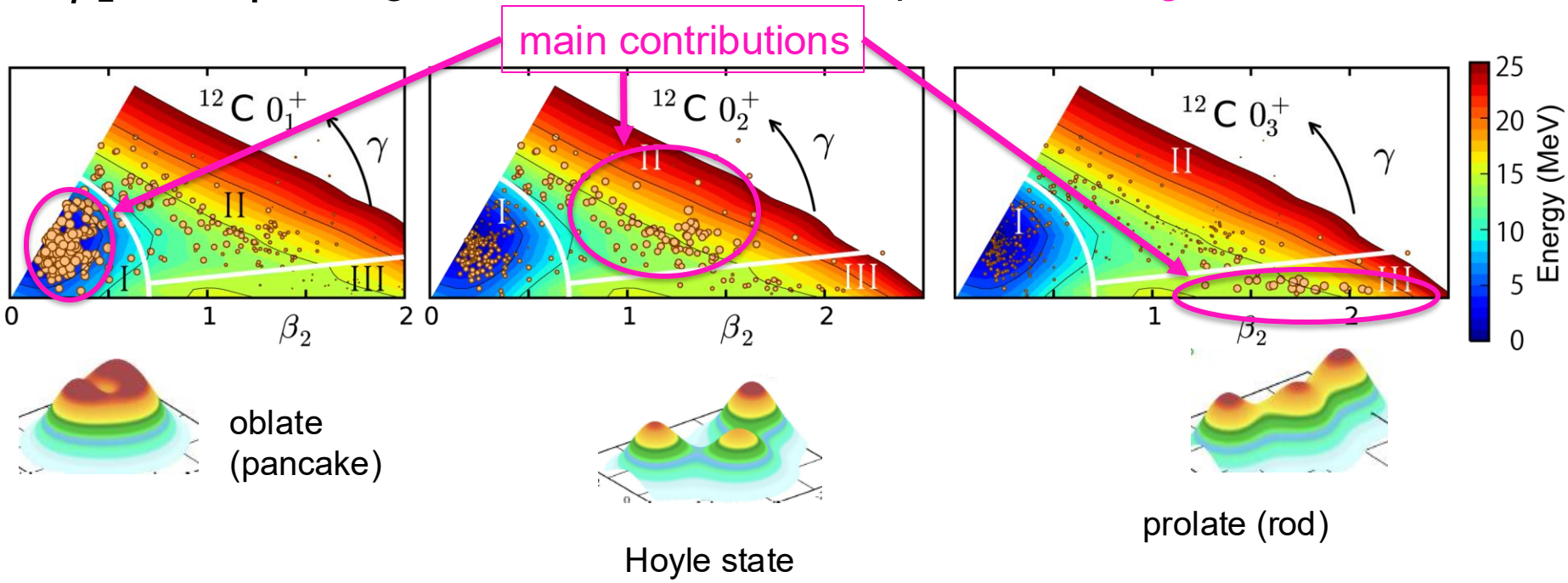
^{12}C : Basis vectors classified by quadrupole shapes (T plot)

T plot circles are spread in the case of ^{12}C. A characteristic feature.

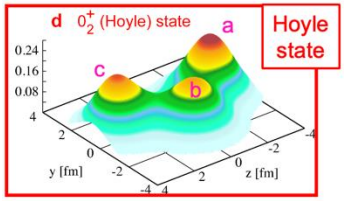
Completely different structures appear at low excitation energies … quite unique

PES is divided into three
- I $\beta_2 < 0.7$, oblate basin in the PES
- II triaxial（clusters come here）
- III near prolate

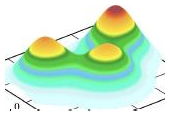
β_2=0.7, γ=6 deg ➔ basis vectors decomposed into regions I, II and III



Mixing and the clustering in the ground state



components of the ground state

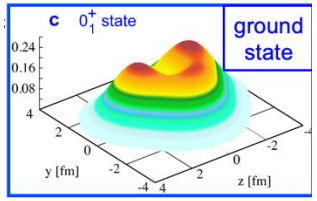


energy

components of the Hoyle state

expanding

Hoyle state



mixing

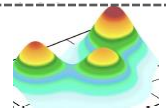
6%

94%

2.9 MeV

-80.4 MeV

cluster



1.5 MeV

-81.9 MeV

3.5 MeV

-84.2 MeV

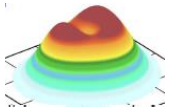
61%

33%

Ground state

0.8 MeV

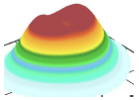
-91.8 MeV



-91.0 MeV

liquid (~uniform density)

-86.0 MeV



compact (closer to sphere)

mixing (repulsive effect) & rearrangement

Two modes of the localization due to the force can talk, and can be mixed.

The Hoyle state can be at a lower excitation energy (< 7 MeV), if there were no mixing.

1. No-core *ab initio* Monte Carlo Shell Model

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Be isotopes were discussed a lot besides ^{12}C.

nature COMMUNICATIONS

NATURE COMMUNICATIONS | (2022) 13:2234 |
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ARTICLE

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Check for updates

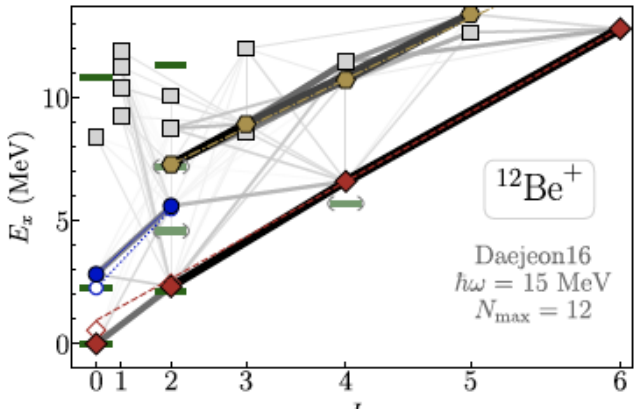
α-Clustering in atomic nuclei from first principles with statistical learning and the Hoyle state character

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]

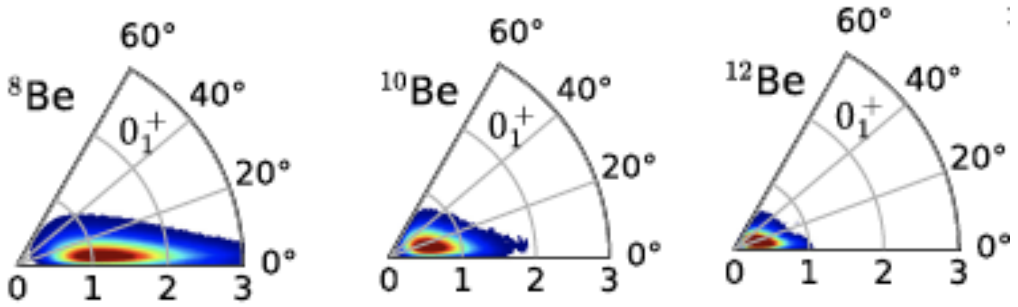
Many works in the past

- Ab initio approaches are rather recent

^{12}Be: McCoy et al., Phys. Lett. B 856, 138870 (2024)



$^{7\text{-}12}$Be: Shen et al., Phys. Rev. Lett. 134, 162503 (2025)



Other conventional works represented, for example, by

Cluster model:

P. Descouvemont, “Microscopic study of α clustering in the 9, 10,11Be isotopes” Nucl. Phys. A, 699 (2002), pp. 463-478,

Molecular Orbital model:

N. Itagaki, S. Okabe, “Molecular orbital structures in 10Be”, Phys. Rev. C, 61 (4) (2000), 044306.

M. Ito, N. Itagaki, H. Sakurai, and K. Ikeda. “Coexistence of Covalent Superdeformation and Molecular Resonances in an Unbound Region of 12Be”, Phys. Rev. Lett. 100, 2008

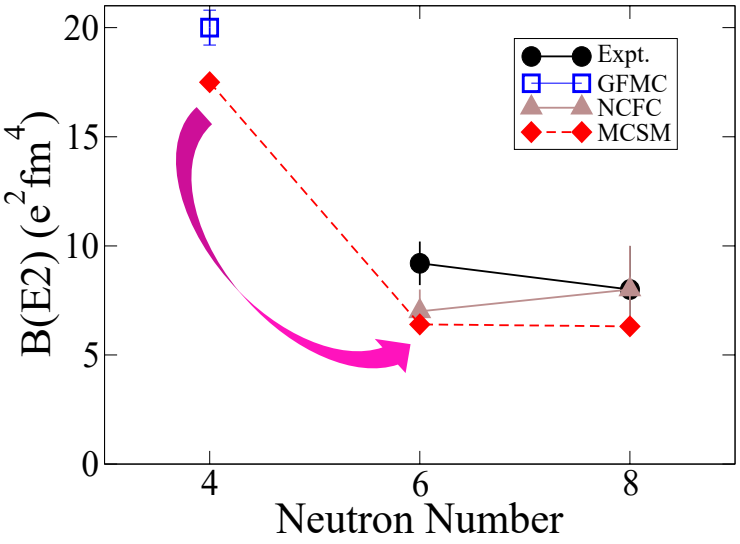
AMD:

Yoshiko Kanada-En'yo , Masaaki Kimura , Akira Ono, “Antisymmetrized molecular dynamics and its applications to cluster phenomena”, Progress of Theoretical and Experimental Physics, Volume 2012, Issue 1, 2012, 01A202,

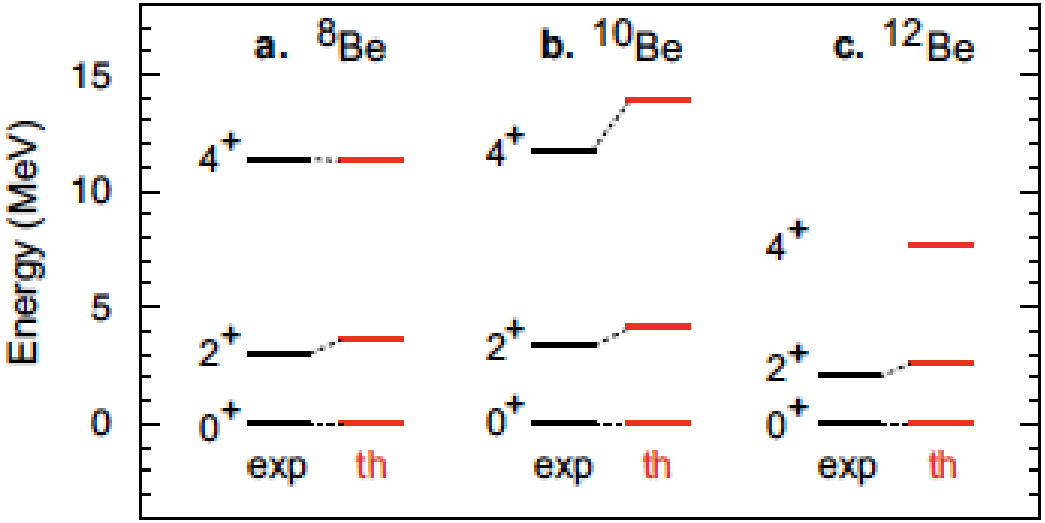
Levels and B(E2)'s of Be isotopes

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



taken from Nature Comm. (2022)



excitation level patterns indicate the occurence of the rotational behavior of a deformed "object"

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

Major points :

Cluster structures in ^{10,12}Be

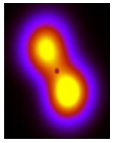
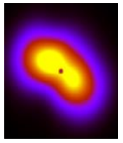
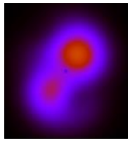
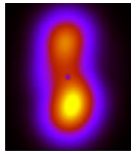
Cluster structure in ^{8}Be is basically trivial, but what about for Others ?

How excess neutrons are configured in ^{10,12}Be

π orbital : on a plane perpendicular to the axis connecting two α clusters and between them

σ orbital : around the axis connecting two α clusters, but mainly outside the clusters

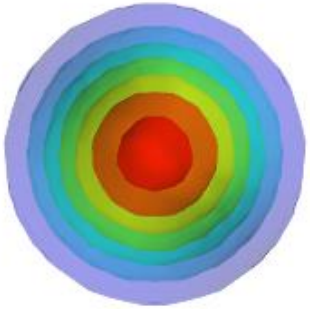
Why do we need the intrinsic density ?
-- in the case of MCSM eigenstate --

$$|\Phi\rangle = \sum_{i=1}^{N_{basis}} c_i |\Phi_i\rangle =$$ c_1  + c_2  + c_3  + c_4  + ...

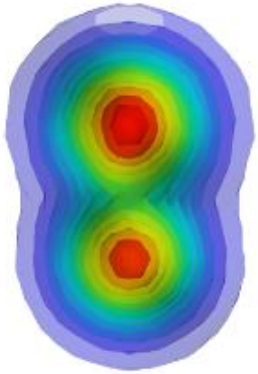
Angular-momentum projection

$$|\Psi\rangle = \sum_{i=1}^{N_{basis}} c_i P^J P^\pi |\Phi_i\rangle$$

We need something like this.



^{8}Be 0^+ ground state

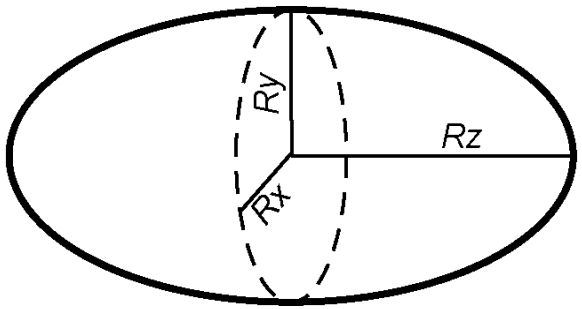


Laboratory frame

Snapshot state
in the body-fixed frame

Calculate Q-moment matrix

$$\begin{bmatrix} Qxx & Qxy & Qxz \\ Qyx & Qyy & Qyz \\ Qzx & Qzy & Qzz \end{bmatrix} \rightarrow \begin{bmatrix} Qz & 0 & 0 \\ 0 & Qy & 0 \\ 0 & 0 & Qx \end{bmatrix}$$



$$Rz = \{1 + 0.63\,\beta_2\,\cos(\gamma)\}\,R_0$$
$$Ry = \{1 + 0.63\,\beta_2\,\sin(\gamma - 30^\circ)\}\,R_0$$
$$Rx = \{1 - 0.63\,\beta_2\,\cos(60^\circ - \gamma)\}\,R_0$$

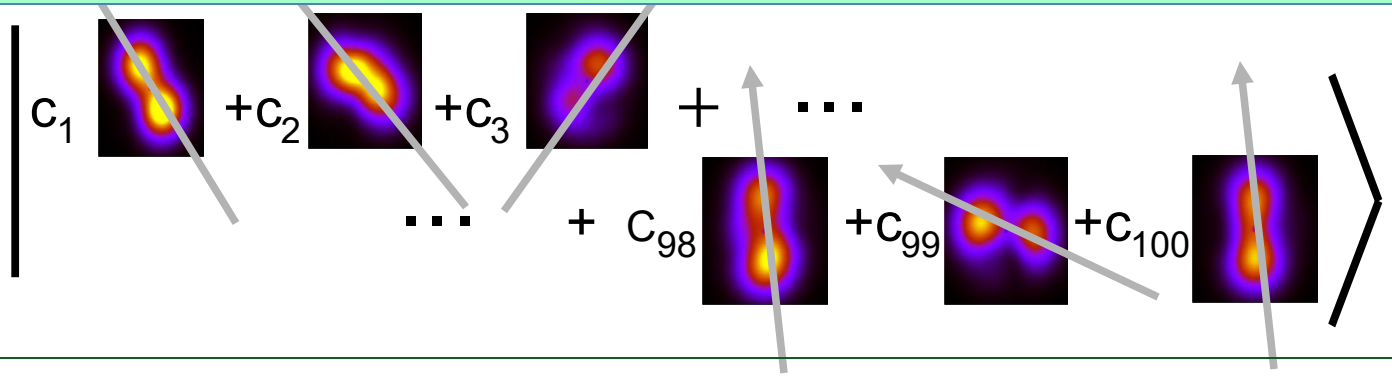
We define the z, y and x axes in this way for each MCSM basis vector

Superpose MCSM basis vectors on the same coordinate axes
➔ Q aligned state

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

Deformed Slater determinant with three axes of ellipsoid

Individual orientations are arbitrary => correlated to form a rotational band

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

For "snapshot 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.

"Q-aligned state"

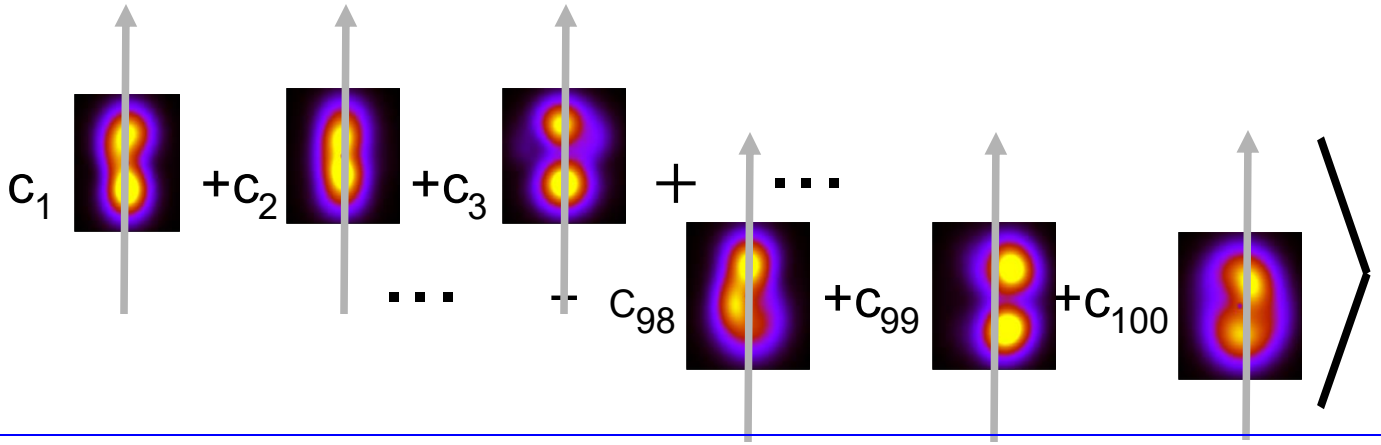
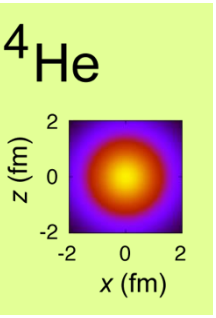
$\left|\Psi_{\text{intr.}}(D)\right\rangle =$ 

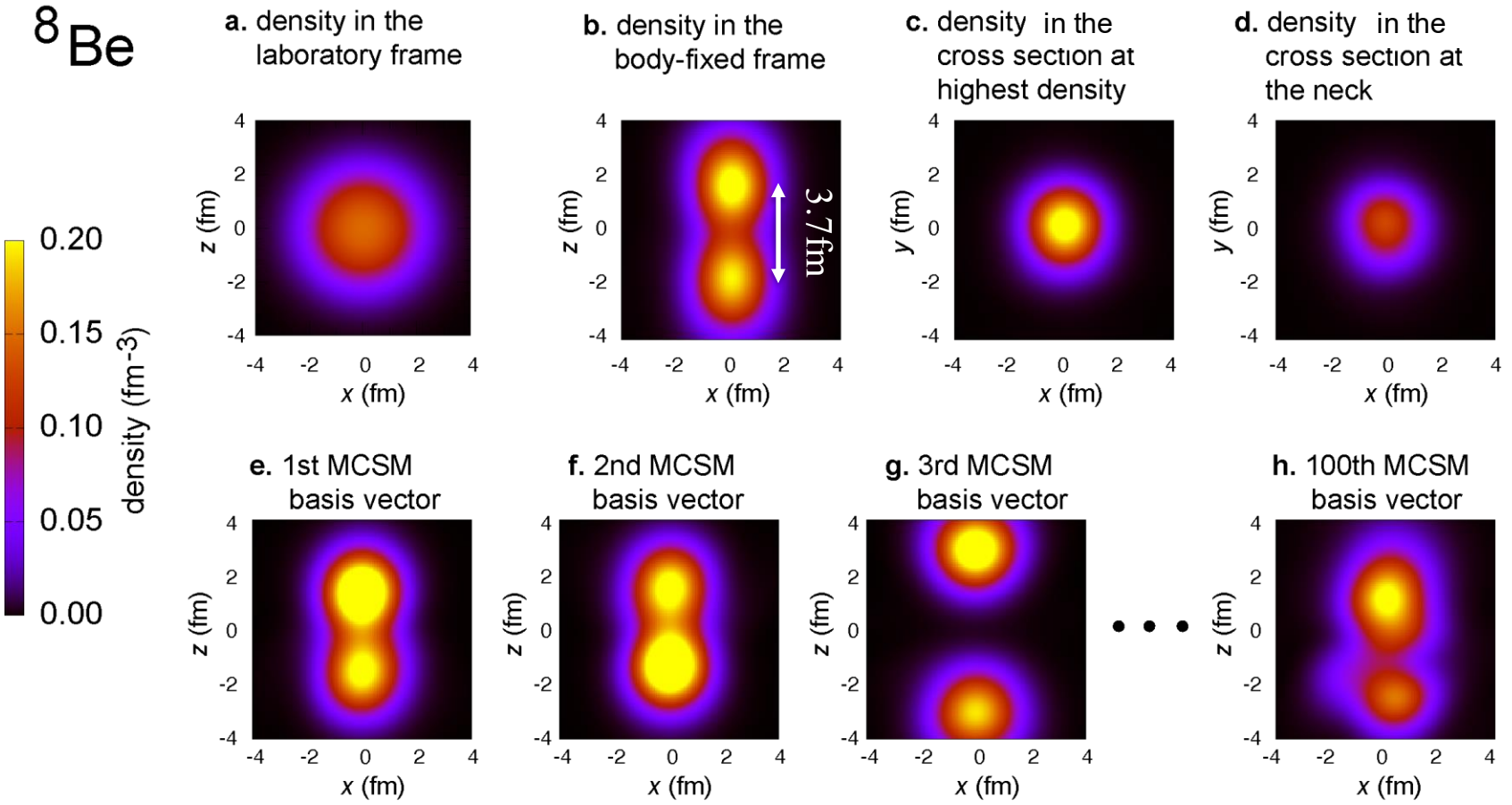
fig. 3 of Nature Comm. (2022)



Body-fixed (intrinsic) frame

Laboratory-frame

Q aligned state



MCSM basis vectors (individually aligned)

Full Fig. 3 of our Nature Comm. Paper (2022)

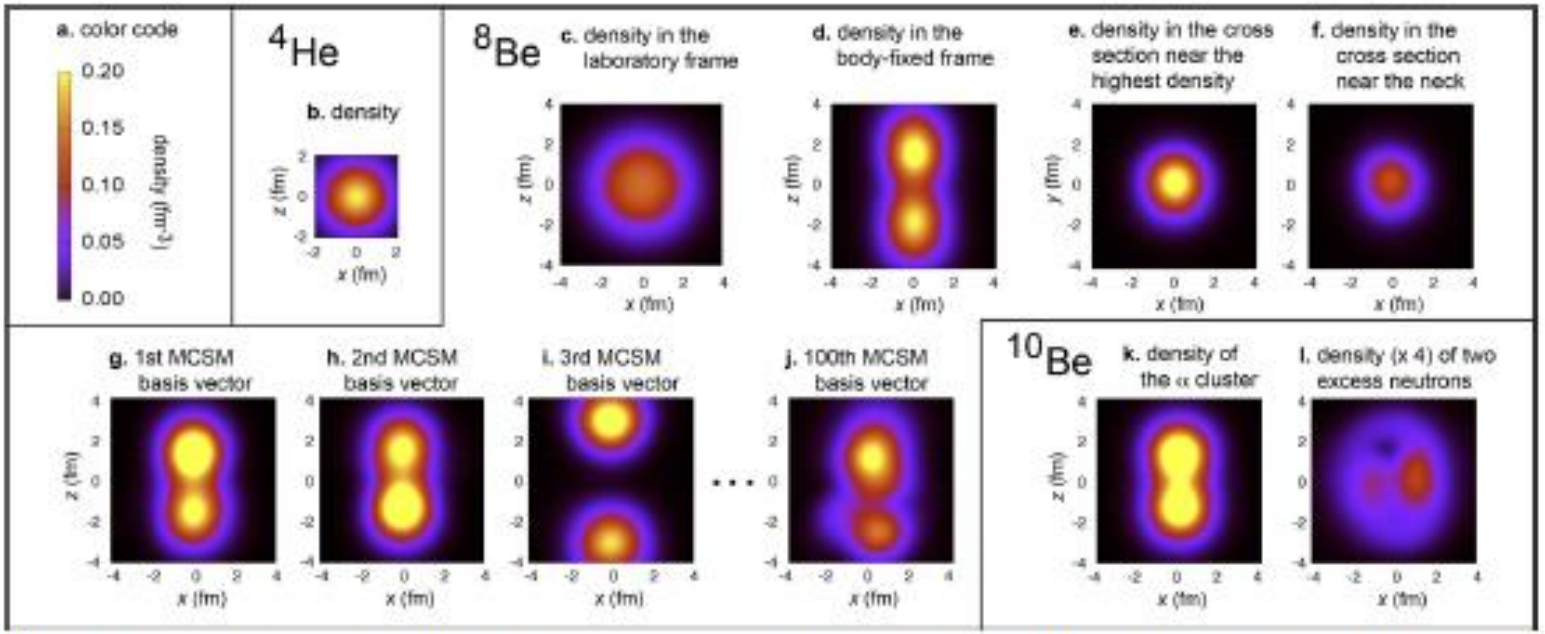


Fig. 3 Density profiles of ^{8,10}Be ground state in the body-fixed frame unless otherwise specified. a Legend. **b** Matter density of ^{4}He (α particle). **c** Matter density of ^{8}Be in the laboratory frame. **d–f** Matter density ^{8}Be on the xz plane (d) and on the xy plane (**e**, **f**). **g–j** Matter density of MCSM basis vectors for ^{8}Be. **k** Matter density of the α-cluster part of ^{10}Be. **l** Density of the excess neutrons of ^{10}Be.

Validity of Intrinsic state

The intrinsic state can give us a snapshot, because it rotates with the nucleus. If the intrinsic state is composed of a single component, the picture is very straightforward.

The intrinsic state fixed for the 0^+ ground state gives the 2^+ excited state by its projection to $J=2^+$

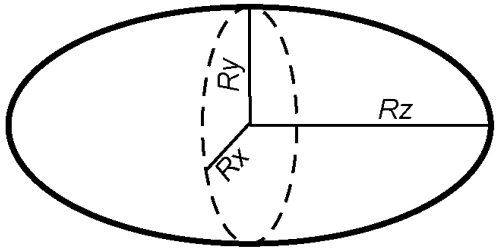
Overlap probability : 99 %

Energy : 99 %

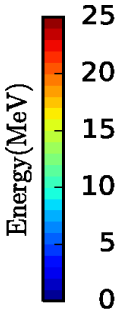
The $J=0^+$ & 2^+ states belong to the same rotational band
→ the present Q-aligned state can be regarded as the intrinsic state at the level of 99%.

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

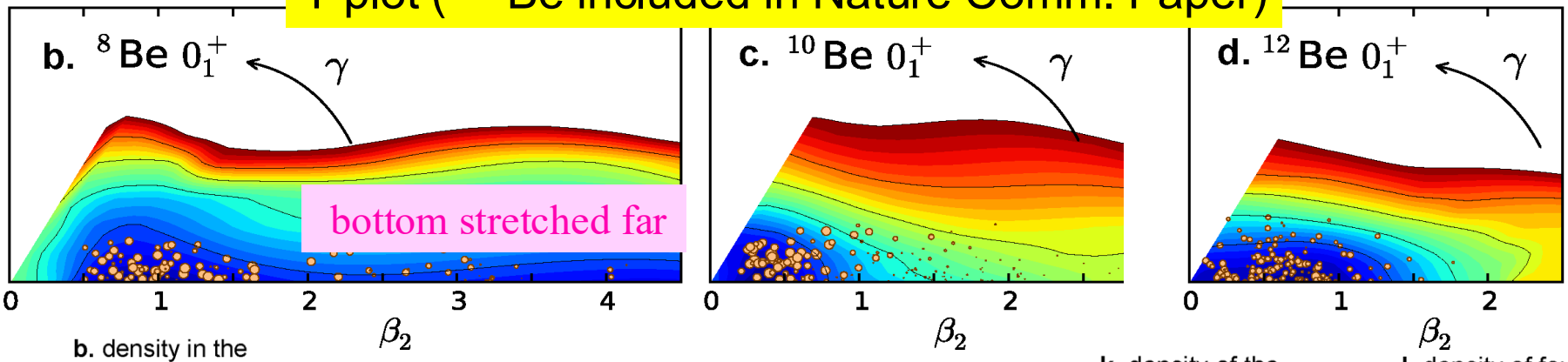
a.



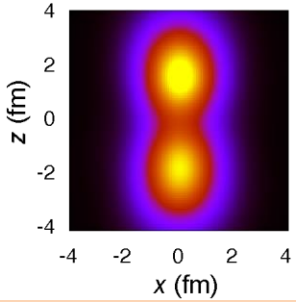
$$Rz = \{1 + 0.63\,\beta_2\,\cos(\gamma)\}\,R_0$$
$$Ry = \{1 + 0.63\,\beta_2\,\sin(\gamma - 30^\circ)\}\,R_0$$
$$Rx = \{1 - 0.63\,\beta_2\,\cos(60^\circ - \gamma)\}\,R_0$$



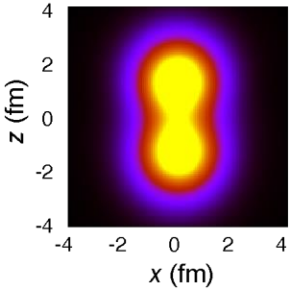
T-plot (^{8,10}Be included in Nature Comm. Paper)



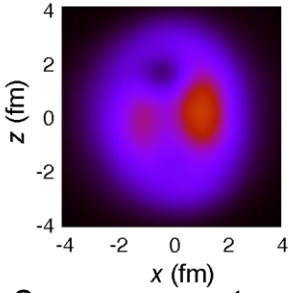
b. density in the body-fixed frame



i. density of the α cluster part (twice proton density)

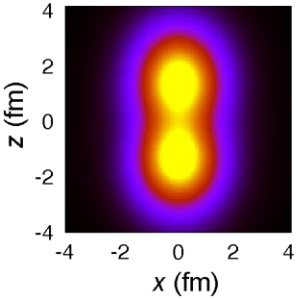


j. density of two excess neutrons

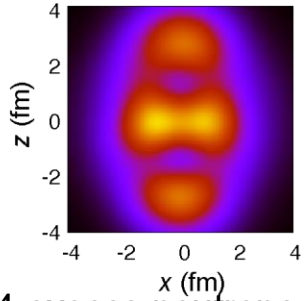


2 excess neutrons

k. density of the α cluster part (twice proton density)



l. density of four excess neutrons



4 excess neutrons

PES minimum stretching to the right direction implies underlying unbound nature

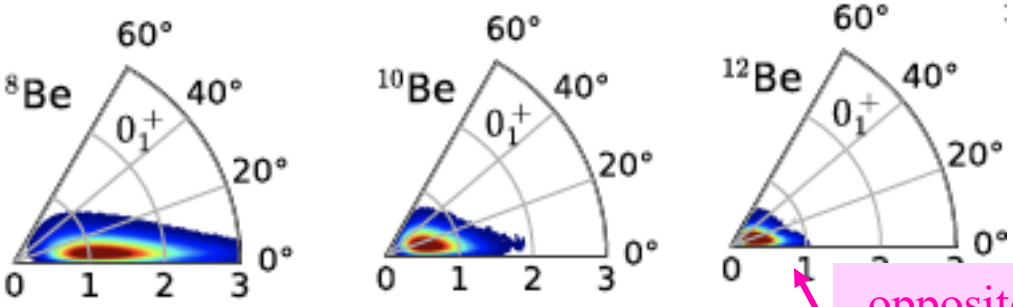
2 α clusters get closer due to neutrons in molecular π orbitals

2 α clusters get a bit apart due to neutrons outside

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

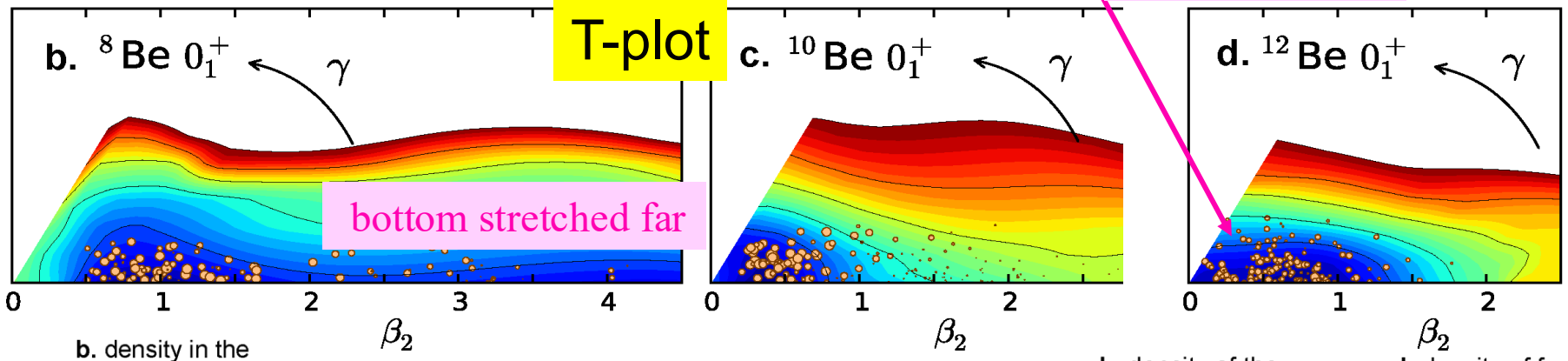
Related analysis in Shen et al.

basic similarities

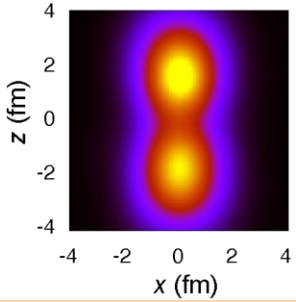


opposite trends

T-plot



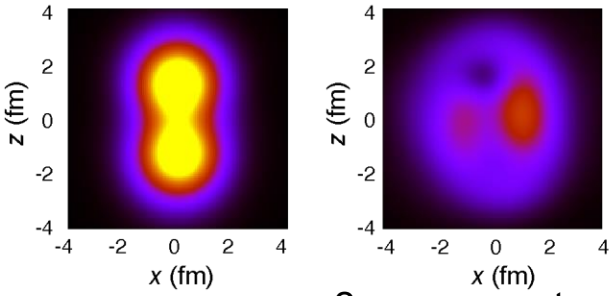
b. density in the body-fixed frame



PES minimum stretching to the right direction implies underlying unbound nature

i. density of the α cluster part (twice proton density)

j. density of two excess neutrons

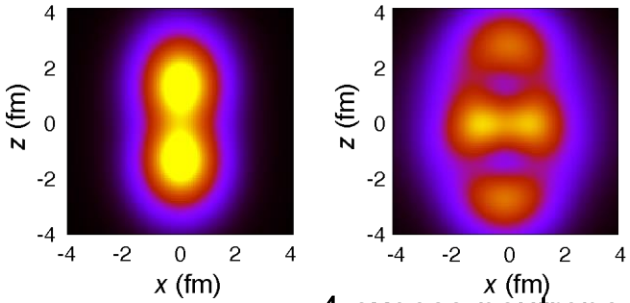


2 excess neutrons

2 α clusters get closer due to neutrons in molecular π orbitals

k. density of the α cluster part (twice proton density)

l. density of four excess neutrons



4 excess neutrons

2 α clusters get a bit apart due to neutrons outside

basis vectors (^{10}Be)

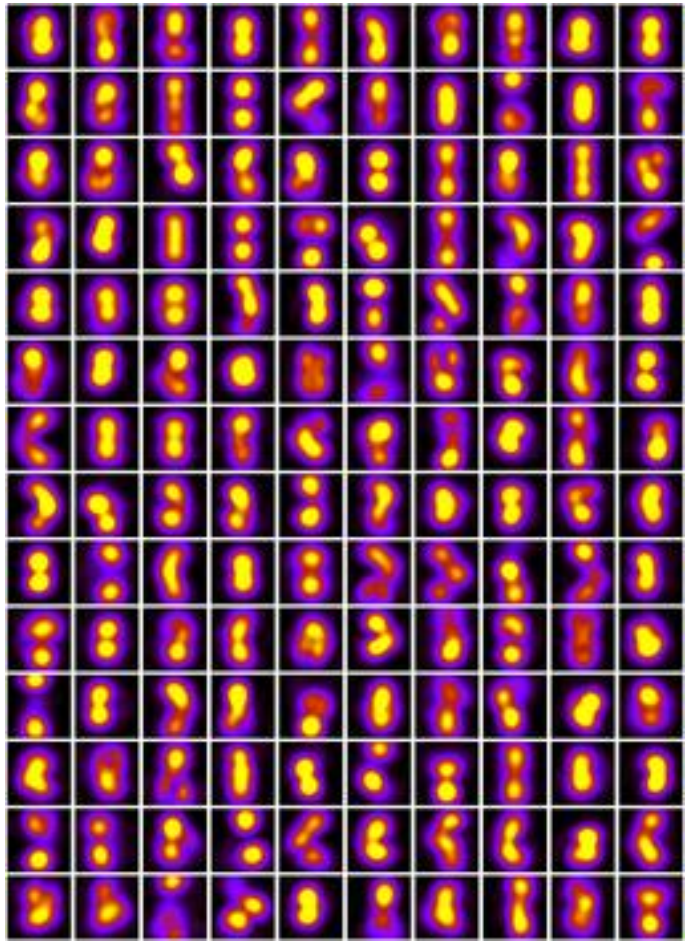
total # = 140

N_{shell} = 6, $\hbar\omega$ = 15 MeV

proton density x 2
= nucleon density of cluster sector

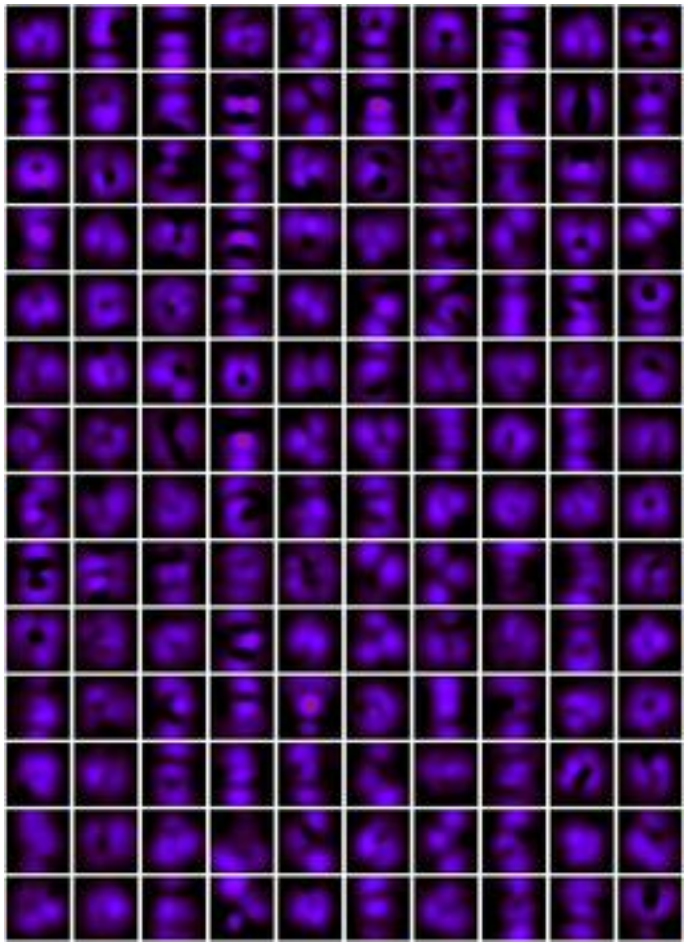
neutron density – proton density
= valence neutron density

basis vector #1, #2, #3, …



basis vector #140

basis vector #1, #2, #3, …



basis vector #140

Density after superposition
(^{10}Be, $0_{1,2}^+$)

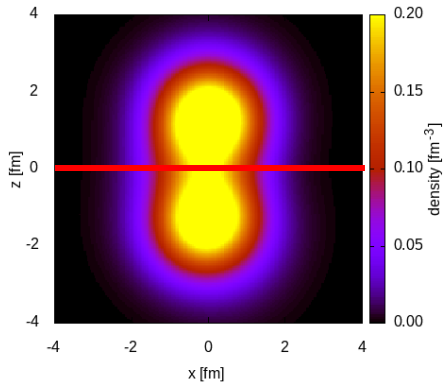
# of bases = 140

N_{shell} = 6,
JISP16,
$\hbar\omega$ = 15 MeV

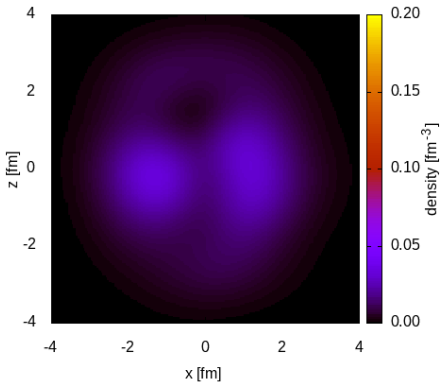
proton density x 2
= nucleon density of cluster sector

neutron density – proton density
= valence neutron density

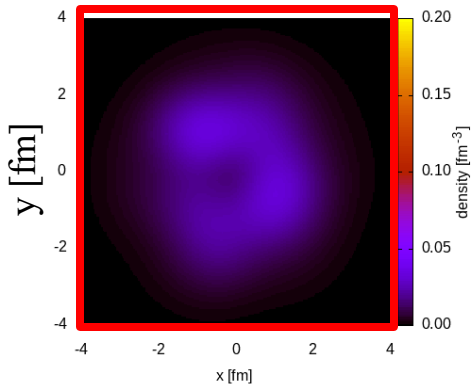
(0_1^+) xz plane (y=0)



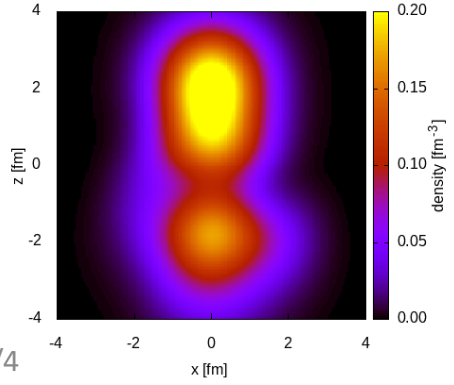
xz plane (y=0)



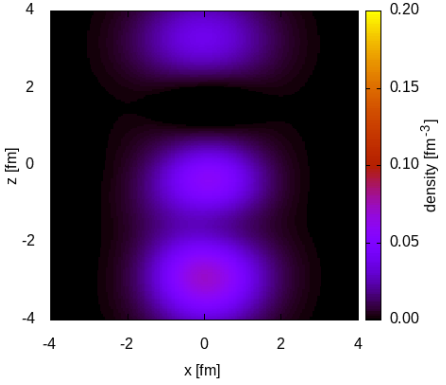
(0_1^+) xy plane (z=0)



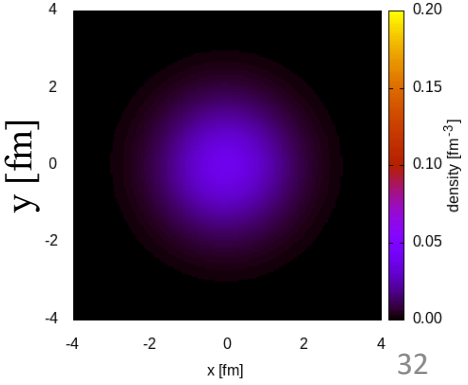
(0_2^+) xz plane (y=0)



xz plane (y=0)



(0_2^+) xy plane (z=0)



basis vectors (^{12}Be)

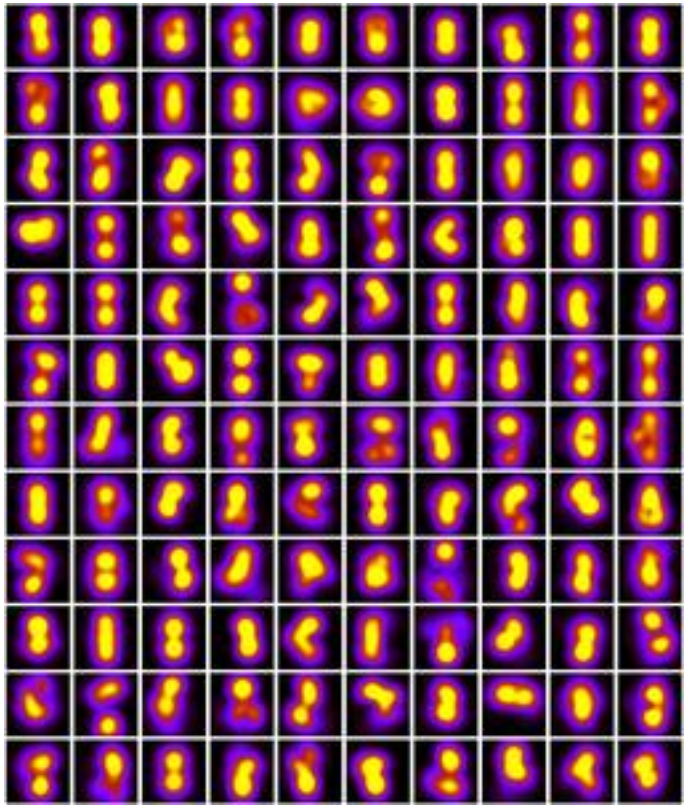
total # = 120

N_{shell} = 6, $\hbar\omega$ = 15 MeV

proton density x 2
= nucleon density of cluster sector

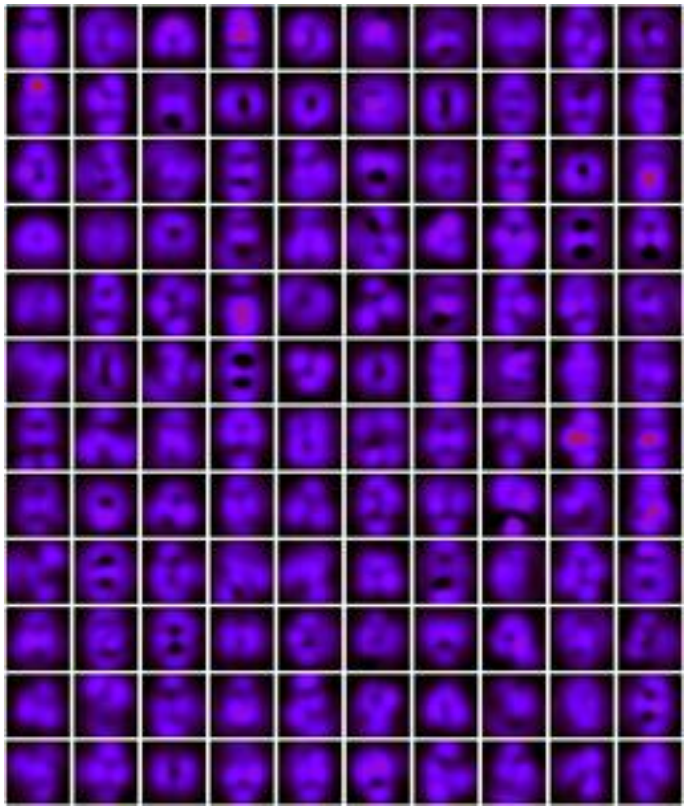
neutron density – proton density
= valence neutron density

basis vector #1, #2, #3, …



basis vector #120

basis vector #1, #2, #3, …



basis vector #120

Density after superposition (^{12}Be, $0_{1,2}^+$)

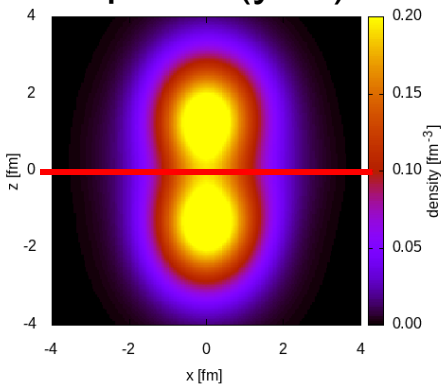
of bases = 120

N_{shell} = 6,
JISP16,
$\hbar\omega$ = 15 MeV

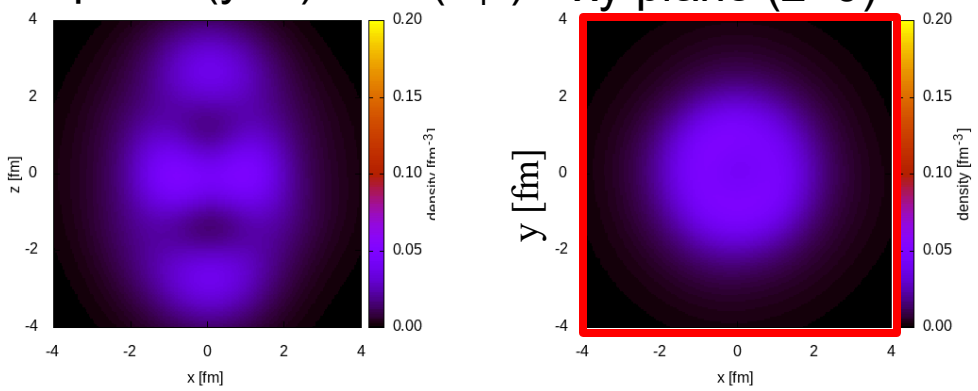
proton density x 2
= nucleon density of cluster sector

neutron density – proton density
= valence neutron density

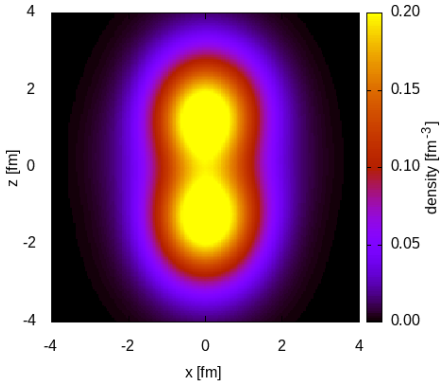
(0_1^+) xz plane (y=0)



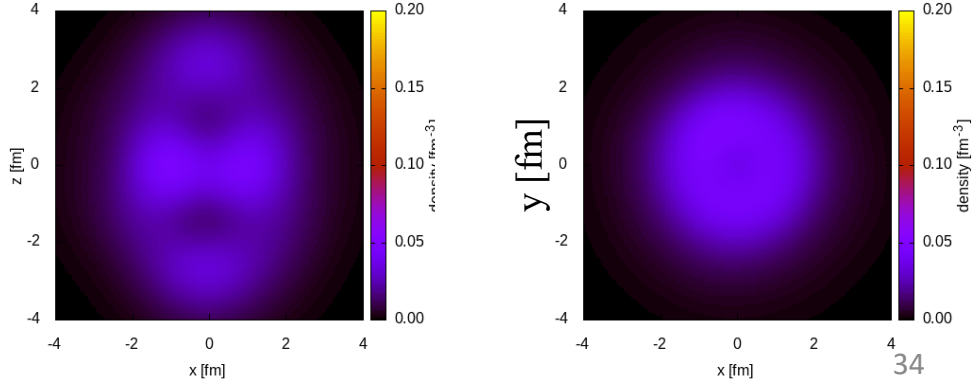
xz plane (y=0) (0_1^+) xy plane (z=0)



(0_2^+) xz plane (y=0)



xz plane (y=0) (0_2^+) xy plane (z=0)



^{12}C : Basis vectors classified by quadrupole shapes (T plot)

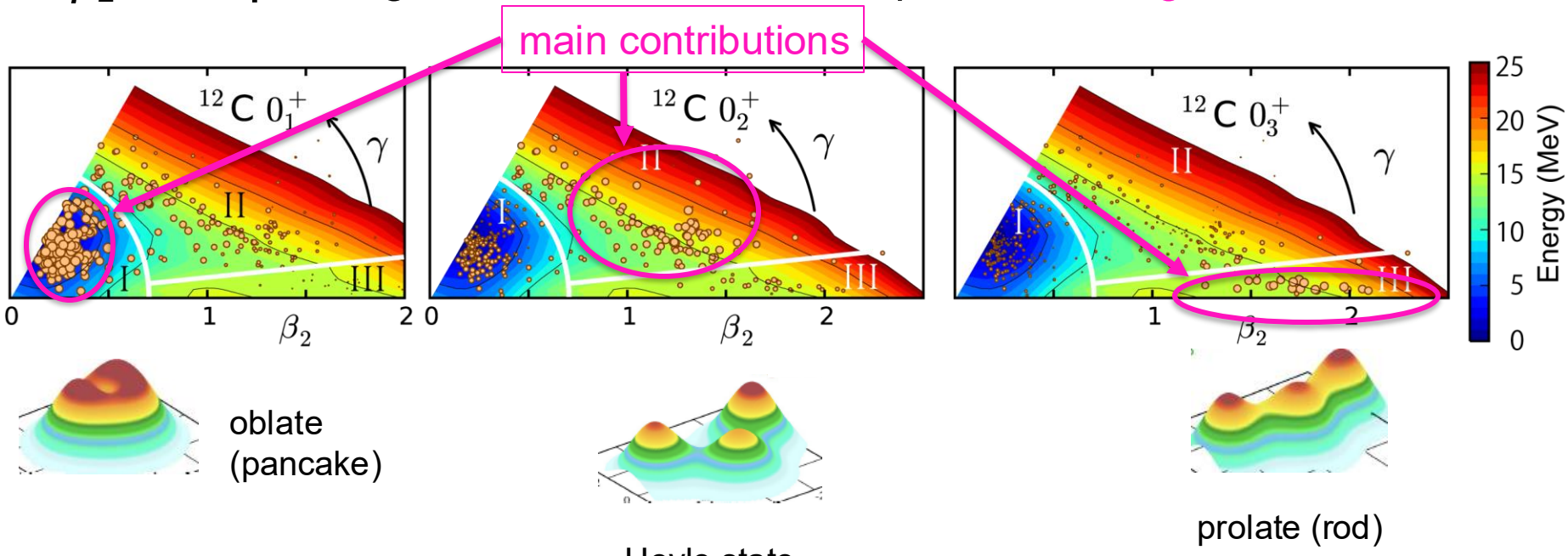
reprise

T plot circles are spread in the case of ^{12}C. A characteristic feature.

Completely different structures appear at low excitation energies … quite unique

PES is divided into three
- I $\beta_2 < 0.7$, oblate basin in the PES
- II triaxial（clusters come here）
- III near prolate

β_2=0.7, γ=6 deg ➔ basis vectors decomposed into regions I, II and III



An alternative analysis … applicable to exotic Be isotopes

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

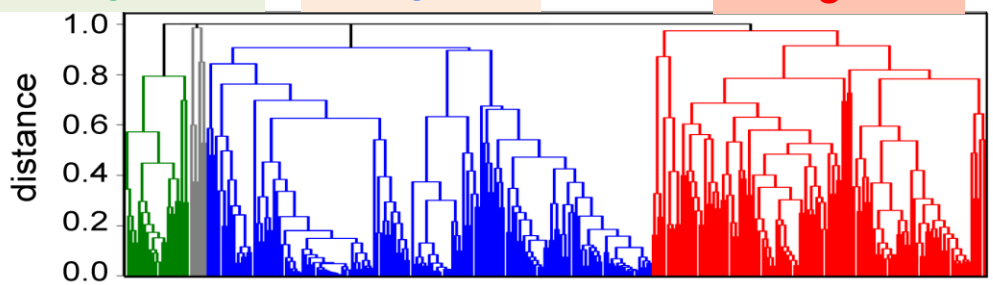
connect basis vectors from the shortest distance to longer up to the threshold

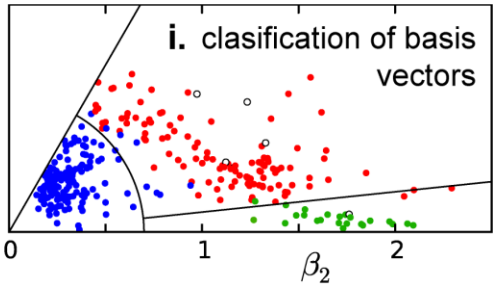
➔ see next page

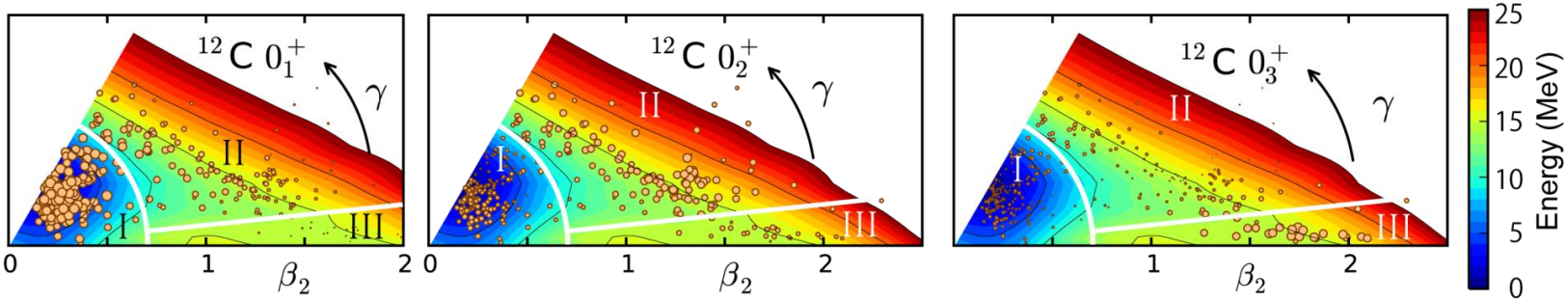
independent confirmation of the validity of the region decomposition

~region III ~region I ~region II

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

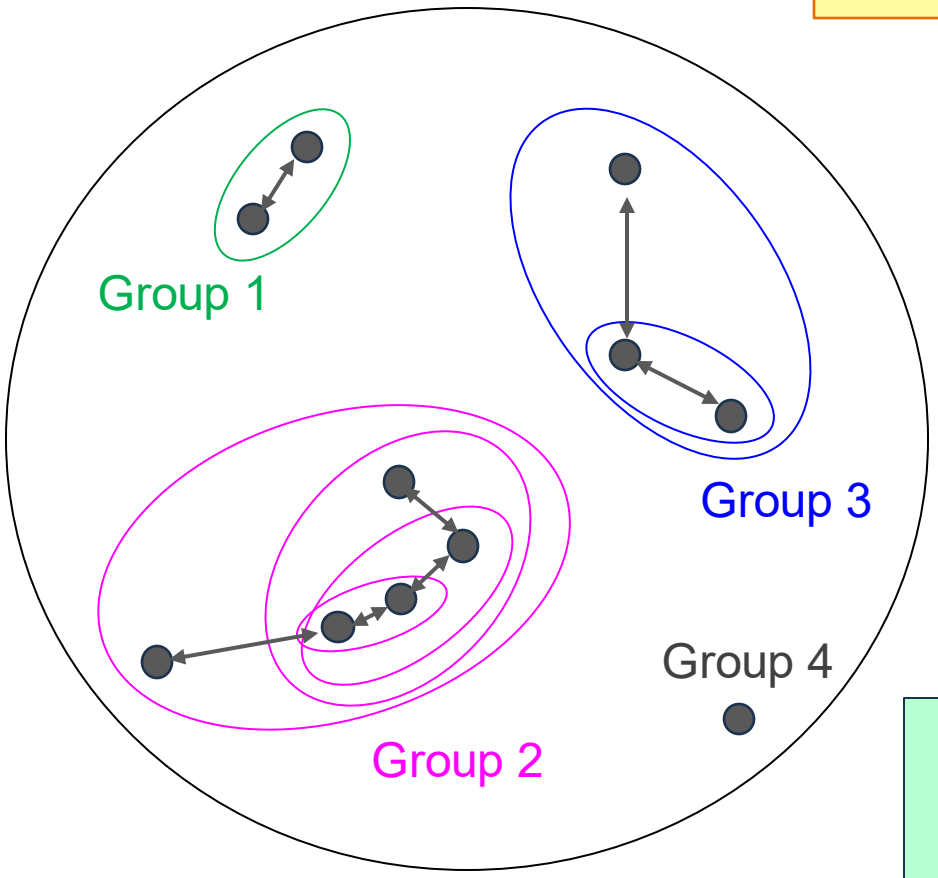






Dendrogram analysis - grouping -

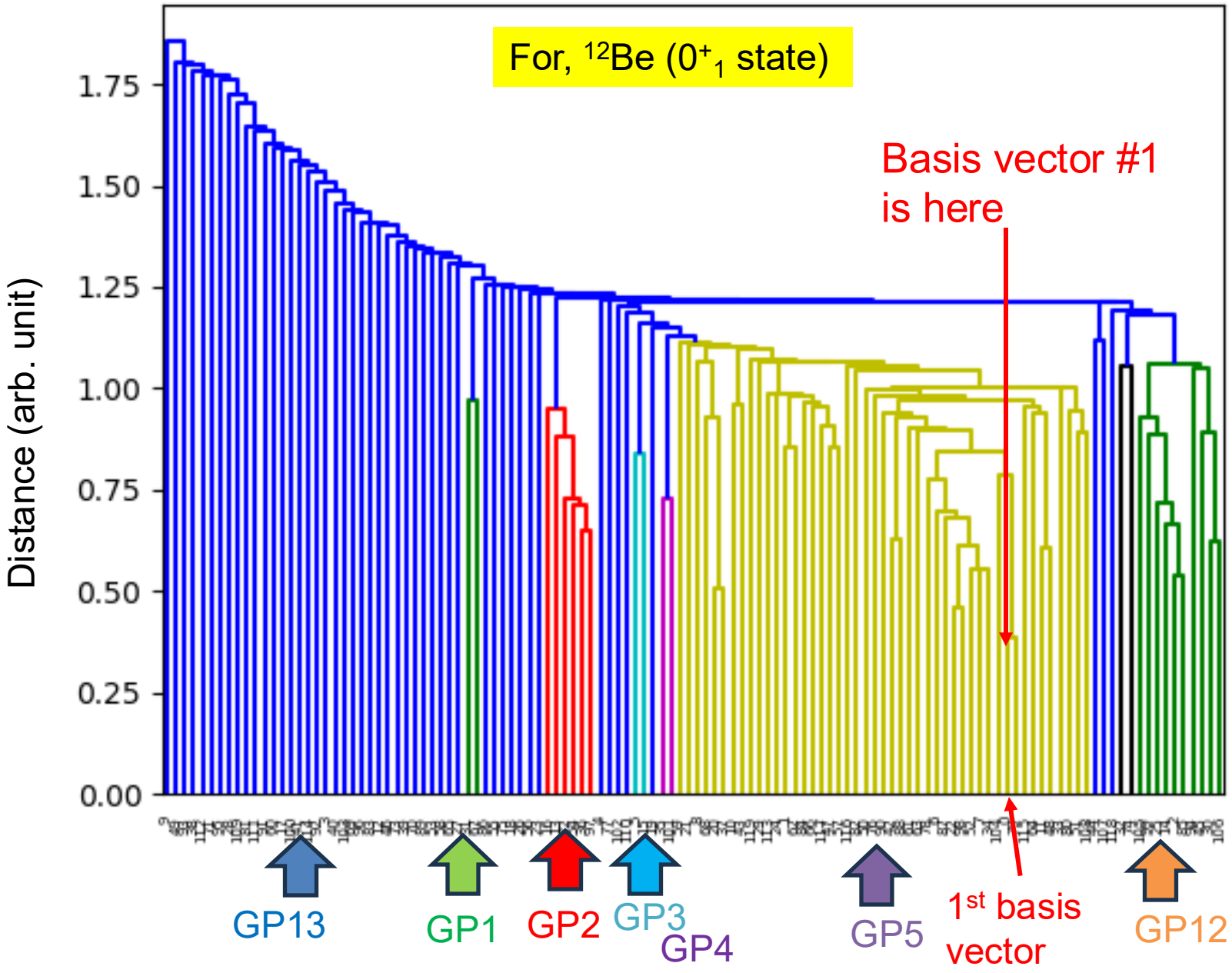
schematic description



: distance between two states

The distance is defined based on the overlap Between two states as vectors in the many-body Hilbert space

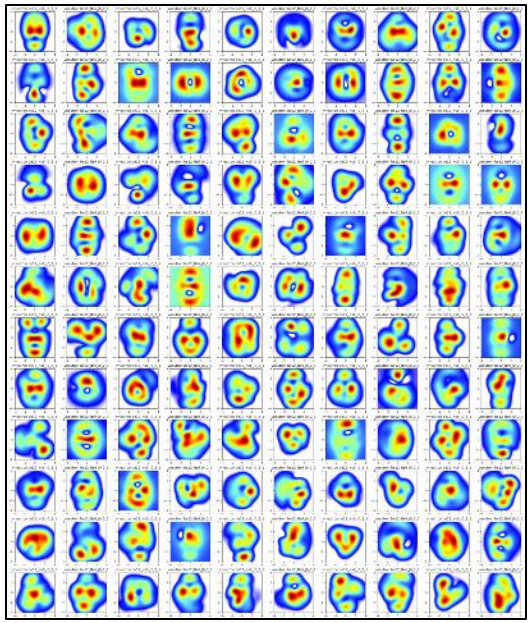
threshold distance (maximal allowed distance)


For, ^{12}Be (0^+_1 state)
Basis vector #1 is here
Distance (arb. unit)
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
GP13
GP1
GP2
GP3
GP4
GP5
1st basis vector
GP12

Dendrogram analysis (^{12}Be, 0_1)

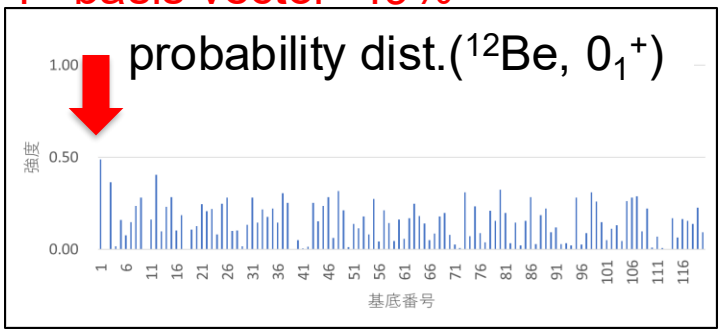
N_{shell}=6,
JISP16,
$\hbar\omega$=15MeV

basis vec=120

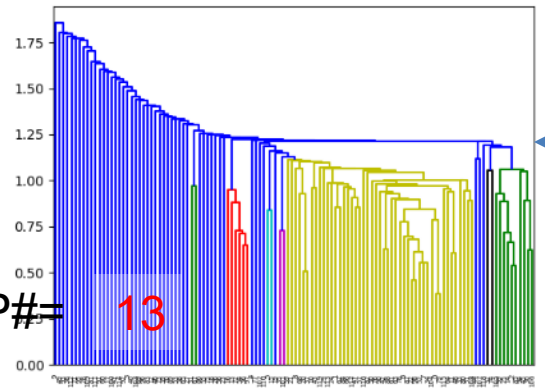


density of excess neutrons

1st basis vector~49%



basis vector #



threshold = 0.6 * max distance

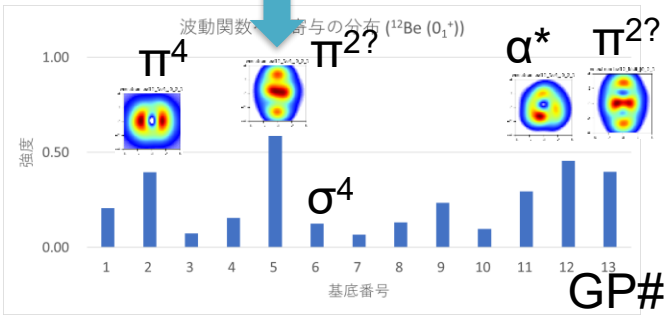
basis vecors

grouping

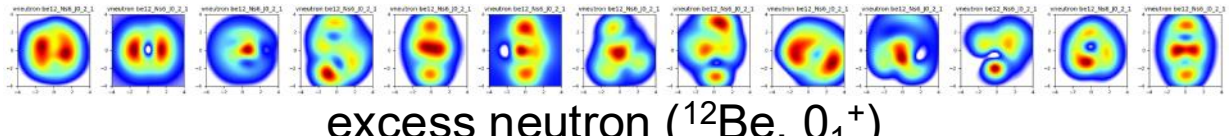
GP5

Dendrogram classification

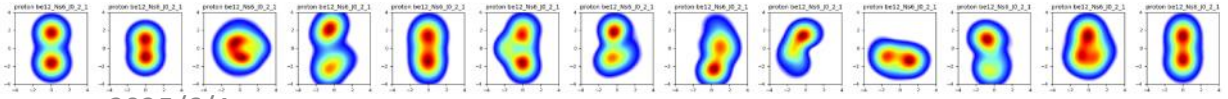
GP5~59%



Probablity of each group



excess neutron (^{12}Be, 0_1^+)



proton (^{12}Be, 0_1^+)

Density of protons ^{12}Be($0_{1,2}^+$) with group decomposition

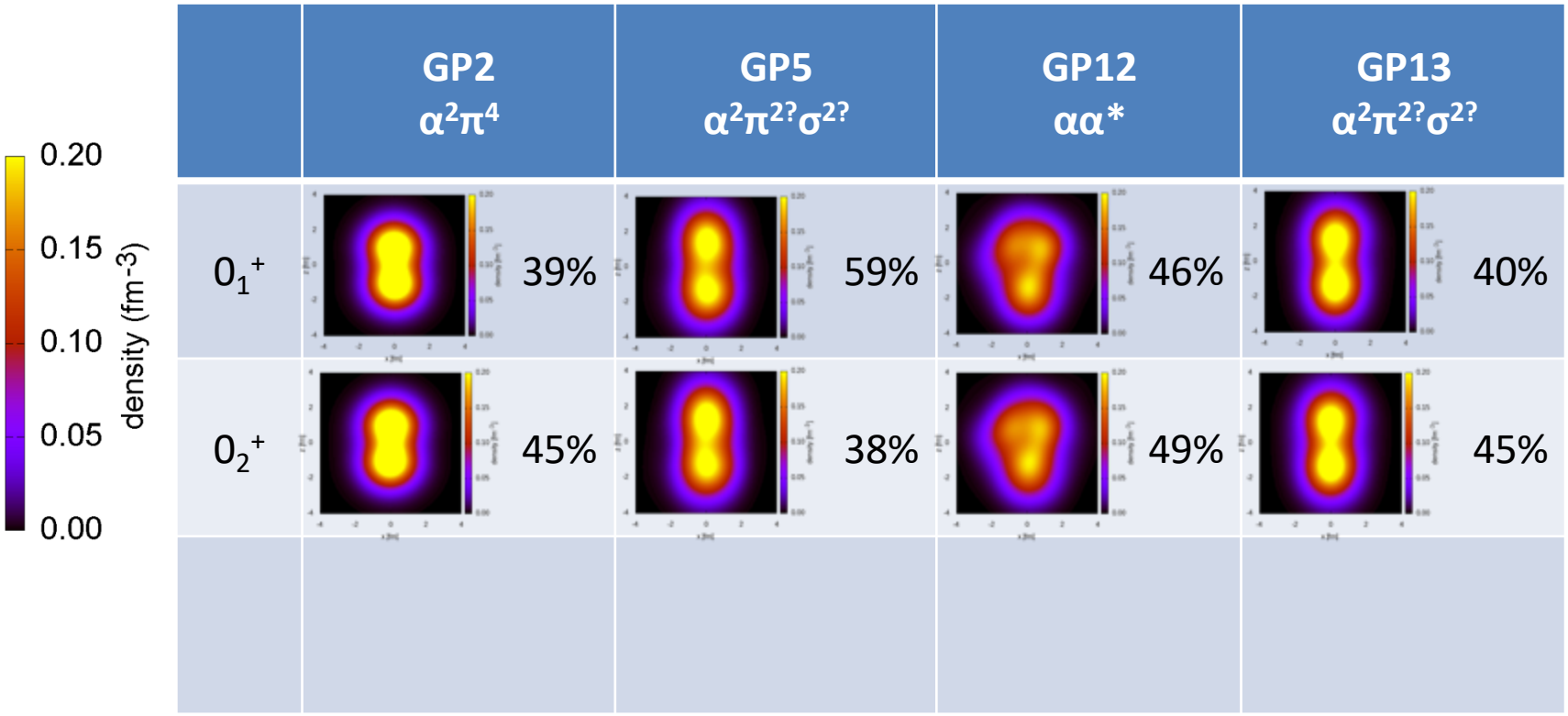
nucleons in the cluster sectors

very preliminary

- Overlap probabilities in 0_1^+

  $|\langle GP2|GP5\rangle|^2 = 0.01$, $|\langle GP2|GP12\rangle|^2 = 0.80$, $|\langle GP2|GP13\rangle|^2 = 0.10$,
  $|\langle GP5|GP13\rangle|^2 = 0.15$, $|\langle GP12|GP13\rangle|^2 = 0.10$

Density profiles of



Density of excess neutrons ^{12}Be($0_{1,2}^+$) with group decomposition

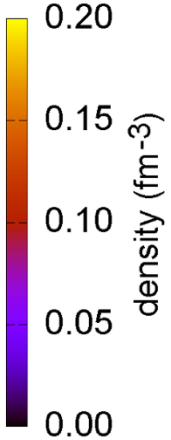
- Overlap probabilities in 0_1^+

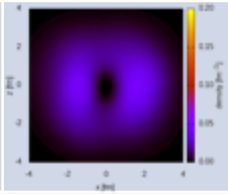
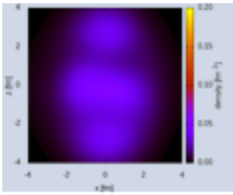
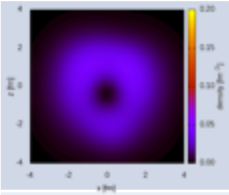
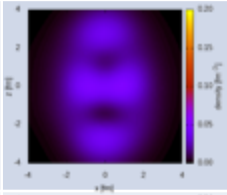
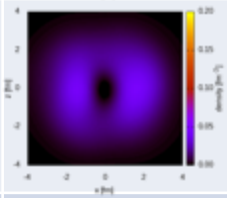
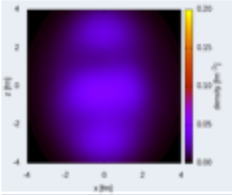
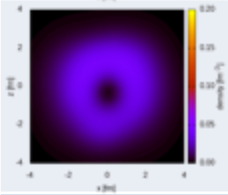
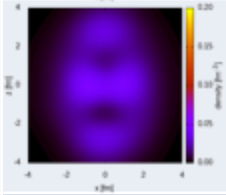
  $|\langle GP2|GP5\rangle|^2 = 0.01$, $|\langle GP2|GP12\rangle|^2 = 0.80$,

  $|\langle GP2|GP13\rangle|^2 = 0.10$, $|\langle GP5|GP13\rangle|^2 = 0.15$,

  $|\langle GP12|GP13\rangle|^2 = 0.10$

very preliminary



	GP2 $\alpha^2\pi^4$	GP5 $\alpha^2\pi^{2?}\sigma^{2?}$	GP12 $\alpha\alpha^*$	GP13 $\alpha^2\pi^{2?}\sigma^{2?}$
0_1^+	 39%	 59%	 46%	 40%
0_2^+	 45%	 38%	 49%	 45%

Density of excess neutrons ^{12}Be($0_{1,2}^+$) with group decomposition

variations emphasized

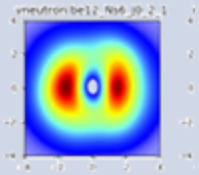
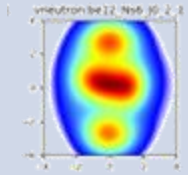
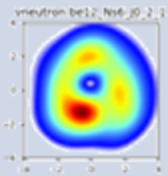
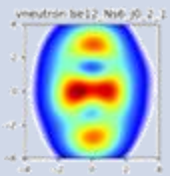
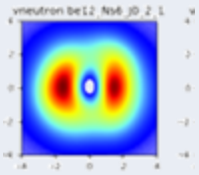
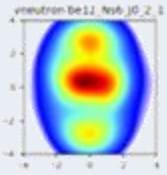
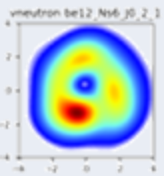
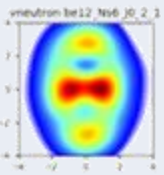
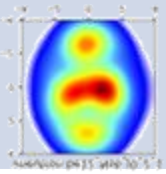
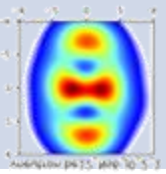
- Overlap probabilities in 0_1^+

  $|\langle GP2|GP5\rangle|^2 = 0.01$, $|\langle GP2|GP12\rangle|^2 = 0.80$,

  $|\langle GP2|GP13\rangle|^2 = 0.10$, $|\langle GP5|GP13\rangle|^2 = 0.15$,

  $|\langle GP12|GP13\rangle|^2 = 0.10$

very preliminary

	GP2 $\alpha^2\pi^4$	GP5 $\alpha^2\pi^{2?}\sigma^{2?}$	GP12 $\alpha\alpha^*$??	GP13 $\alpha^2\pi^{2?}\sigma^{2?}$
0_1^+	 39%	 59%	 46%	 40%
0_2^+	 45%	 38%	 49%	 45%
0_3^+		 94%		 35%

Summary

1. *Ab initio* no-core MCSM can describe the structure of ^{8,10,12}Be and ^{12}C, focusing on α clustering and molecular orbiting without assuming them.

2. The density profile in the body-fixed frame is presented as a snapshot. Because of *ab initio* nature, the nucleon density are obtained directly.

3. ^{8}Be is a perfect di-cluster system. The ^{12}C ground state is mainly quantum liquid with a 6% mixing of α-clustering. (Similar mixings in heavy nuclei may be an origin of α decay, which is still to be clarified.)
   The Hoyle state is a three-α-cluster state with the probability ~2/3, in tri-angular configurations. The rest is a quantum-liquid. A unique case of possible "crossover" between the liquid and the cluster "phases".

4. ^{10}Be is a di-α-cluster system plus π-orbital two excess neutrons, with a shorter distance between the α's.

5. ^{12}Be is a di-α-cluster system plus **various** molecular orbital configurations of the four excess neutrons, with somewhat longer distance between the α's than in ^{10}Be. It does not seem to be a standard ellipsoidal object.

6. The unsupervised statistical learning used in data science can be utilized, clarifying a variety of clustering and molecular structures.

The paper shown below has been published online on June 2.

It shows, I believe, many new aspects of nuclear shapes and rotations.

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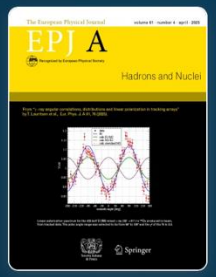
Prevailing triaxial shapes in atomic nuclei and a quantum theory of rotation of composite objects

Regular Article - Theoretical Physics | Open access | Published: 02 June 2025

Volume 61, article number 126, (2025) Cite this article



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T. Otsuka, Y. Tsunoda, N. Shimizu, Y. Utsuno, T. Abe & H. Ueno

Are atomic nuclei like rugby ball or almond ?

Thank you !

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)	$\sqrt{\langle \hat{r}^2 \rangle_{\rm pp}}$ (fm) MCSM $N_{\rm shell}=7$	MCSM $N_{\rm shell}\to\infty$	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

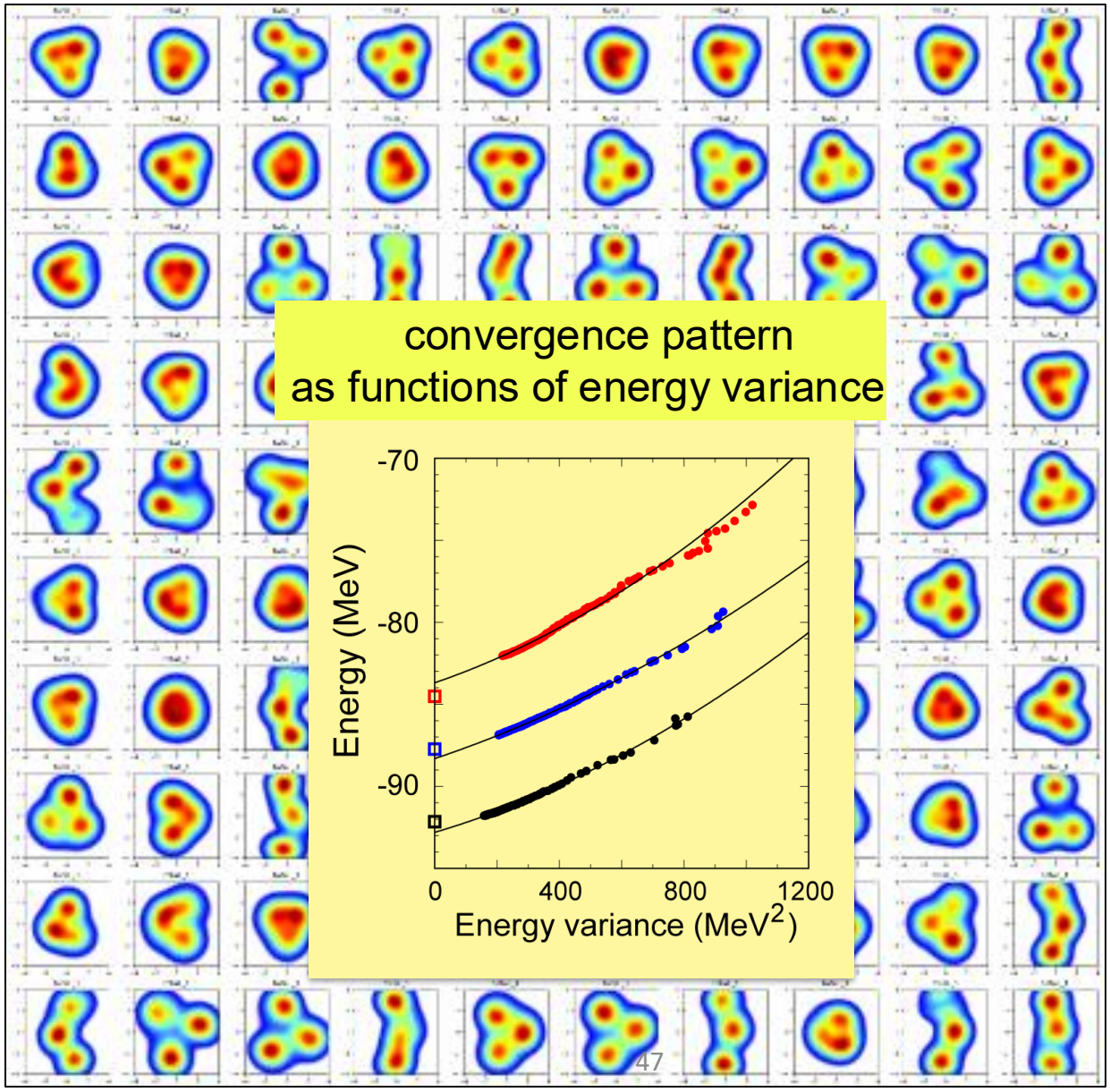
Ground-state properties of light 4*n* self-conjugate nuclei in *ab initio* no-core Monte Carlo shell model calculations with nonlocal *NN* interactions

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*
[5]*Advanced Science Research Center, Japan Atomic Energy Agency, Tokai, Ibaraki 319-1195, Japan*

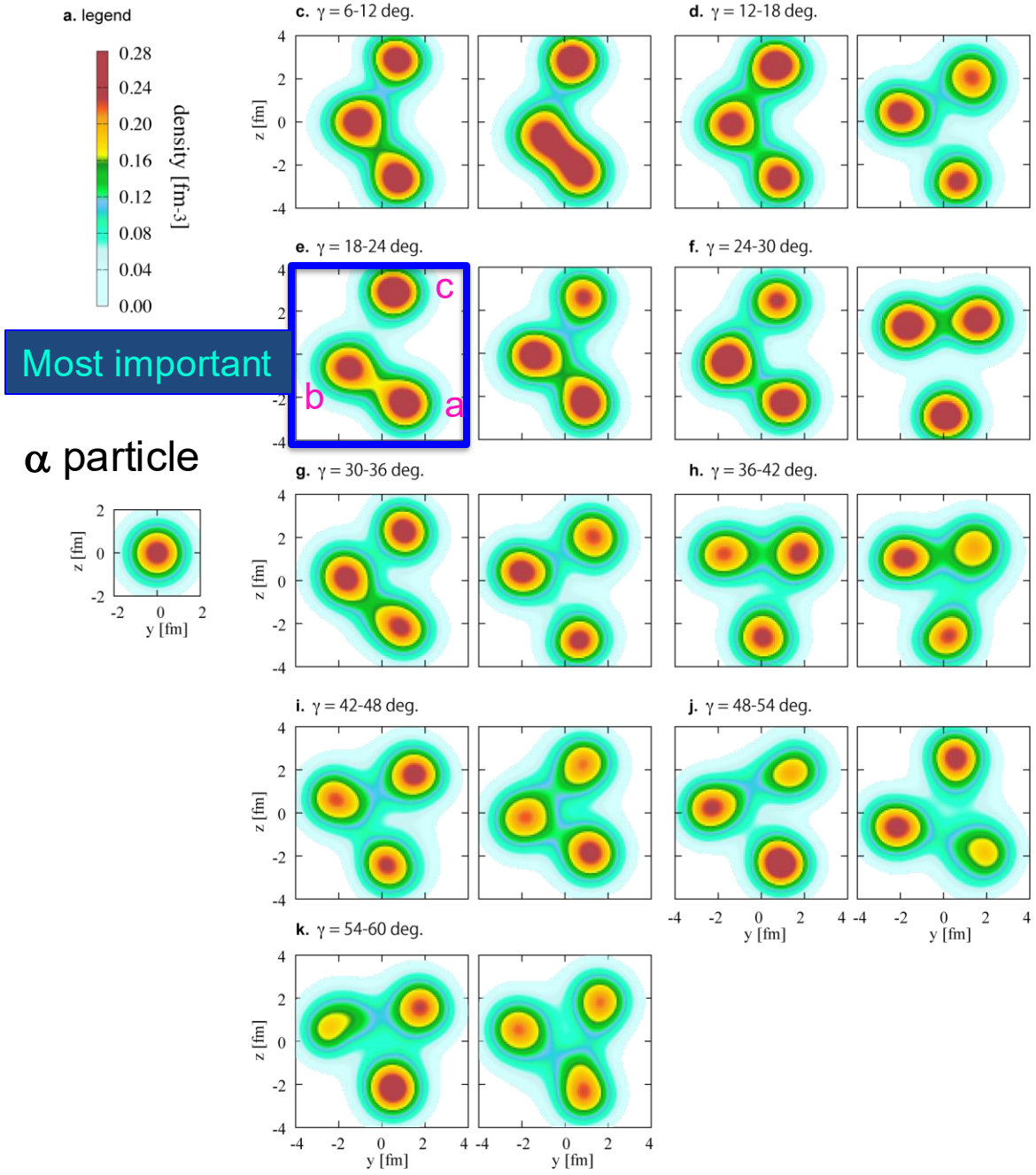
(Received 29 June 2021; accepted 5 October 2021; published 24 November 2021)

Generated basis vectors (^{12}C, $0_{1,2,3}^{+}$)

N_{shell} = 7, Daejeon16 int., $\hbar\omega$ = 20 MeV



convergence pattern
as functions of energy variance



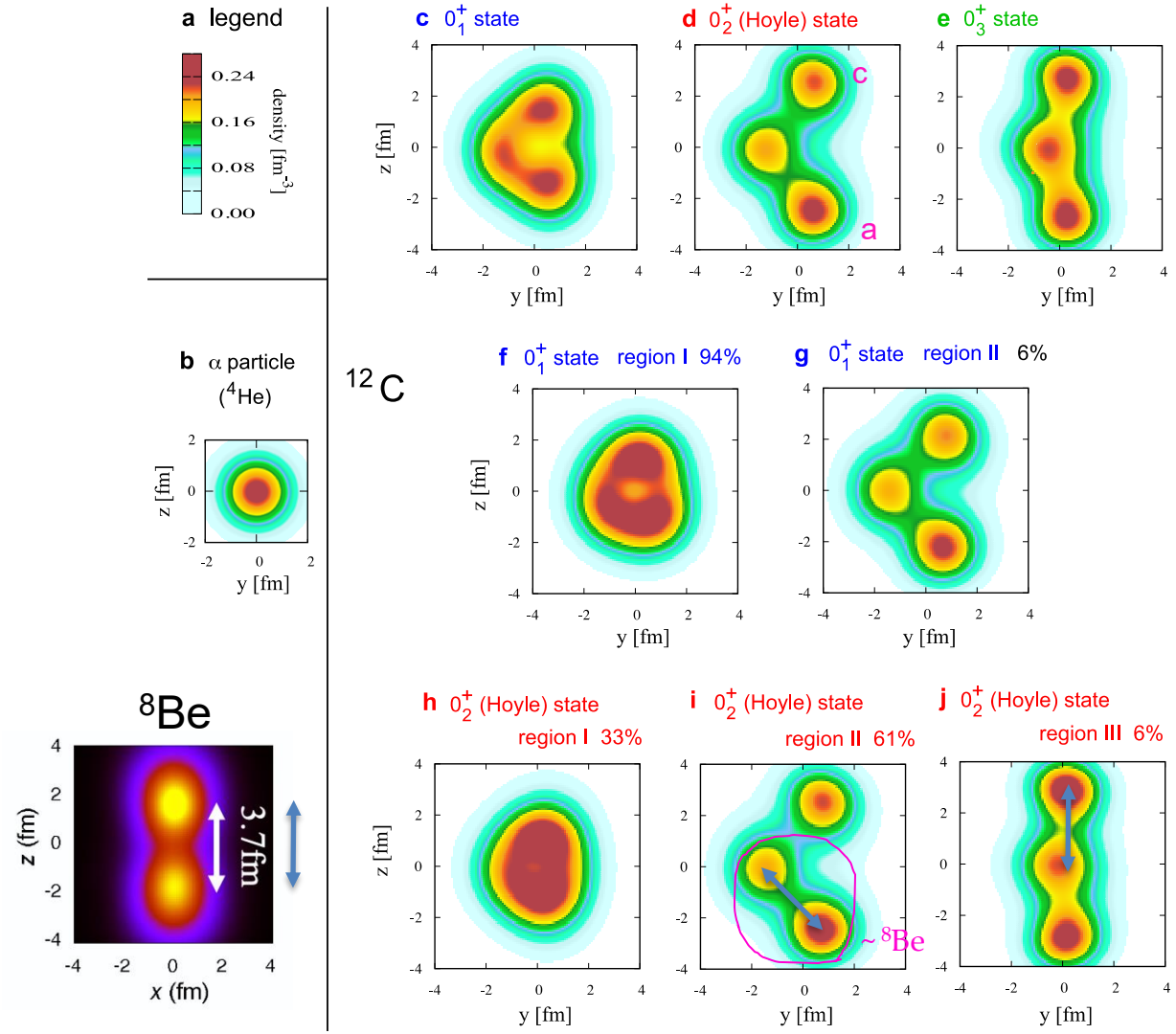
Most important

α particle

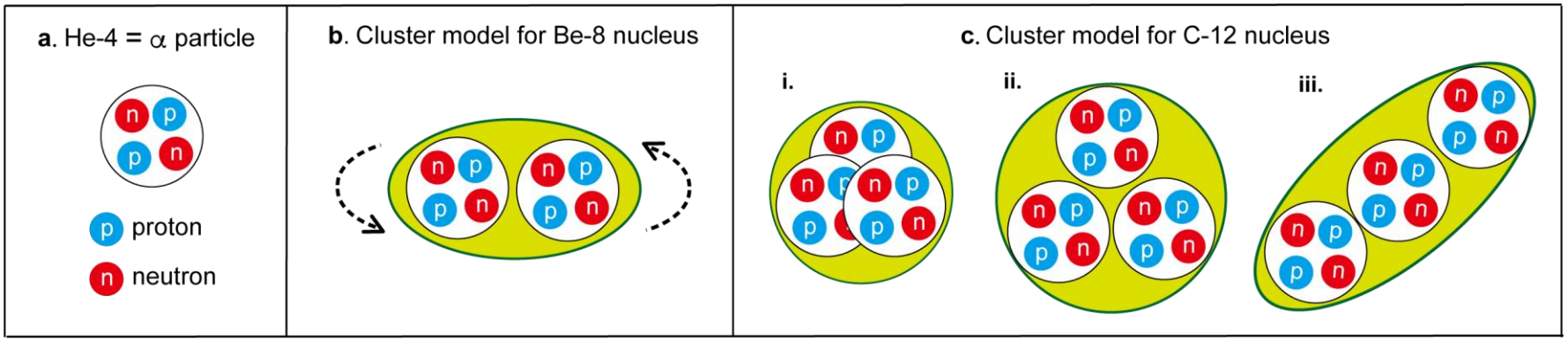
density profiles of major MCSM basis vectors in region II

Triangle configurations with three α clusters are favored (compare to single α)

Fluctuations within such configurations


a legend
0.24
0.16
0.08
0.00
density [fm^{-3}]
b α particle
(^{4}He)
z [fm]
y [fm]
^{12}C
c 0_1^+ state
d 0_2^+ (Hoyle) state
e 0_3^+ state
c
a
f 0_1^+ state region I 94%
g 0_1^+ state region II 6%
h 0_2^+ (Hoyle) state
region I 33%
i 0_2^+ (Hoyle) state
region II 61%
j 0_2^+ (Hoyle) state
region III 6%
~ ^{8}Be
^{8}Be
3.7fm
z (fm)
x (fm)

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.

(*We obtain states in the lab. frame by rotating it, a la Nambu-Goldstone mode.*)

This snapshot state gives the snapshot of density profile.

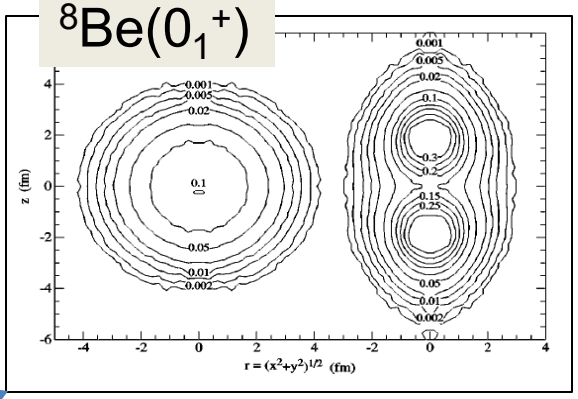
(*The snapshot state is nothing but the intrinsic state in some literatures.*)

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

The clustering is one of the fundamental problems in physics.

From contemporary works

$^8Be(0_1^+)$



***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

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

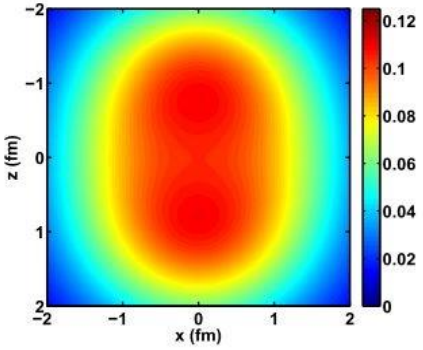
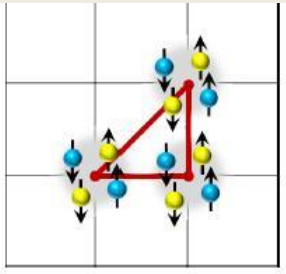


FIG. 12: (Color online) The $y = 0$ slice of the translationally-inv
density for the same state is on the right. These densities were

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

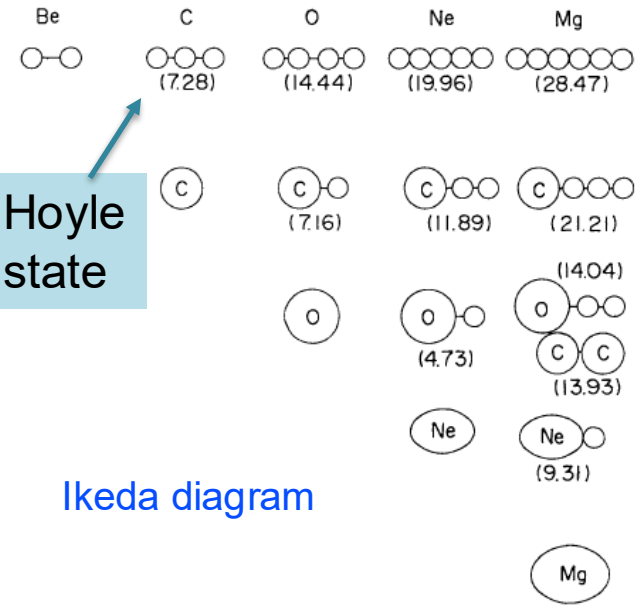


- ***ab initio No-Core* Monte Carlo Shell Model (MCSM)**

  This work -> clustering in Be and C isotopes

  its emergence and variation + Hoyle state

Alpha formation near the threshold energy



Hoyle state

Ikeda diagram

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 is considered to occur near the threshold energy, as a complementary binding mechanism.
This is a nice idea, and sounds plausible.

This has been a strong guiding principle for half a century.
We investigate whether this principle dominates the alpha clustering or not.

Shell Model calculations

Solve the eigenvalue problem : $\mathbf{H\,\Psi = E\,\Psi}$

$$\begin{pmatrix} \langle \phi_1 |H| \phi_1 \rangle & \langle \phi_1 |H| \phi_2 \rangle & \cdots \\ \langle \phi_2 |H| \phi_1 \rangle & \langle \phi_2 |H| \phi_2 \rangle & \cdots \\ \langle \phi_3 |H| \phi_1 \rangle & \cdots & \cdots \\ \langle \phi_4 |H| \phi_1 \rangle & \cdots & \cdots \\ \cdots & \cdots & \cdots \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ \cdots \\ \cdots \end{pmatrix} = E \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ \cdots \\ \cdots \end{pmatrix}$$

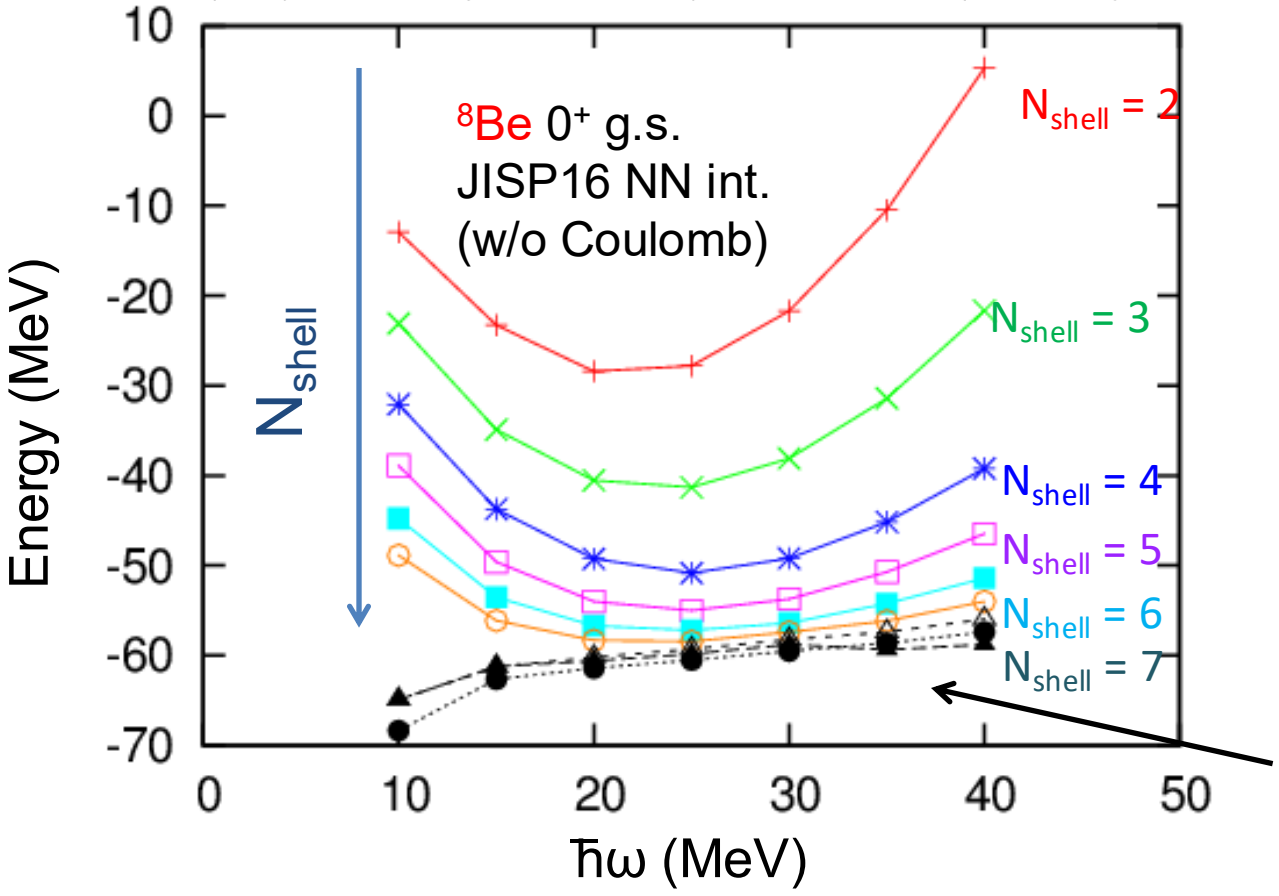
$\Psi = c_1\,\phi_1 + c_2\,\phi_2 + c_3\,\phi_3 + \ldots..$

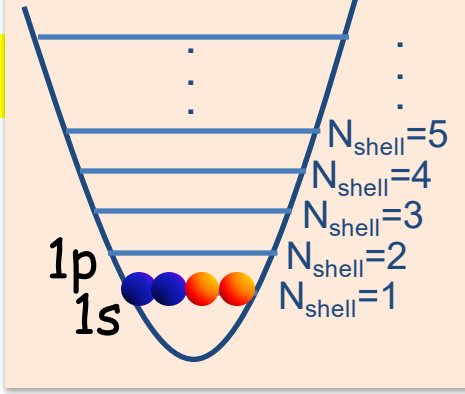
ϕ_i **Slater determinants,** c_i **probability amplitudes**

Extrapolation to infinite basis space in *ab initio* calculations

Energy eigenvalue at $N_{\rm shell} = N$ is expressed empirically as

$$E(N) = E(N=\infty) + a\exp(-bN)$$





Energy eigenvalue depends also on ħω

But, the eigenvalue in the infinite space should be independent of it, *i.e.*, flatness.

Extrapolation with
$N_{\rm shell}$ = 2 – 7 (●)
$N_{\rm shell}$ = 3 – 7 (▲)
$N_{\rm shell}$ = 4 – 7 (△)

c.f.) NCFC: -59.1(1) MeV
Extrapolated results to infinite $N_{\rm max}$

MCSM: -59.3(1.0) MeV
($N_{\rm shell}$ = 3 - 7, ħω = 20 - 35 MeV)

Density of protons ^{12}Be($0_{1,2}^+$) with group decomposition

nucleons in the cluster sectors

variations emphasized

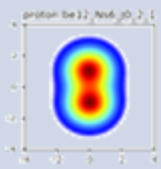
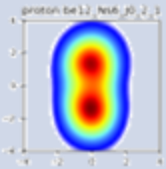
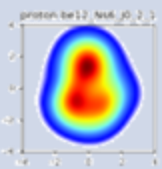
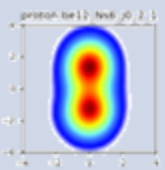
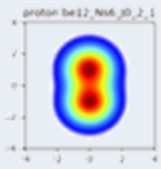
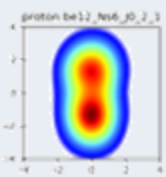
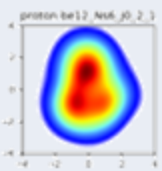
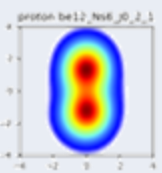
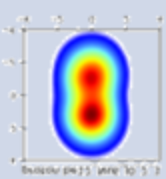
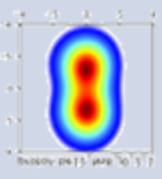
very preliminary

- Overlap probabilities in 0_1^+

  $|\langle GP2|GP5\rangle|^2 = 0.01$, $|\langle GP2|GP12\rangle|^2 = 0.80$, $|\langle GP2|GP13\rangle|^2 = 0.10$,

  $|\langle GP5|GP13\rangle|^2 = 0.15$, $|\langle GP12|GP13\rangle|^2 = 0.10$

Density profiles of each group

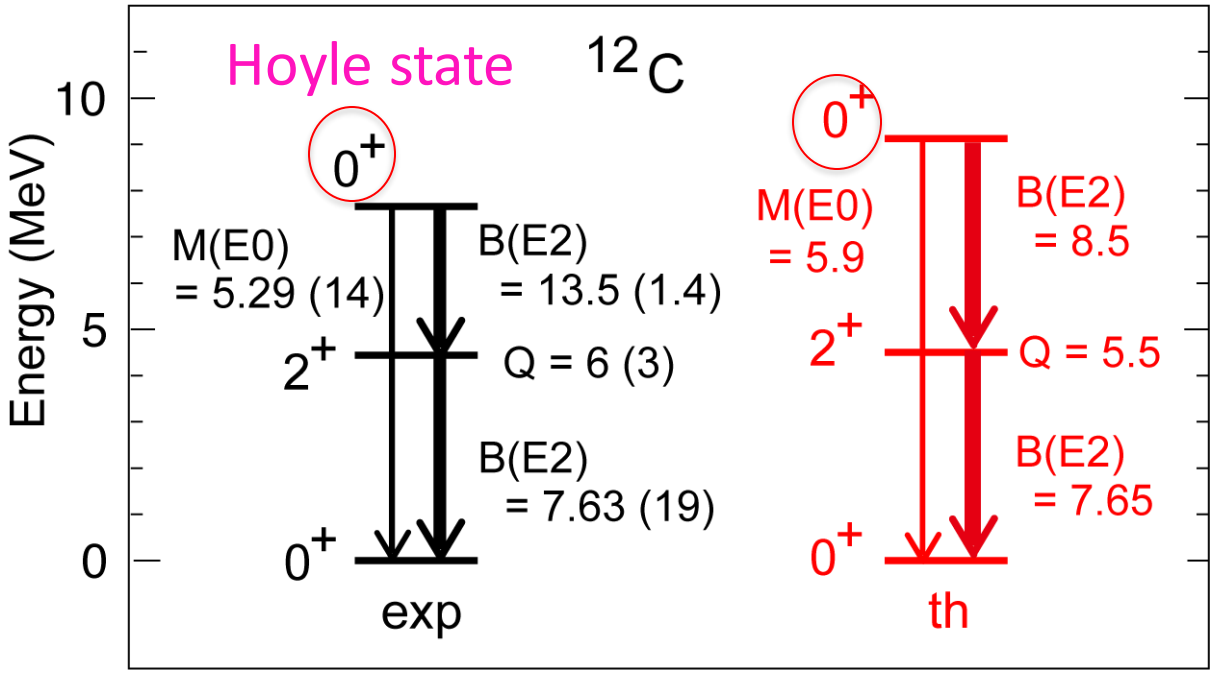
	GP2 $\alpha^2\pi^4$	GP5 $\alpha^2\pi^{2?}\sigma^{2?}$	GP12 $\alpha\alpha^*??$	GP13 $\alpha^2\pi^{2?}\sigma^{2?}$
0_1^+	 39%	 59%	 46%	 40%
0_2^+	 45%	 38%	 49%	 45%
0_3^+		 94%		 35%

Energy level & transition strength of ^{12}C

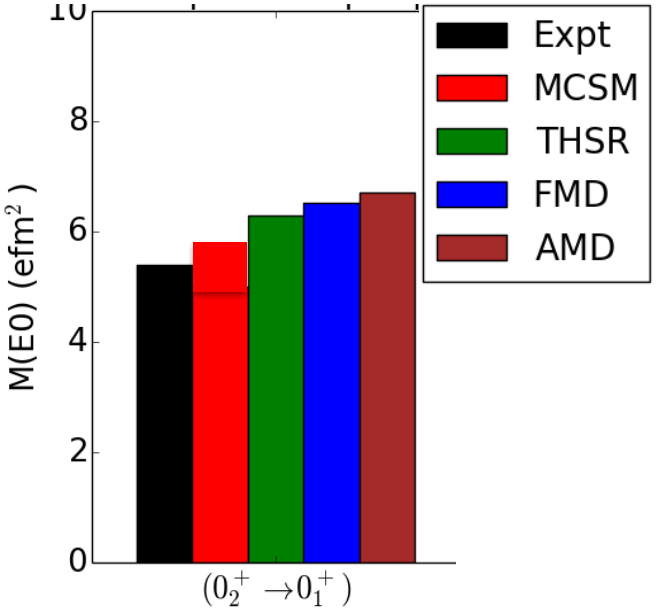
correlation effects are explicitly treated
(no medium correction needed)

charges protons 1e
neutrons 0e

0^+ Linear ?



$M(E0; 0^+_2 \rightarrow 0^+_1)$



M(E0) = 5.29 e fm^2
(Daejeon, 7shell, hw=20MeV)

Expt.: ENSDF
THSR: Y. Funaki 2015
FMD: M. Chernykth 2007
AMD: Y. Kanada-En'yo 2007

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.