MCD2022 –3rd week, YKIS
Yukawa Institute
May 25 (23-27), 2022

New facets of alpha-clustering and deformation towards driplines depicted by nuclear forces

Takaharu Otsuka

This work was supported 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.

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

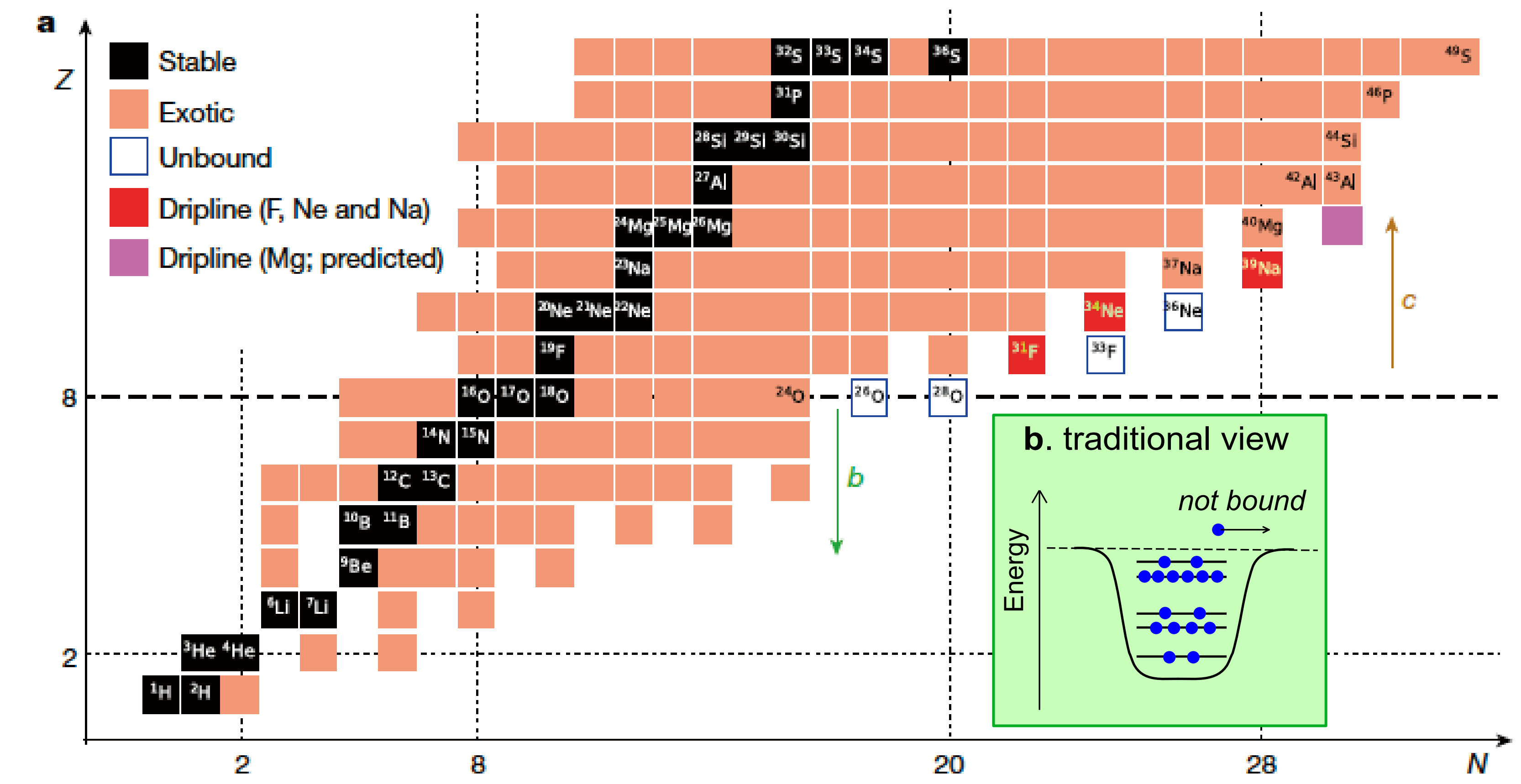
First topic (very brief)

ab initio interaction EEdf1

and

emerging driplines

Neutron driplines and its traditional view



nature

Article | Published: 04 November 2020

The impact of nuclear shape on the emergence of the neutron dripline

Naofumi Tsunoda, Takaharu Otsuka, Kazuo Takayanagi, Noritaka Shimizu, Toshio Suzuki, Yutaka Utsuno, Sota Yoshida & Hideki Ueno

Nature **587**, 66–71(2020) | Cite this article

Chiral EFT *NN* int. + Fujita-Miyazawa 3*N* int. with averaging

(to be replaced by EFT N2LO 3*N* int.)

$V_{\text{low k}}$: treatment of high-momentum components

EKK : in-medium correction (core polarization)
(*conventional MBPT may diverge in two major shells*)

Krenciglwa and Kuo (1971) -> Extended KK (by Takayanagi)

ab initio effective interaction : EEdf1

Shell model (or Configuration Interaction; CI) calculation
by the conventional matrix diagonalization
or by the Monte Carlo Shell Model

Energy levels, electromagnetic matrix elements
(diagonalization of Hamiltonian matrix)

A development starting from chiral EFT

EKK method* to handle consistently
two (or more) major shells
-> Effective shell-model interaction
(i) without fit of two-body m. e.,
(ii) applicable to broken magicity, or
merging two shells,
both are crucial for exotic nuclei.

*) Extended Krenciglwa-Kuo method is a magic by Takayanagi

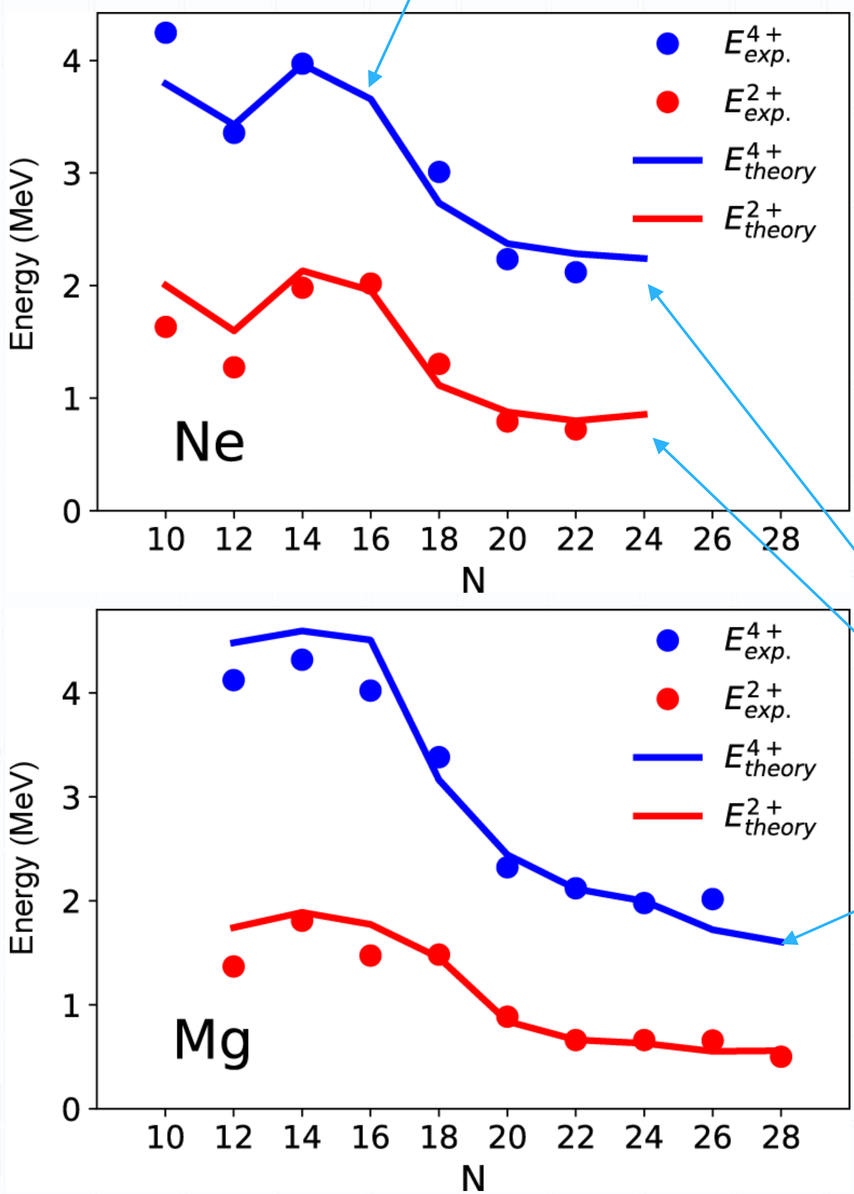
K. Takayanagi, Nucl. Phys. A 852, 61 (2011).

N. Tsunoda, **K. Takayanagi**, M. Hjorth-Jensen, and T. Otsuka, Phys. Rev. C 89, 024313 (2014).

K. Takayanagi, Annals of Physics 350, 501 (2014).

Ne and Mg systematics

We use the EEdf1 interaction derived from the N3LO chiral EFT interaction + Fujita-Miyazawa three-nucleon force.



The EEdf1 Hamiltonian appears to be reasonable up to N~28 for Z=9-12.

Levels do not exist as bound states, because their energies are above the threshold of neutron emission.

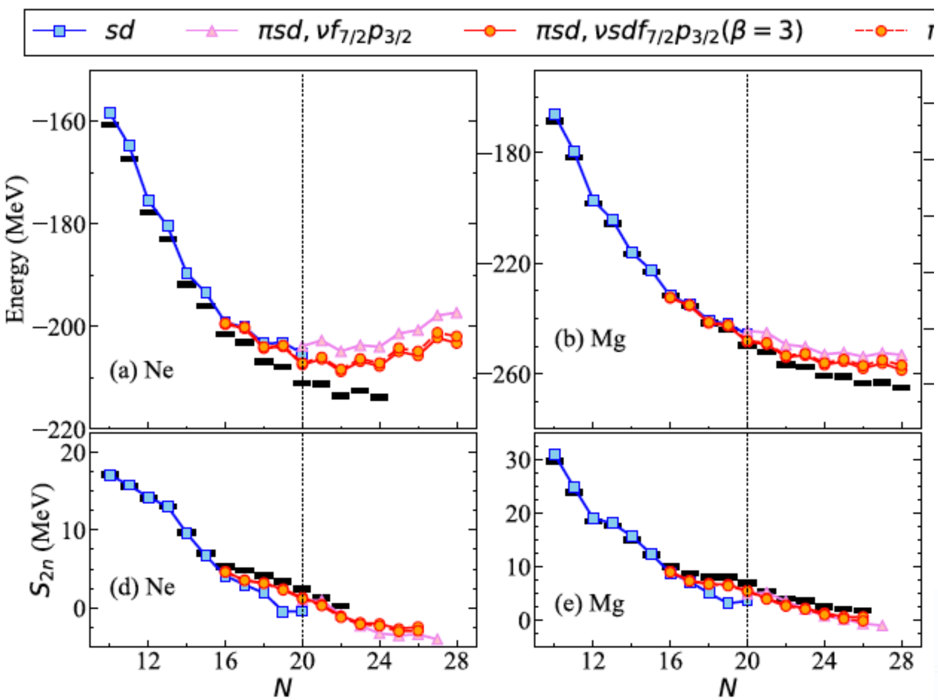
Recent *ab initio* calculation (IM-SRG)

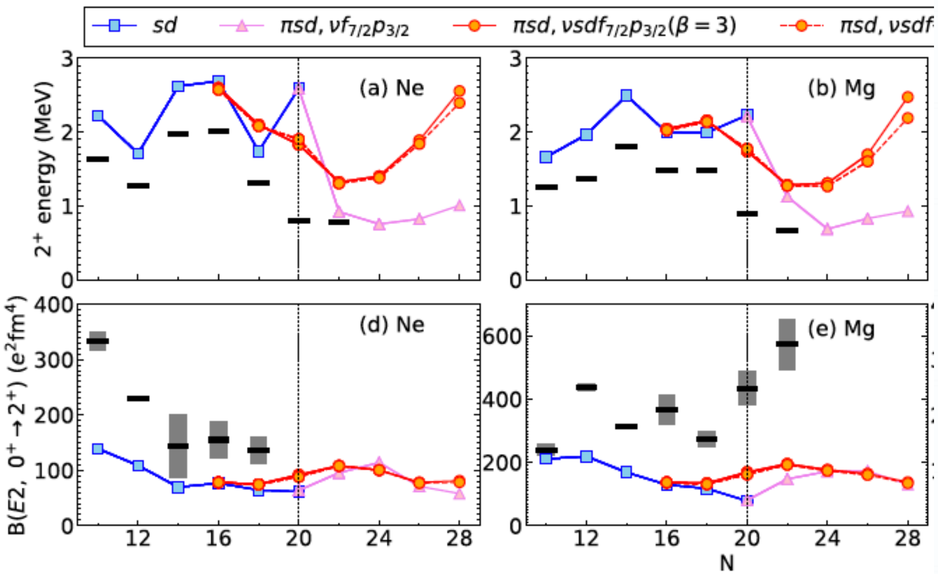
PHYSICAL REVIEW C **102**, 034320 (2020)

Editors' Suggestion

Ab initio multishell valence-space Hamiltonians and the island of inversion

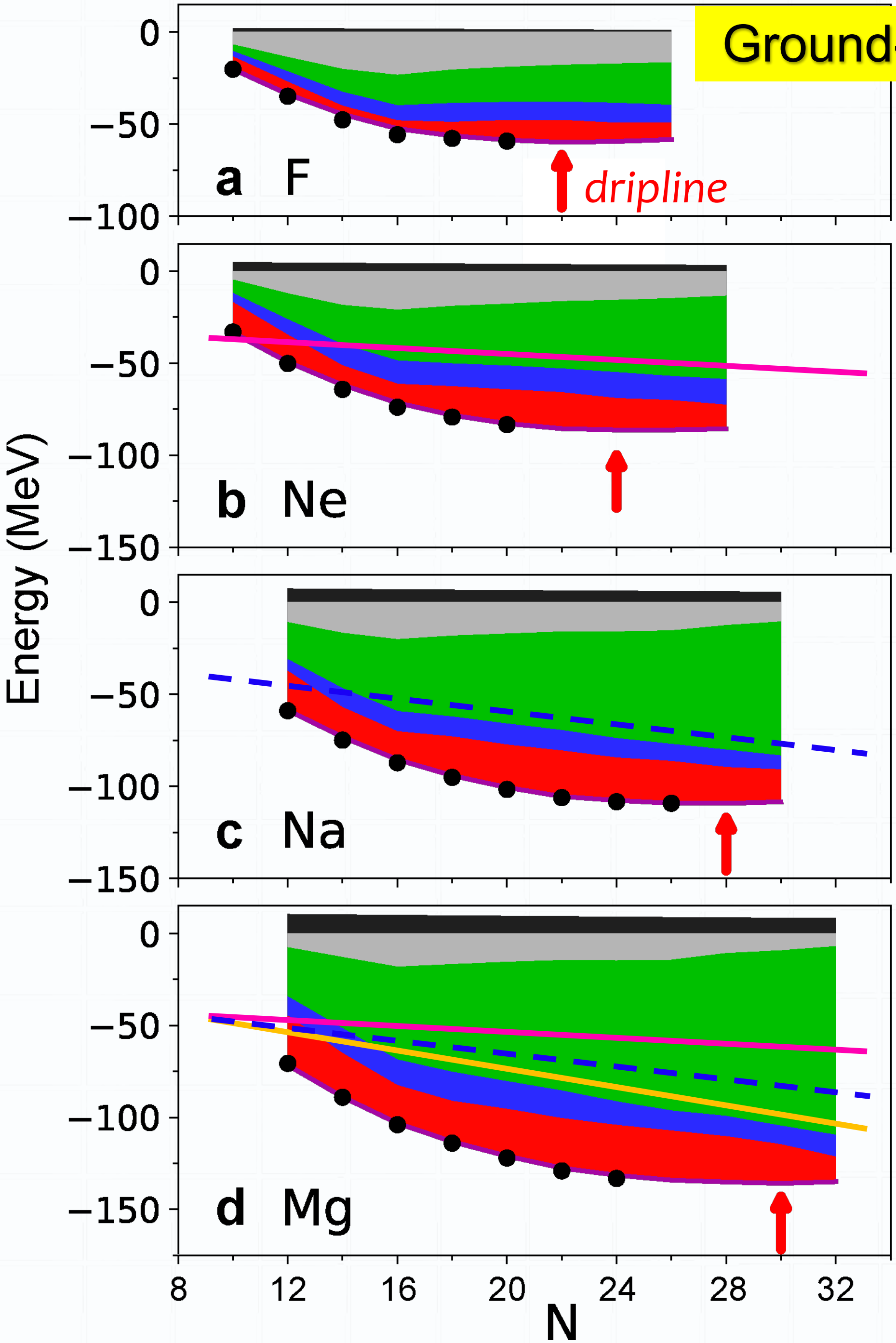
T. Miyagi,[1] S. R. Stroberg,[2] J. D. Holt,[1,3] and N. Shimizu[4]

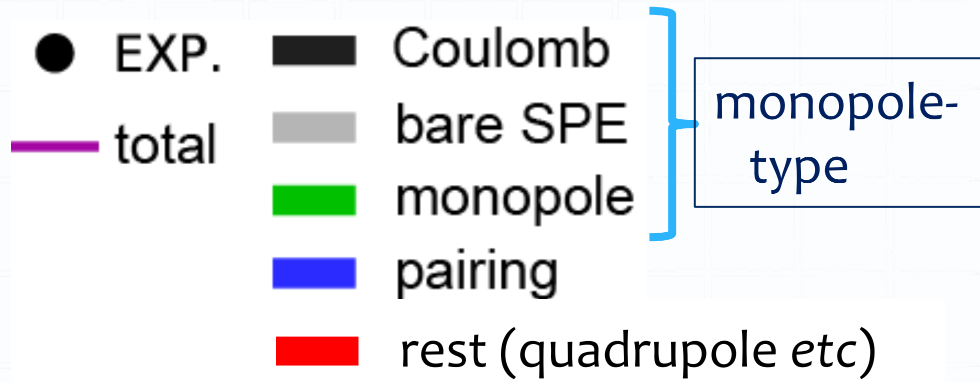




Large deformation seems to be a challenge.

Ground-state energy is decomposed (EEdf1 int.)





The monopole effect (lower edge of green part) lowers the energy as a function of *N*, and its slope becomes steeper as *Z* because of the p-n monopole int., as shown by three lines fitted to different slopes.

The rest (~quadrupole deformation) effect (red part) varies locally.

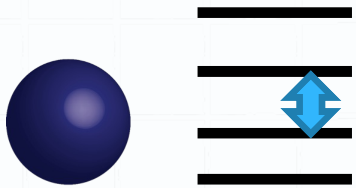
… see next page

Decomposition of the Hamiltonian

monopole part

bare SPE $\sum \epsilon_i a_i^+ a_i$

monopole $\sum_{i,j} V^{ab}_{\mathrm{mono}} a_i^+ a_j^+ a_j a_i$ $\quad V^{ab}_{\mathrm{mono}} = \sum_J \frac{(2J+1)\langle ab|V|ab\rangle_J}{2J+1}$

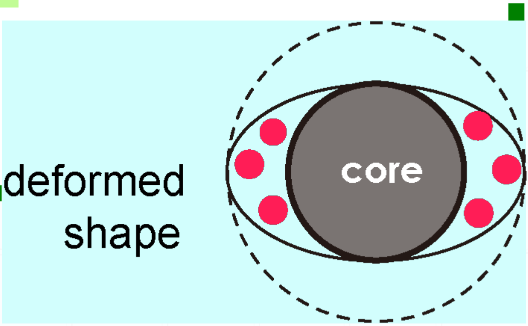


monopole: shift of SPE

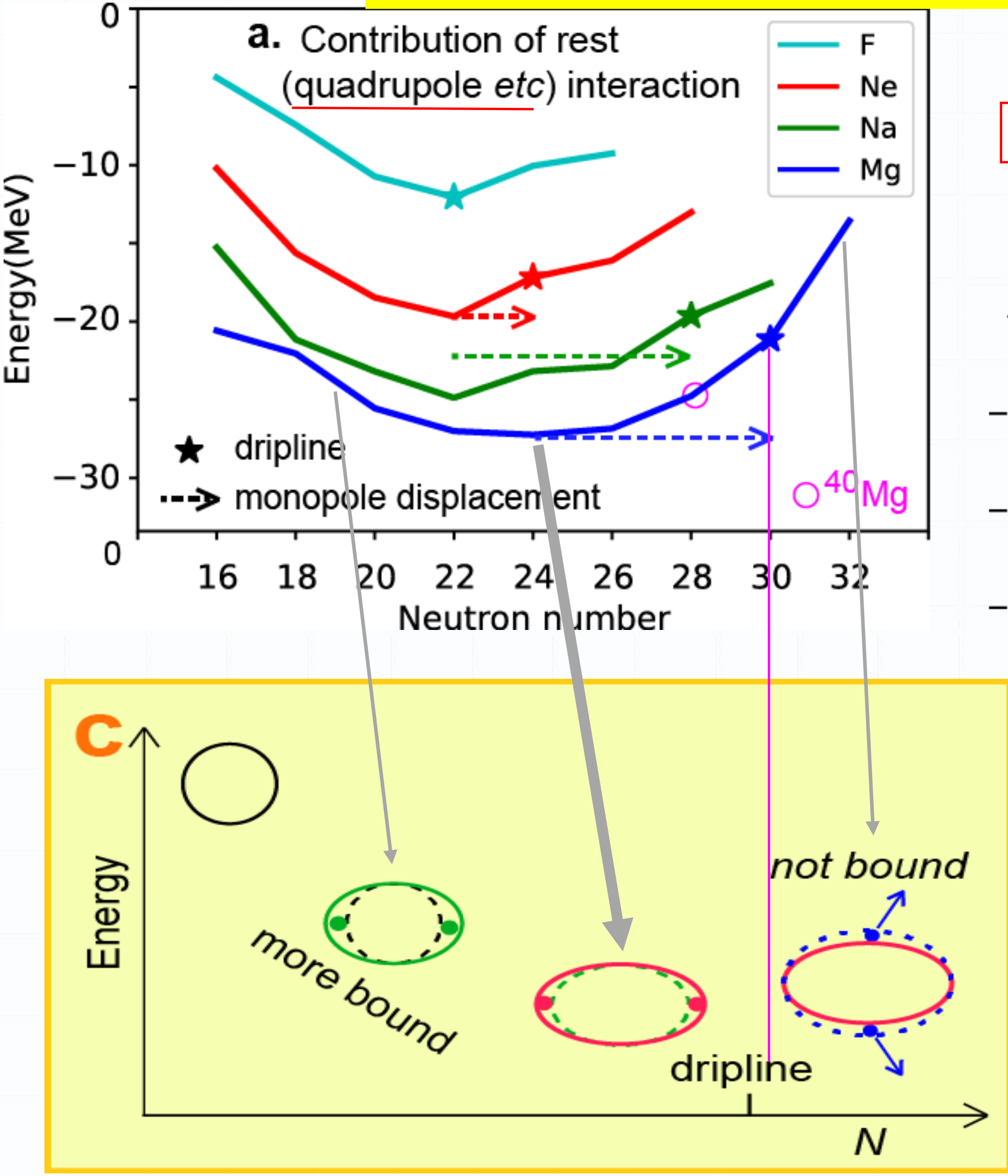
multipole part

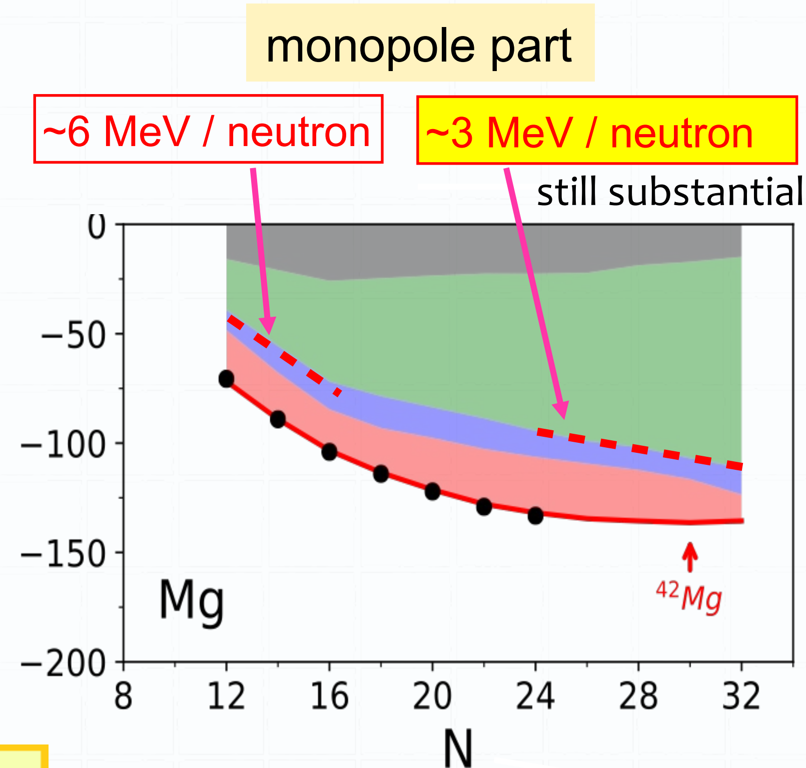
pairing J=0 nn + pp pairing correlations

rest quadrupole deformation, *etc*



Two driving forces: example from Mg isotopes

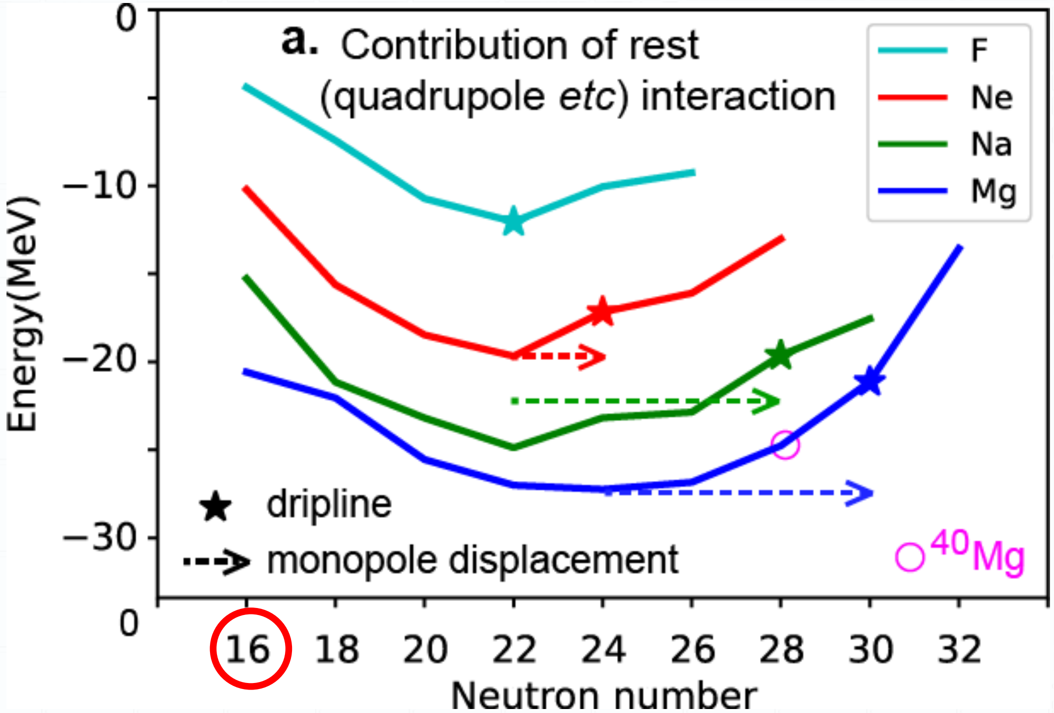


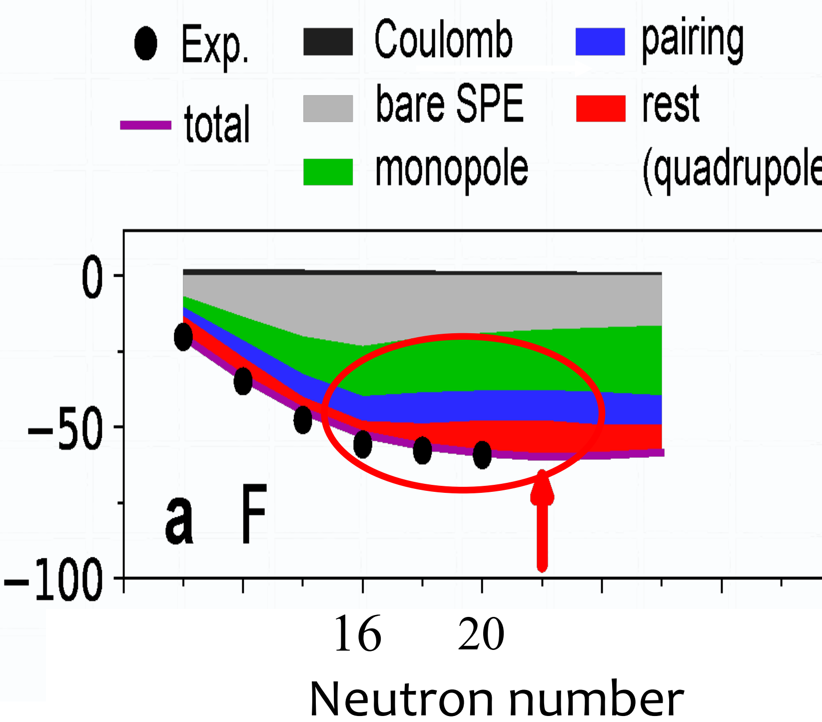


The rest (mainly deformation energy) part is saturated at *N*=24

The monopole effects compensate it, and pushes the dripline away (dashed arrows).

Dripline of F isotopes



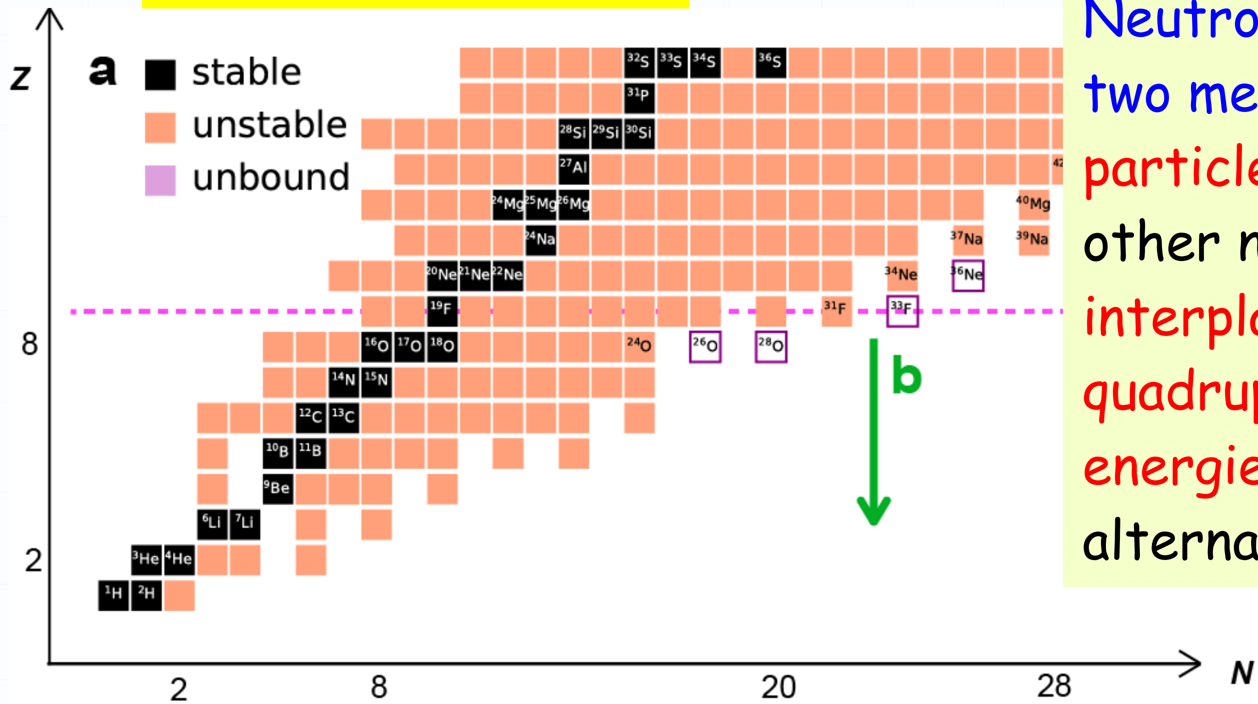


Monopole effect (edge of green part) becomes weaker for N > 16 in F isotopes. It even decreases because of high-lying d3/2 (see gray edge).

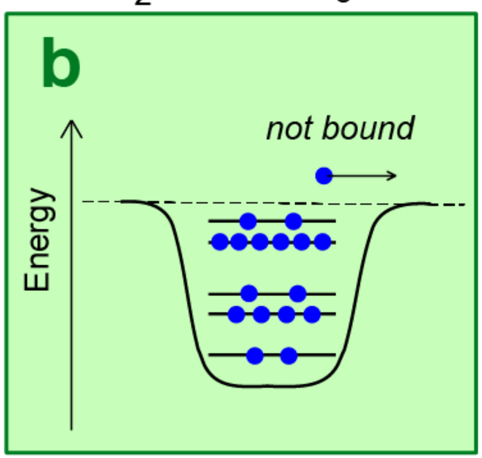
If there were no "rest" (~ quadrupole deformation) effect (red part), the dripline would be at N = 16, which is the same as oxygen isotopes.

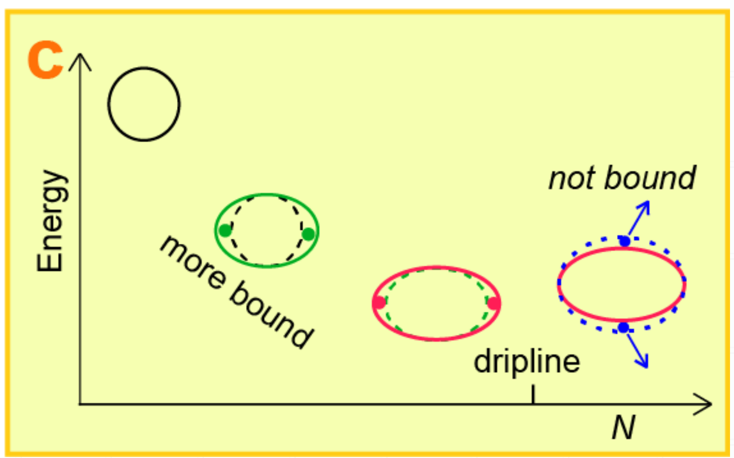
Loose binding phenomena may be seen (?), in contrast to Ne, Na or Mg.

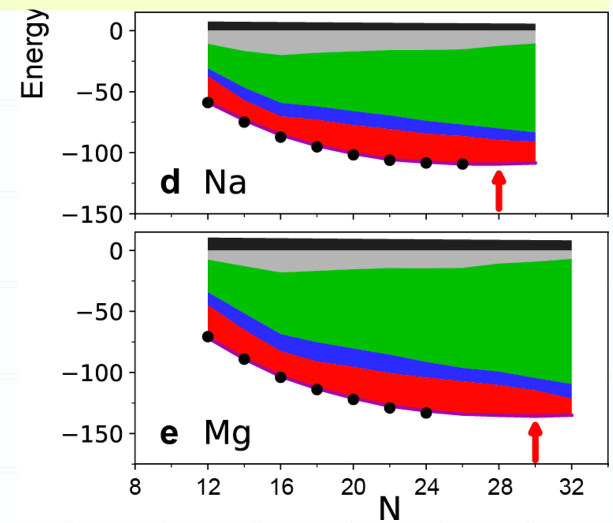
Dripline mechanisms



Neutron driplines are due to two mechanisms: one has single-particle origin (b), while the other new one (c) is due to the interplay of monopole and quadrupole (deformation) energies. They may appear alternatively as Z increases.







Traditional (vague) view
-> extreme: neutron halo

New view

Intermedaite case: ^{22}C

Suzuki, O, Yuan & Alahari, PLB 753, 199 (2016).

Main topic

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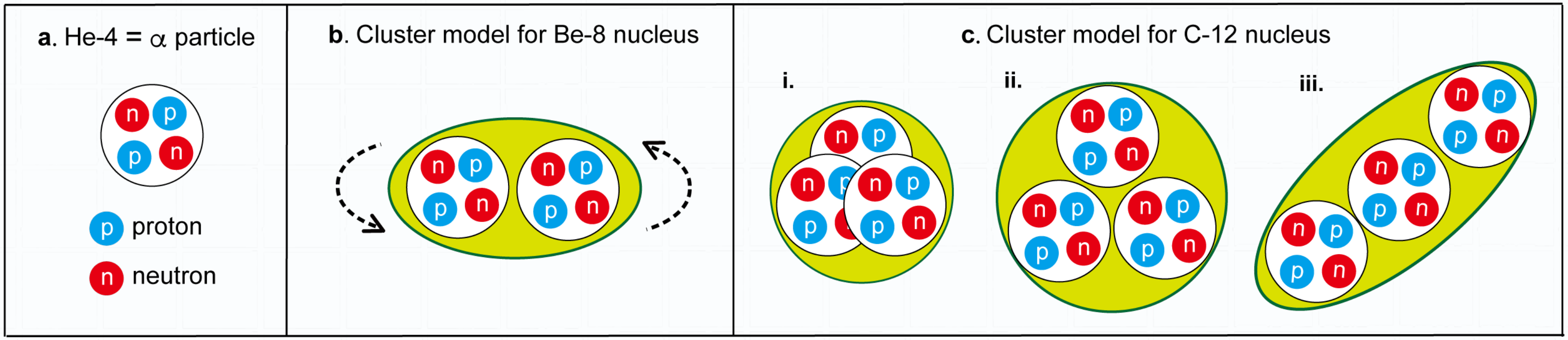
α cluster formation - intuitive image -



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

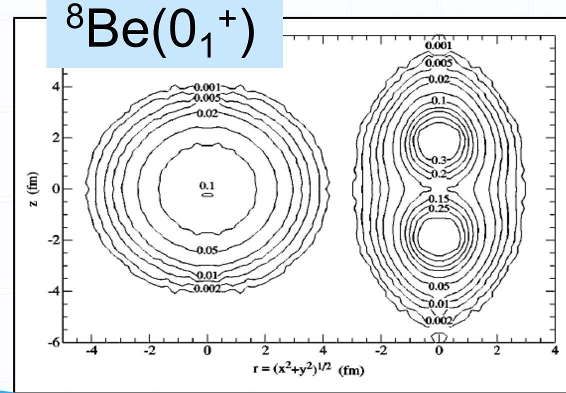
Brink, D., Alpha-Particle Model of Light Nuclei. The Proc. Intl. School of Physics Enrico Fermi, Course, 36 (1966), p. 247.
Ikeda, K., Takigawa, N. and Horiuchi, H., The systematic structure-change into the molecule-like structures in the self-conjugate 4n nuclei. Prog. Thoer. Phys. Suppl., **E68**, 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.

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

Foundation from sound underlying bases

^{8}Be(0_1^+)



Its contemporary versions

Ab initio **calculations on clustering aspects**

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

  Variational Monte Carlo (VMC)

  [Wiringa et al. 2000]

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

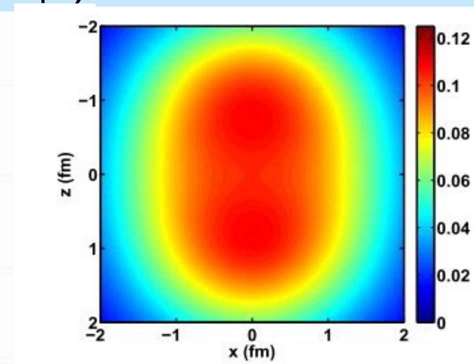


FIG. 12: (Color online) The $y = 0$ slice of the translationally-inv density for the same state is on the right. These densities were

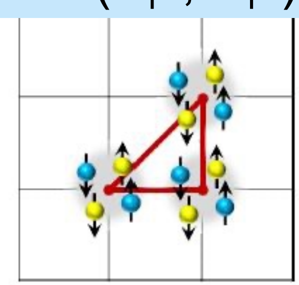
- No Core Full Configuration (NCFC) :

  [Cockrel et al. 2012] *Not clustering*

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

  Initial setup

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



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

  This work -> clustering in Be and C isotopes

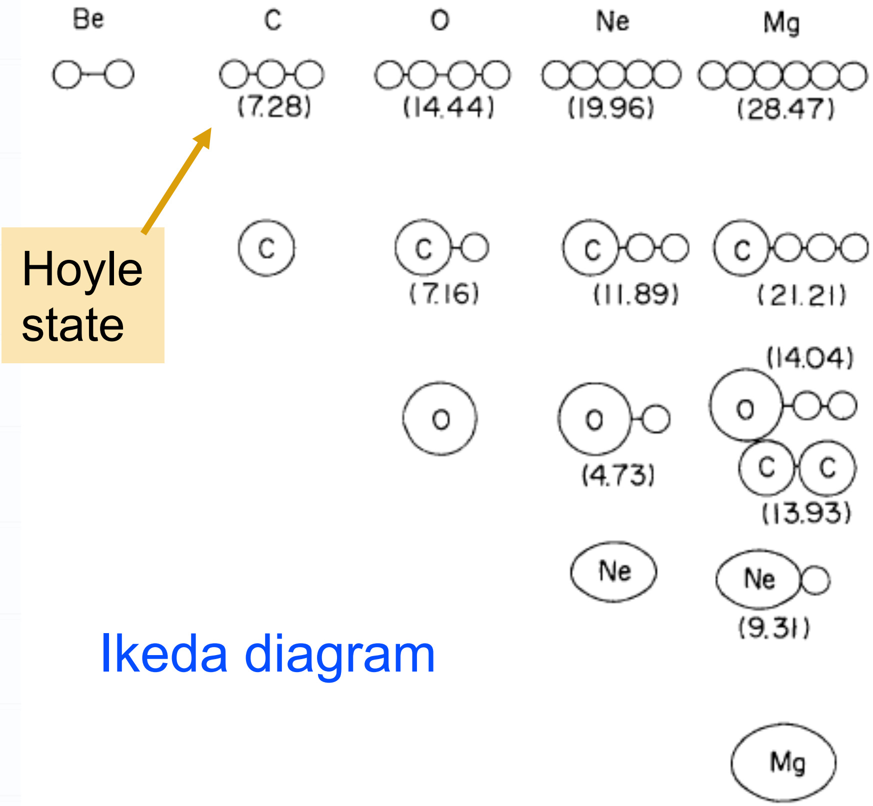
  its emergence and fading + Hoyle state

Alpha formation near the threshold energy

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



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.

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.

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How to calculate ?

ab initio No-Core Monte Carlo Shell Model

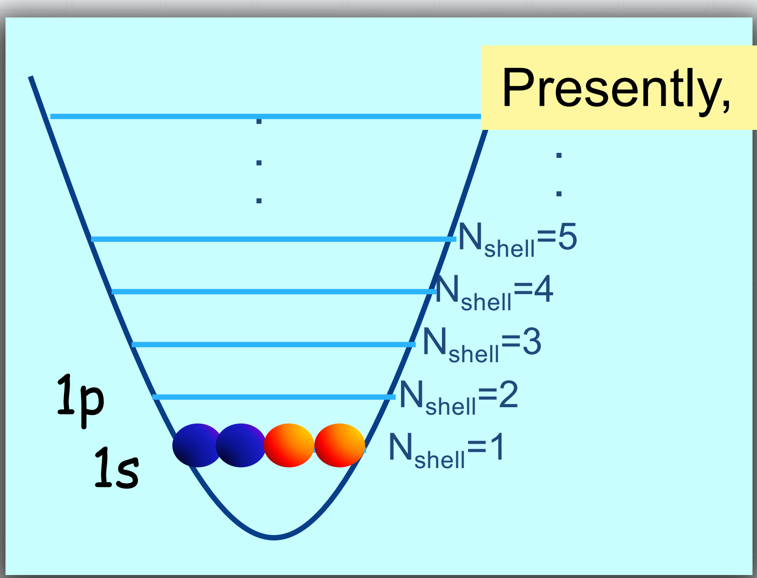
(MCSM)

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.

Note: The first part was done with the sd+pf shell with the ^{16}O *core.*
So, it is different !

Single-particle states included



Presently, up to Nshell =7 (6 hw)

Solve the Schrödinger equation

$$H\Psi = E\Psi$$

E : eigenenergy

Ψ : eigenstate

+ kinetic energy

Nucleon-Nucleon interaction

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).

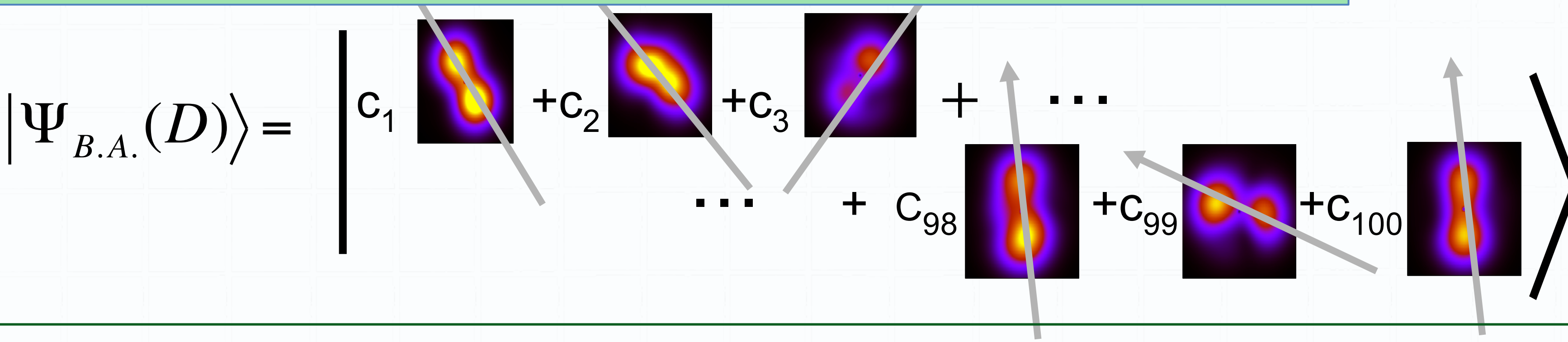
Machleidt, R. & Entem, D. R., Chiral effective field theory and nuclear forces, Phys. Rep. **503**, 1 (2011).

The interactions are fixed prior to the present calculation.

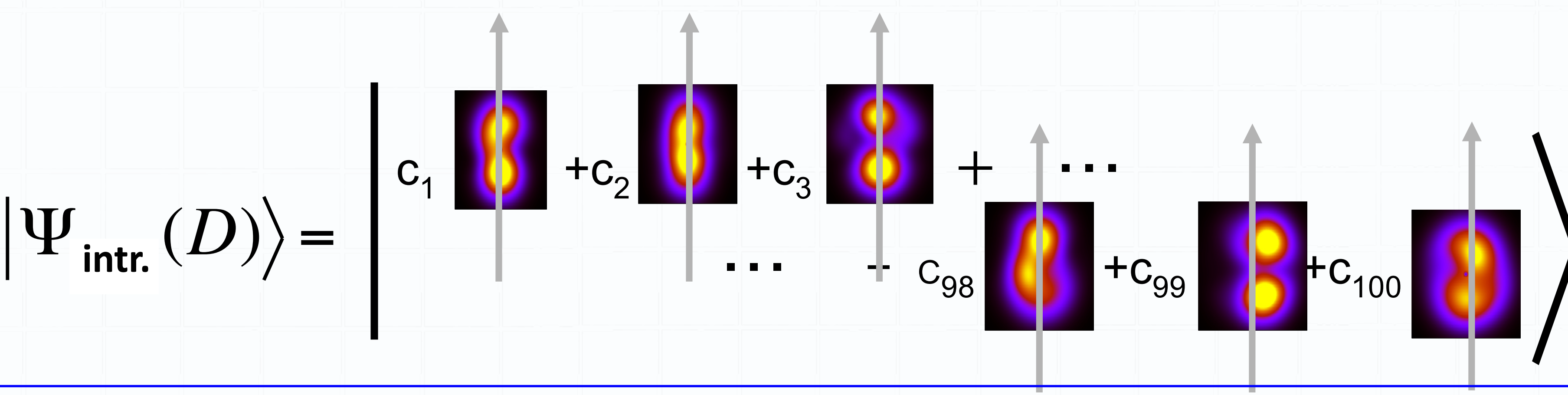
MCSM eigenstate : $\left|\Psi(D)\right\rangle = \sum_{n=1}^{N_B} c_i P^{J,\Pi} \left|\phi(D^{(n)})\right\rangle$

Deformed Slater determinant with three axes of ellipsoid

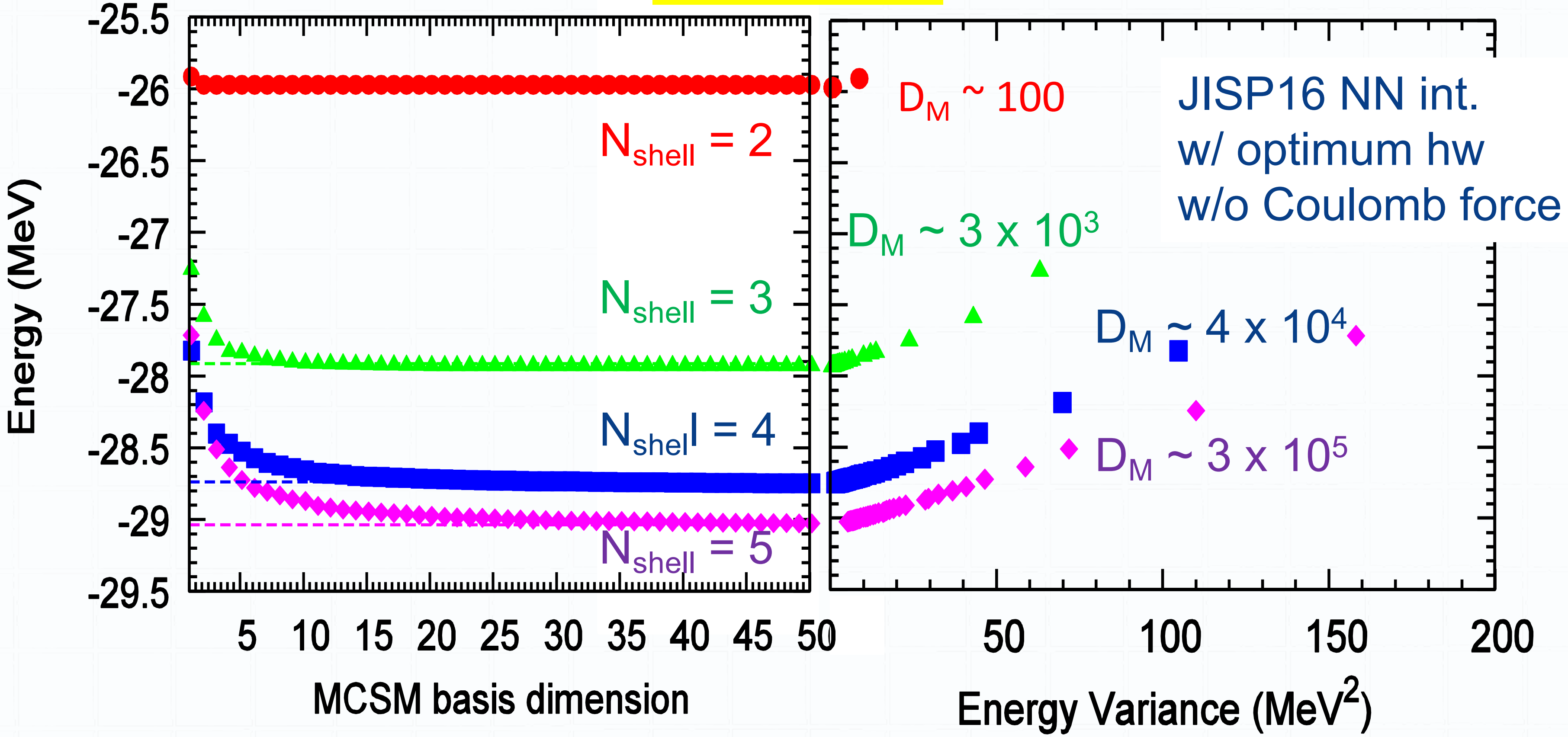
For J^{π} projected states, individual orientations are not relevant.



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.



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



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)

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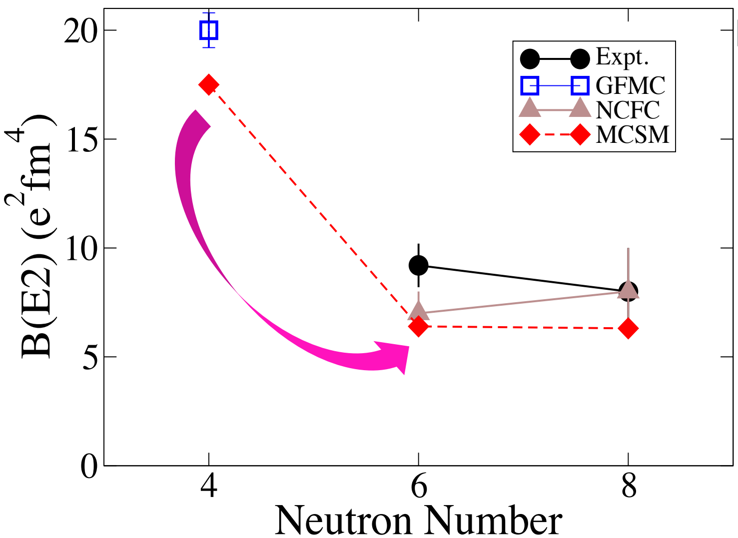
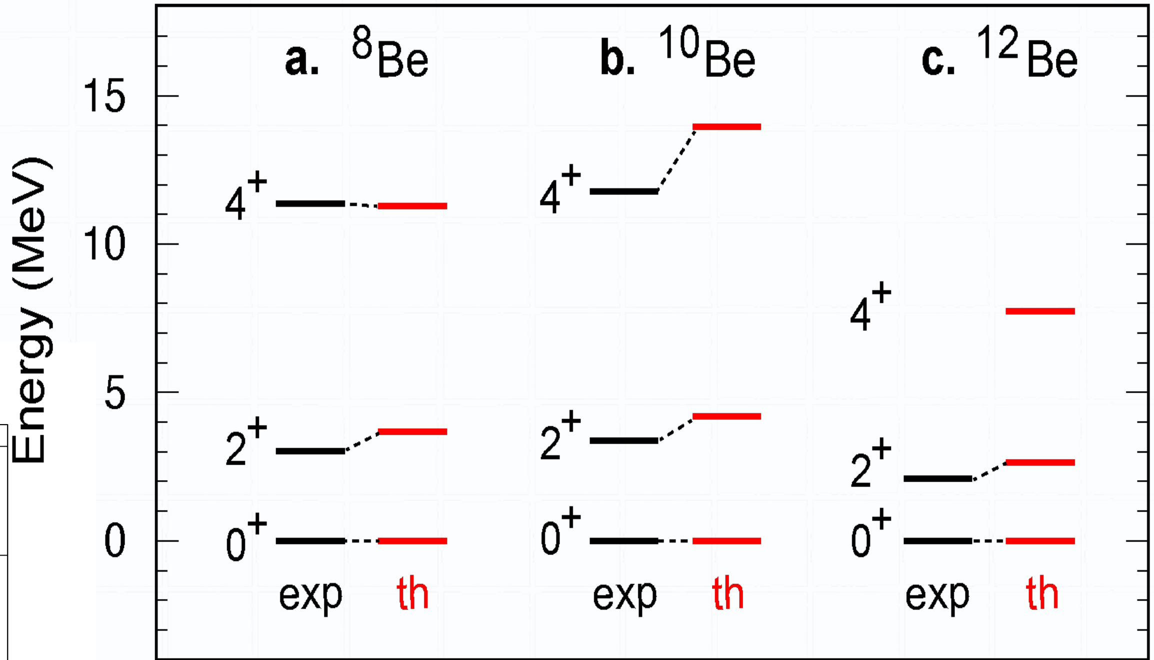
Levels and B(E2)'s of Be isotopes

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



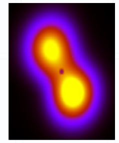
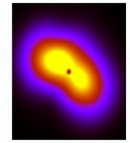
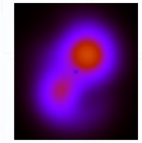
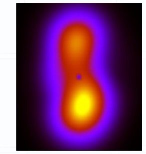


excitation level patterns indicate the occurance of the rotational motion of a deformed "object"

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

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

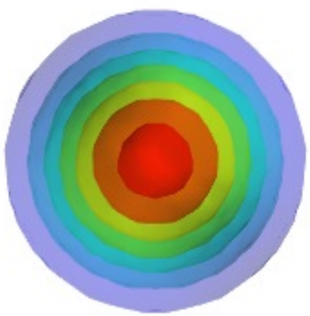
$$|\Phi\rangle = \sum_{i=1}^{N_{basis}} c_i|\Phi_i\rangle =$$

c_1  $+ c_2$  $+ c_3$  $+ c_4$  $+ \dots$

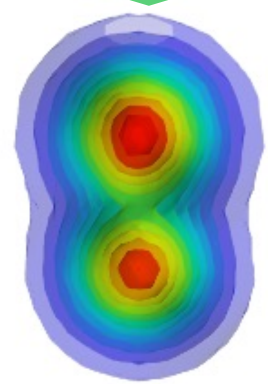
Angular-momentum projection

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

We need something like this.

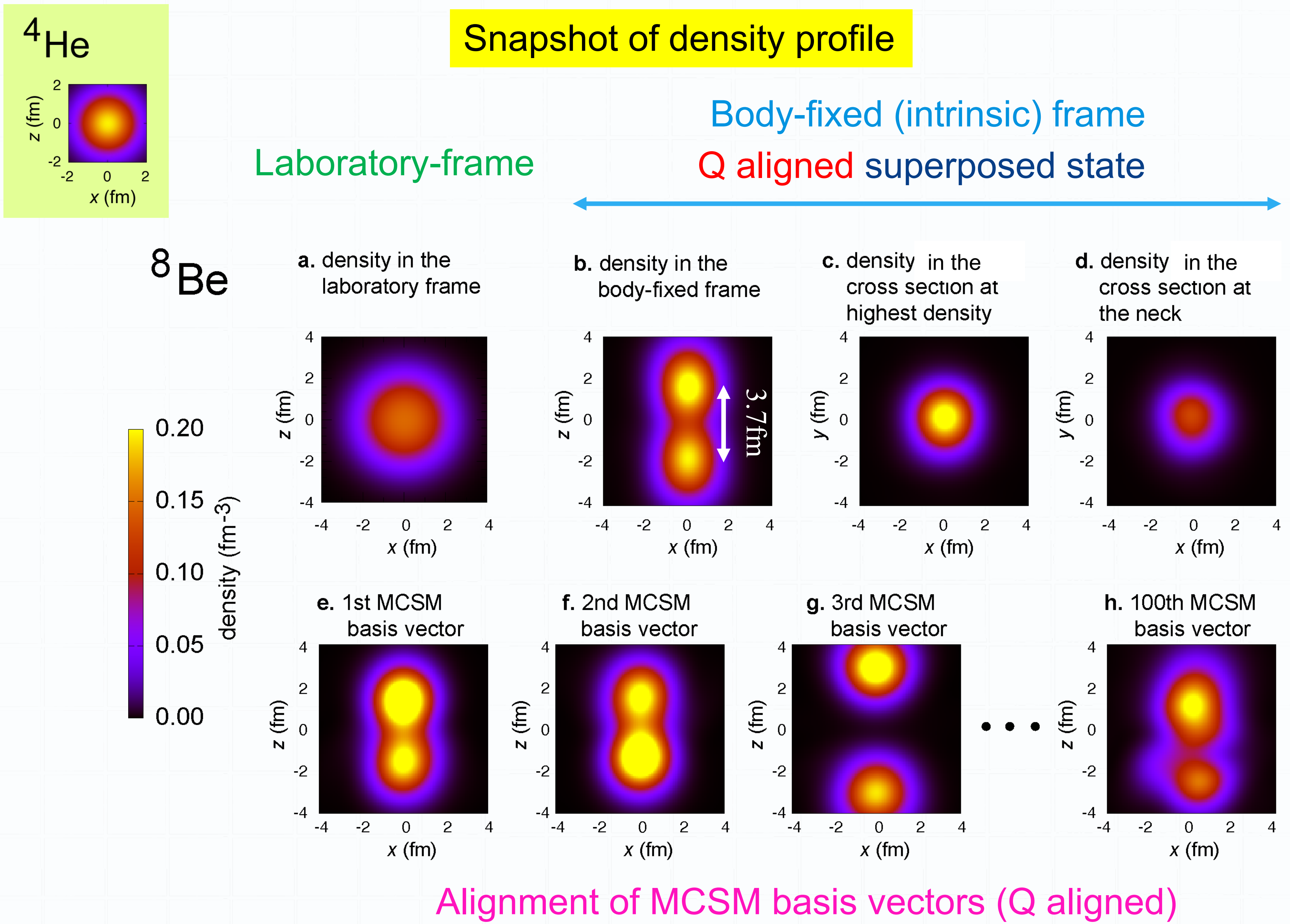


^{8}Be 0$^+$ ground state



Laboratory frame

"Intrinsic" (body-fixed) frame



Snapshot of density profile
4He
z (fm)
x (fm)
Laboratory-frame
Body-fixed (intrinsic) frame
Q aligned superposed state
8Be
a. density in the laboratory frame
b. density in the body-fixed frame
3.7 fm
c. density in the cross section at highest density
d. density in the cross section at the neck
y (fm)
0.20
0.15
0.10
0.05
0.00
density (fm-3)
e. 1st MCSM basis vector
f. 2nd MCSM basis vector
g. 3rd MCSM basis vector
h. 100th MCSM basis vector
Alignment of MCSM basis vectors (Q aligned)

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

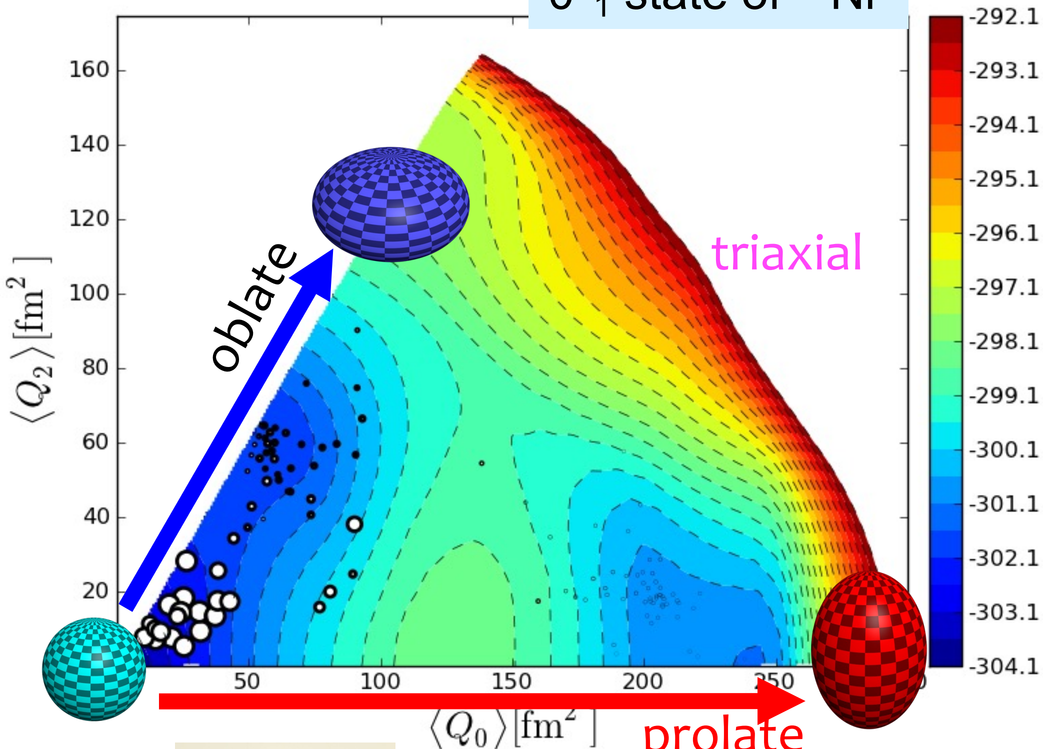
eigenstate $\Psi = \sum_i c_i P[J^\pi] \Phi_i$

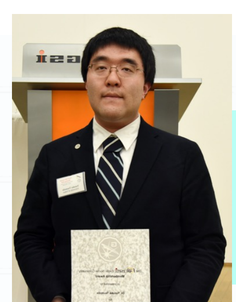
stochastically deformed Slater determinant
→ intrinsic shape

amplitude

projection onto J^π

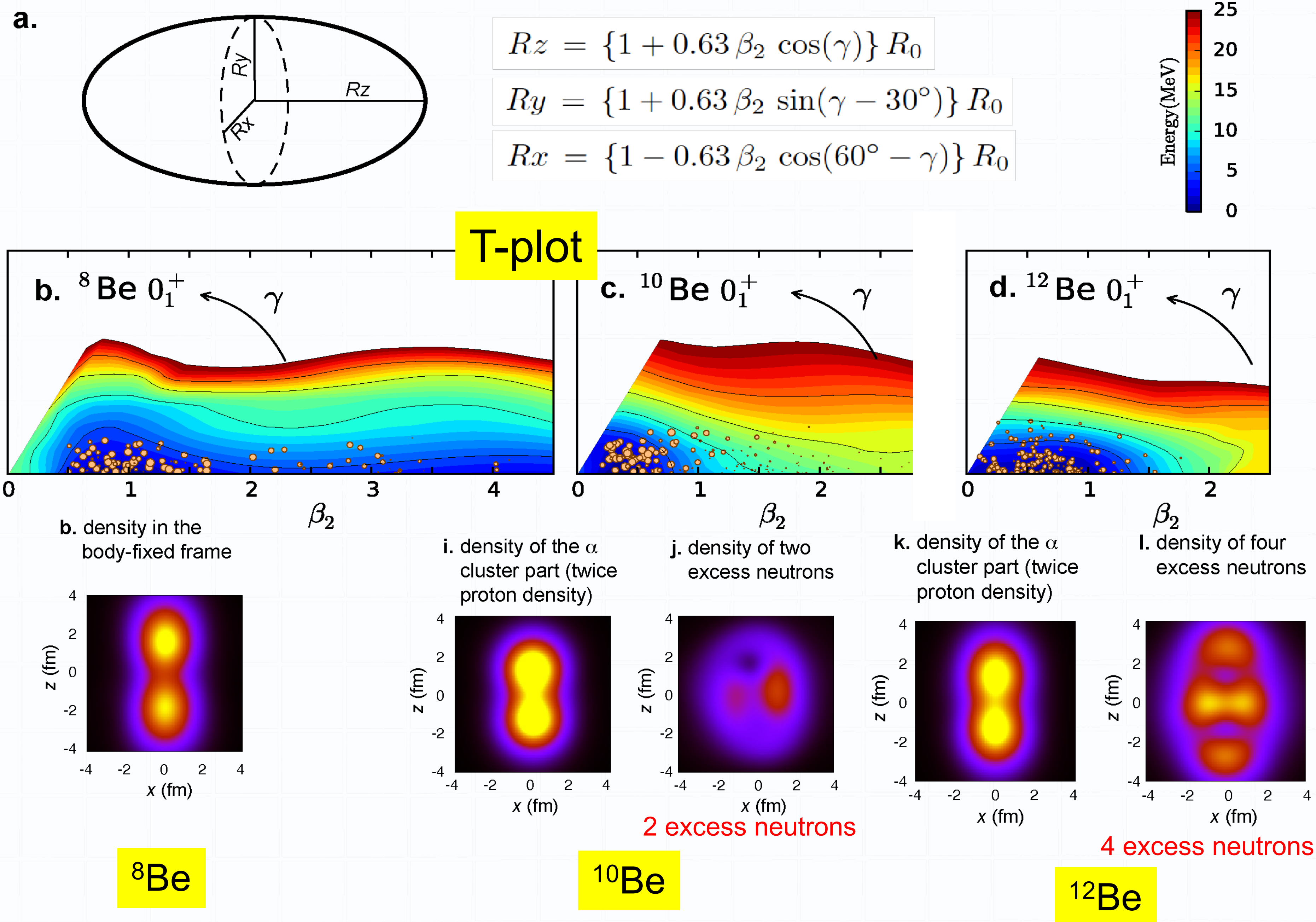
- PES is calculated by CHF for the shell-model Hamiltonian
- Location of circle : quadrupole deformation of unprojected MCSM basis vectors
- Area of circle : overlap probability between each projected basis and eigen wave function





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

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



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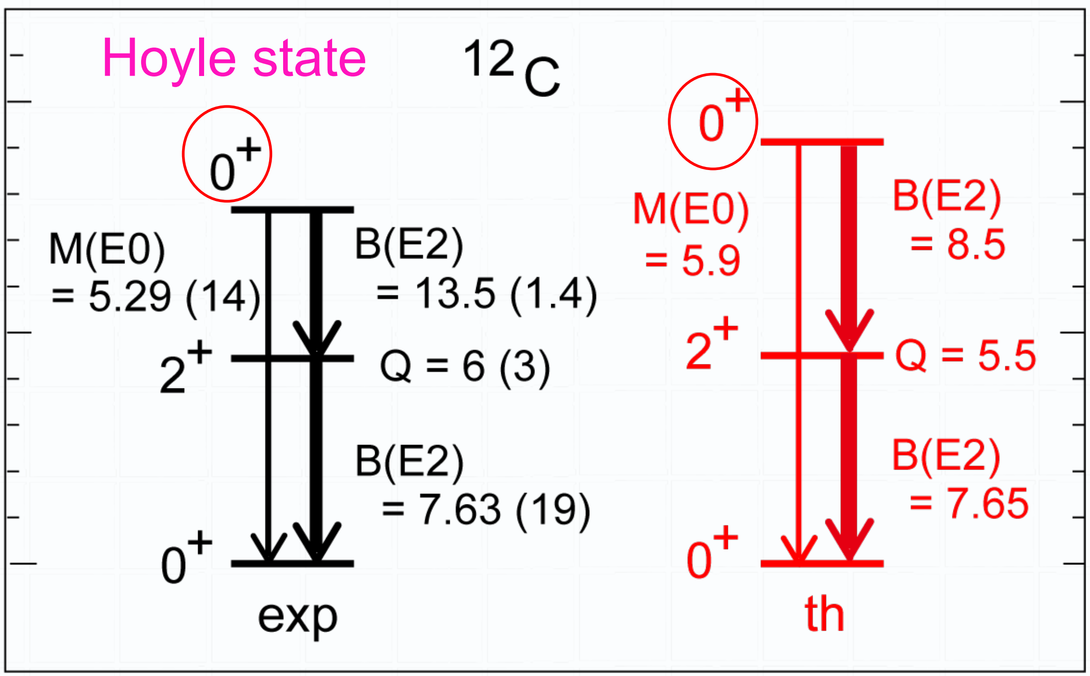
Energy level & transition strength of ^{12}C

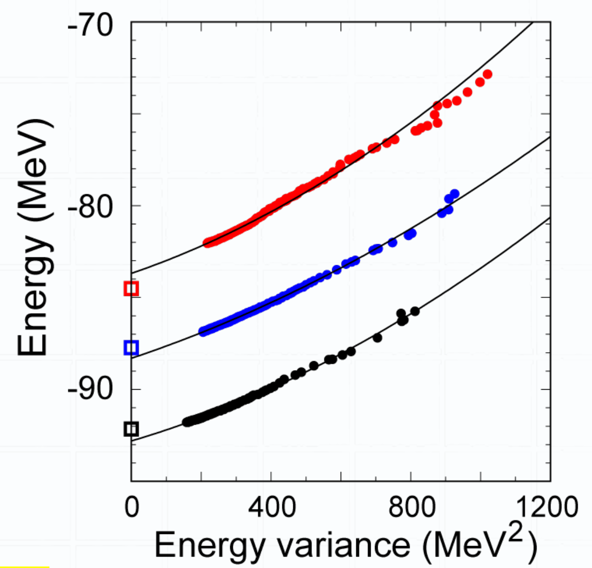
ab initio no-core MCSM + Daejeon 16 interaction (Shirokov et al.) based on chiral EFT (Machleidt-Entem, 2011)

charges protons 1e
neutrons 0e

correlation effects are explicitly treated
(no medium correction needed)



convergence pattern as functions of energy variance

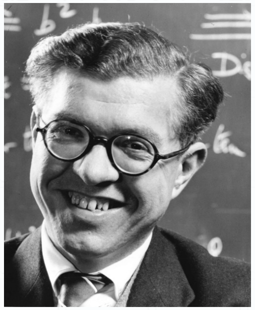


Strong deformation (β_2~0.6, oblate) in the 0^+_1 and 2^+_1 states can now be described from *first principles*.

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

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
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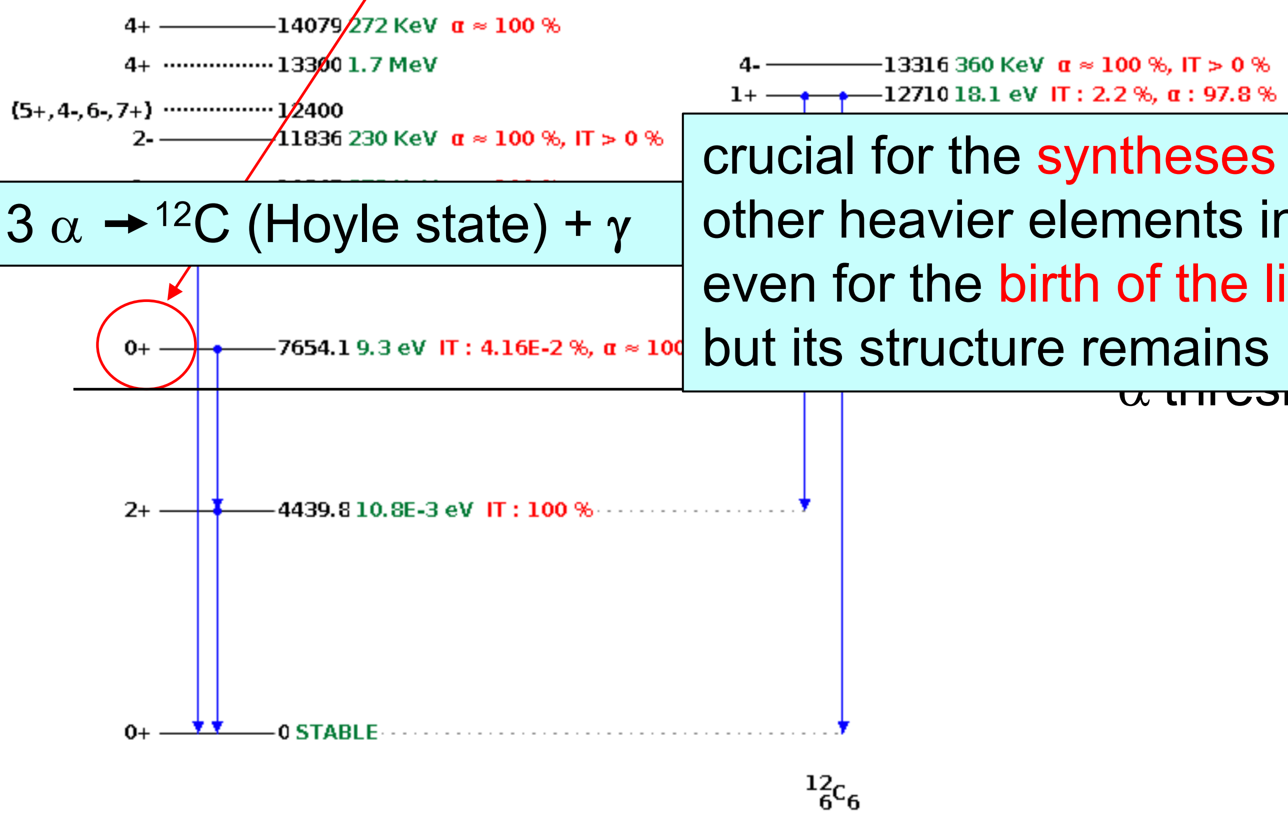
Received December 22, 1953

$A_0 = 4$, $Z_0 = 2$, 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

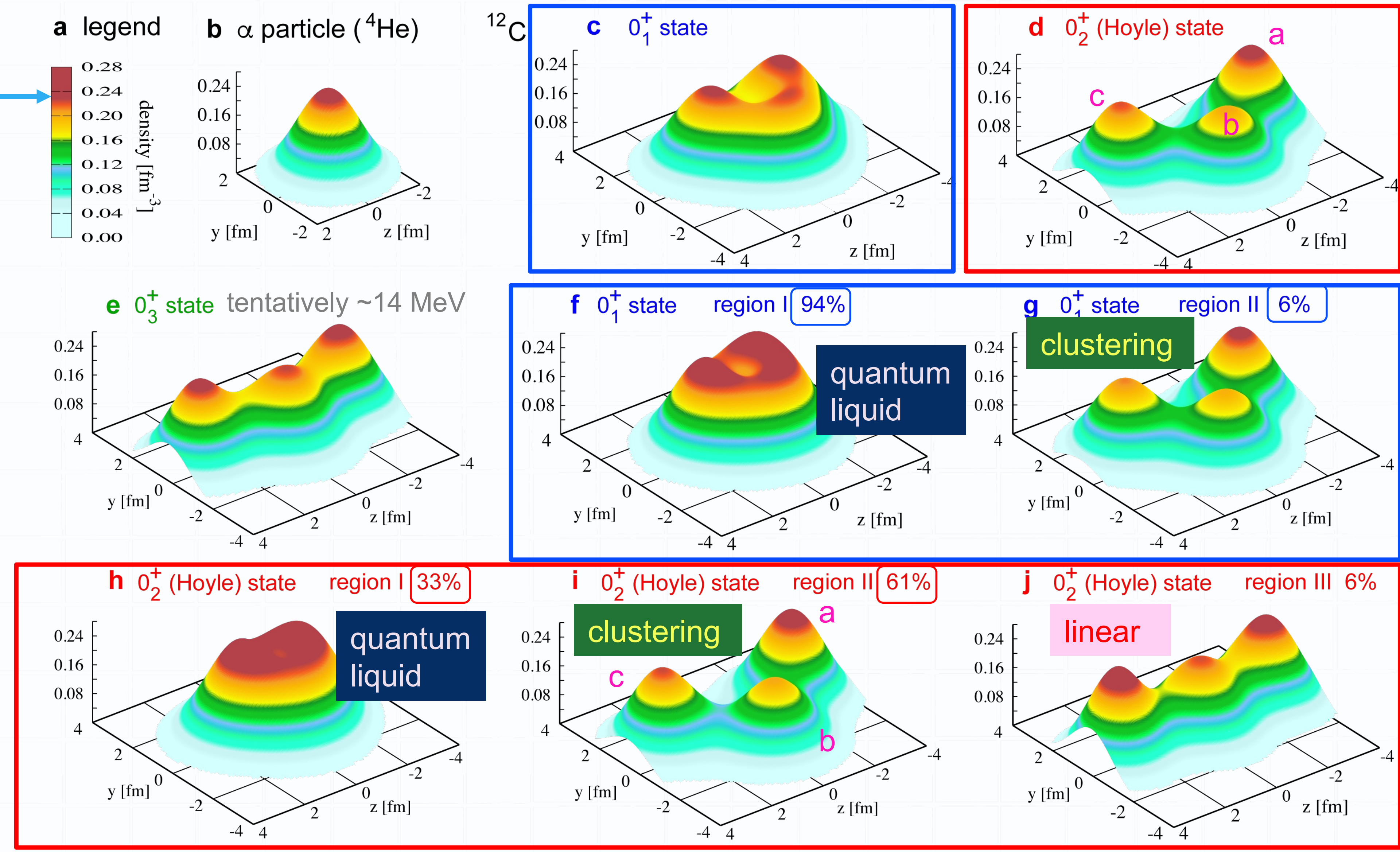


3 α → ^{12}C (Hoyle state) + γ

crucial for the syntheses of carbon and other heavier elements in stars and even for the birth of the life like us, but its structure remains unknown

Nucleon densities in the body-fixed frame

after proper orthogonalization



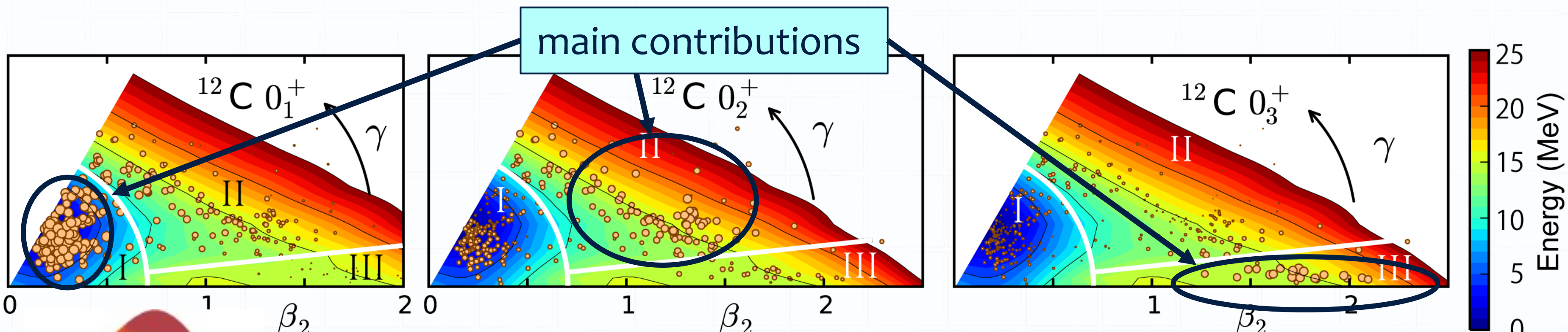
^{12}C : MCSM basis vectors classified by quadrupole shapes (*T plot by Tsunoda*)

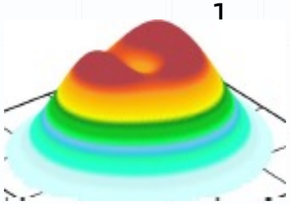
T plot circles are spread in the case of ^{12}C. A characteristic feature.

Unique structures appear at low excitation energies … different from other nuclei

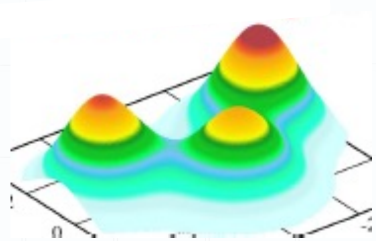
PES is divided into three
- I $\beta_2 < 0.7$, oblate basin in the PES
- II triaxial
- III very prolate

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

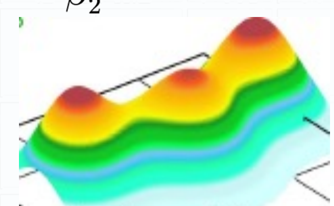




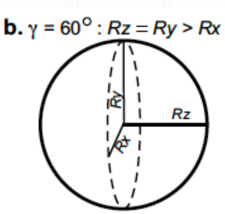
oblate (pancake)



Hoyle state

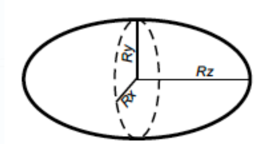


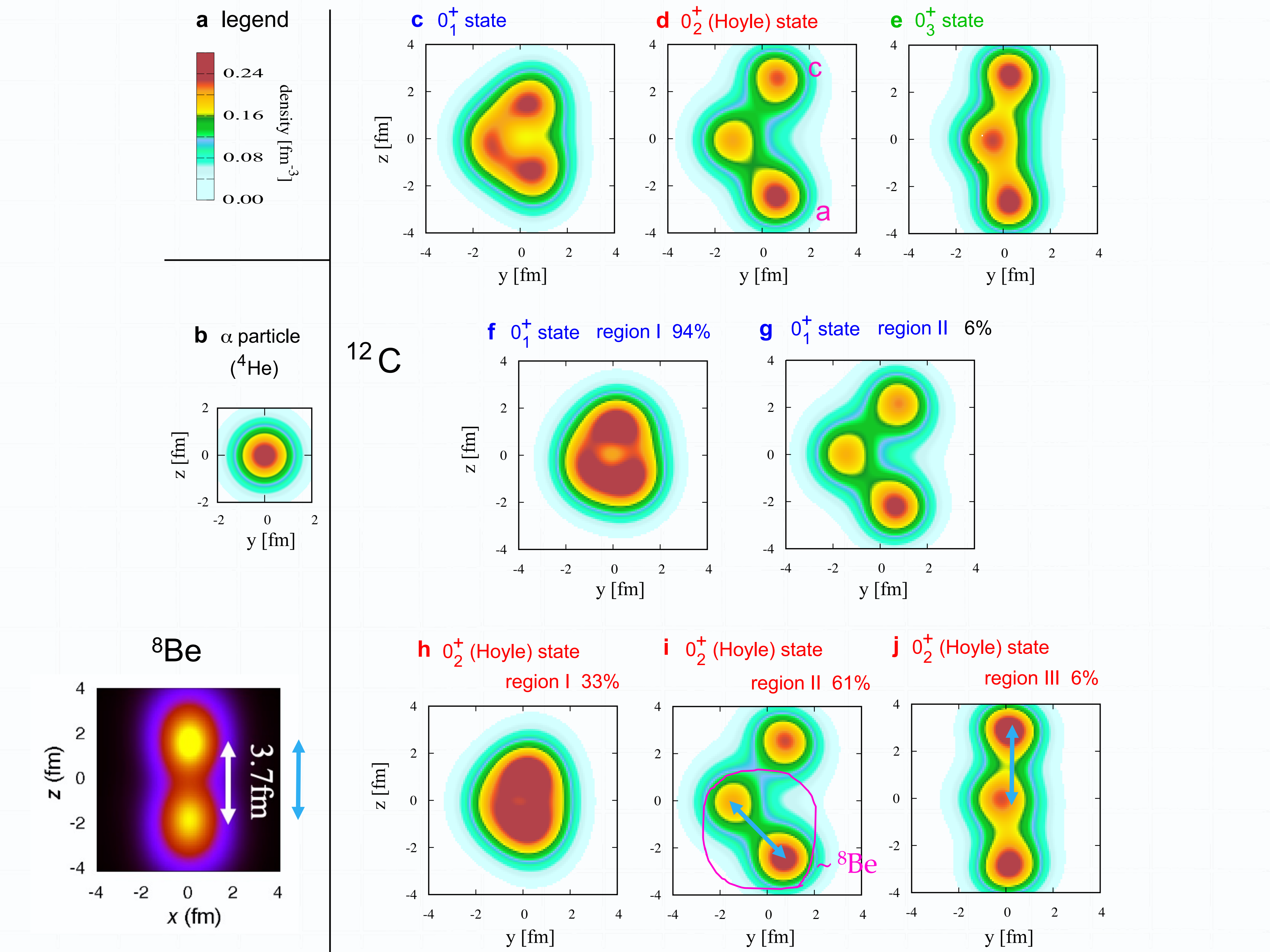
prolate (football)



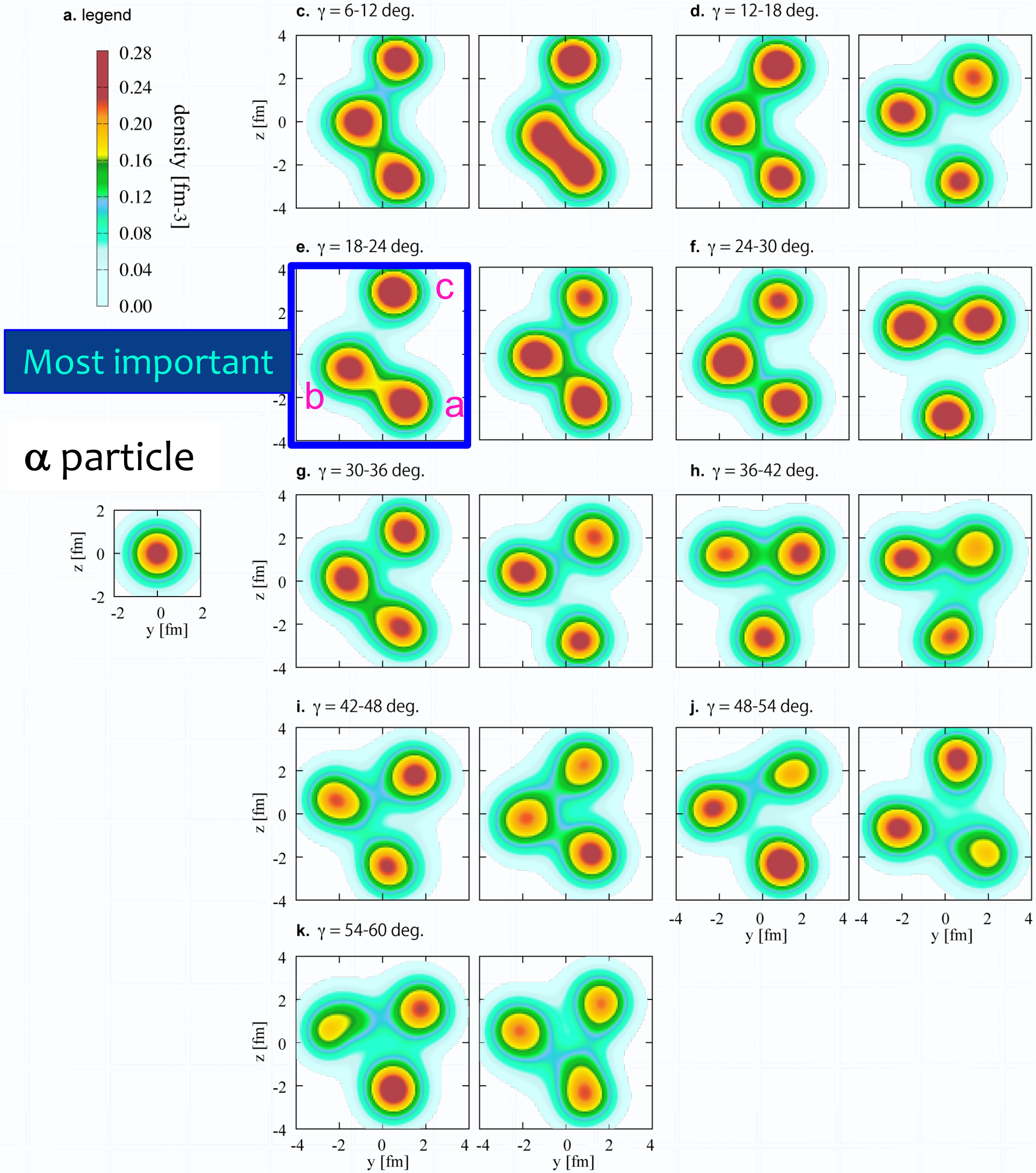
Rz : Ry : Rx = 2 : 2 : 1

Rz : Ry : Rx = 5 : 1 : 1





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

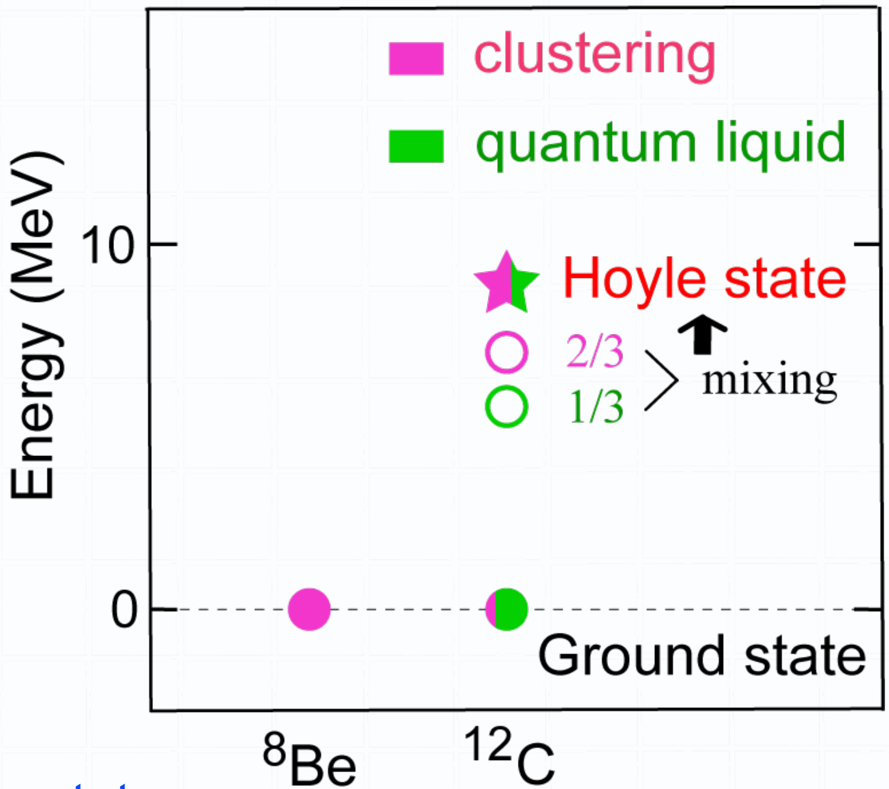


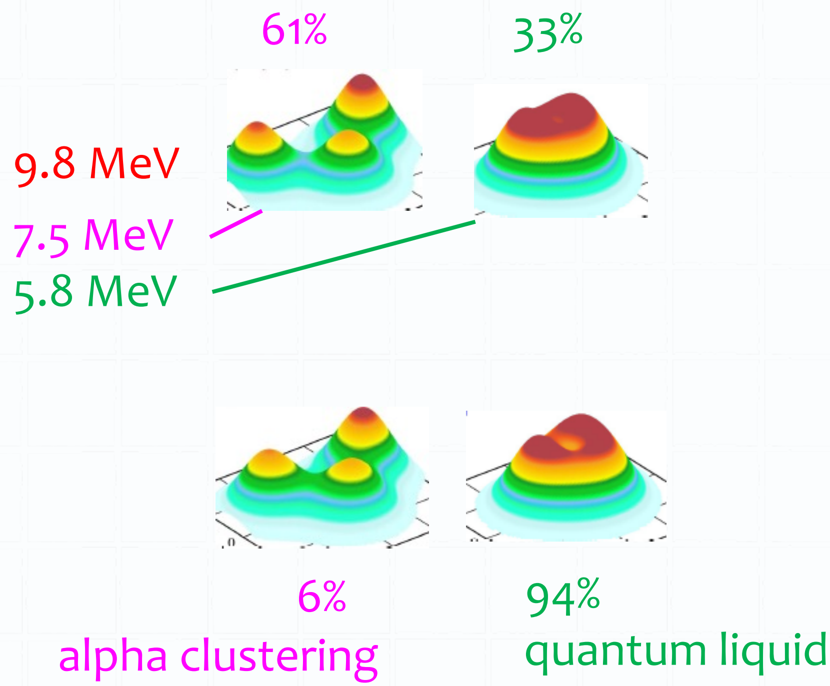
density profiles of major MCSM basis vectors (Slater determinants) in region II, generated by the interaction.

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

Fluctuations within such configurations

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





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).

The present mixing seems to be consistent with the BEC (THSR) model.

Ground state :

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

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

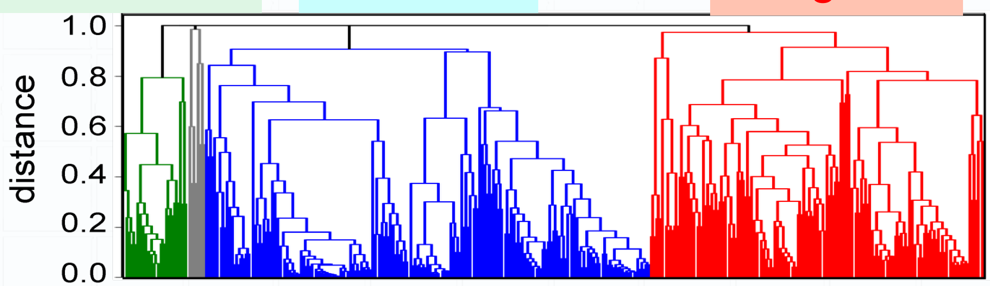
where parenthesis means a scalar product (overlap integral) with the $J^{\pi} = 0^{+}$ projection

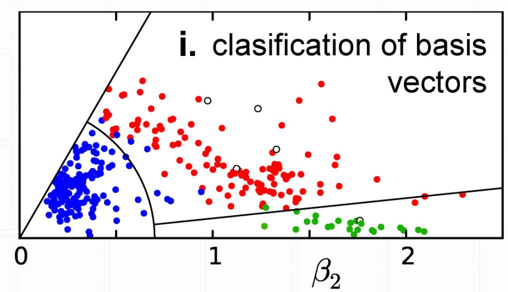
connect basis vectors from the shortest distance to longer up to the threshold

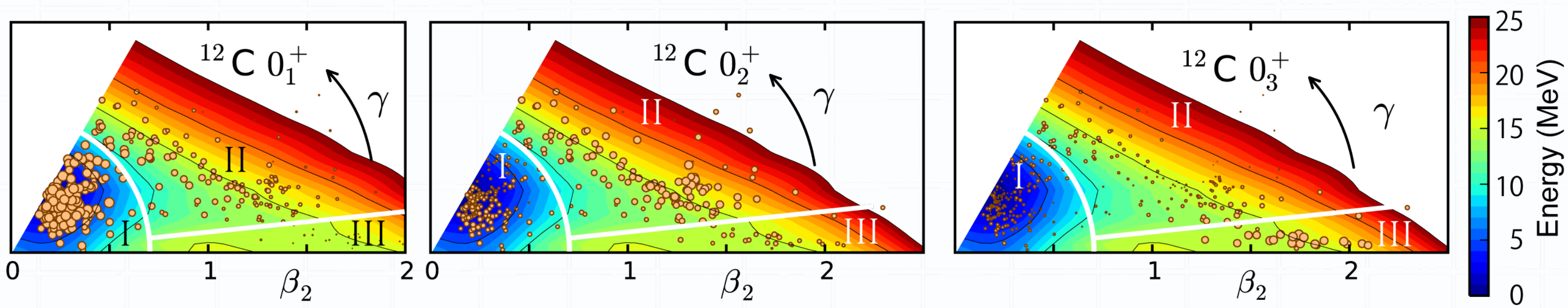
independent confirmation of the validity of the region decomposition

~region III ~region I ~region II

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







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		Expt.
		$N_{shell} = 7$	$N_{shell} \to \infty$	
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

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Summary of the 2nd part

α clustering from first principles without any assumption

Perfect oblate rotational band from first principles in ^{12}C

Nuclear forces favor both quantum liquid and alpha cluster

Transition between them is not a phase transition but a crossover

Alpha cluster emerges without threshold effect (←→Ikeda diagram)

What is crucial is probably shorter range parts of nuclear forces, which has been "uninvited guest" to nuclear structure physics

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

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

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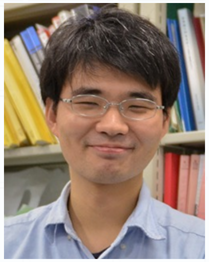
Collaborators



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E N D

Thank you for your attention