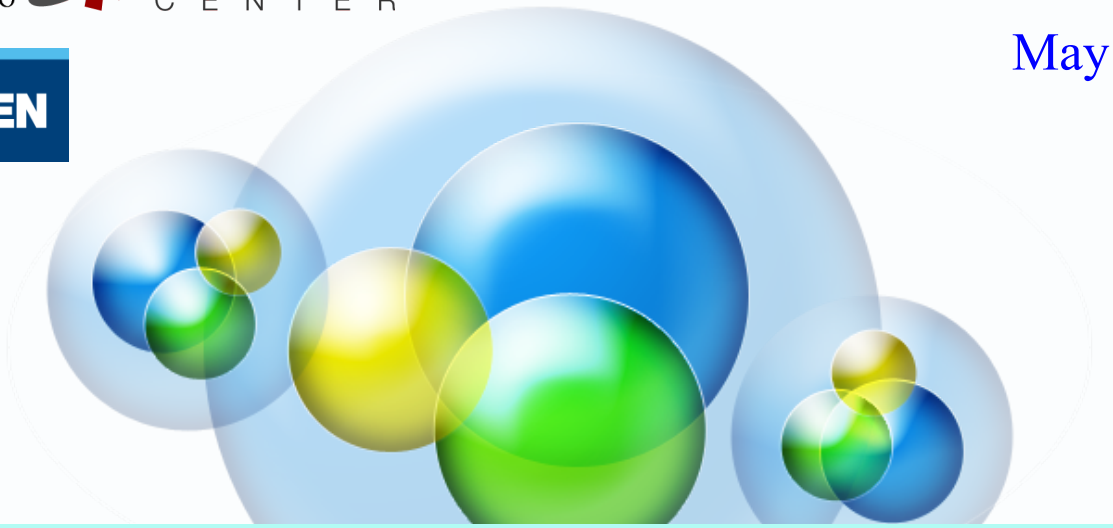
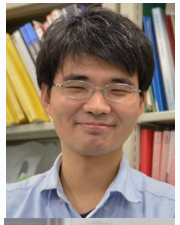
SOTANCP4
Galveston, TX
May 14 (14-18), 2018



Ab initio description of clustering phenomena in atomic nuclei by the Monte Carlo shell model



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Outline

1. Introduction
2. Monte Carlo Shell Model - Quick overview -
3. Be isotopes - Levels, molecular orbits and E0 –
4. C isotopes - Hoyle state, AI-related method –
5. Summary

The clustering is one of the fundamental problems in physics.

Foundation from a certain underlying basis

Its contemporary version

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

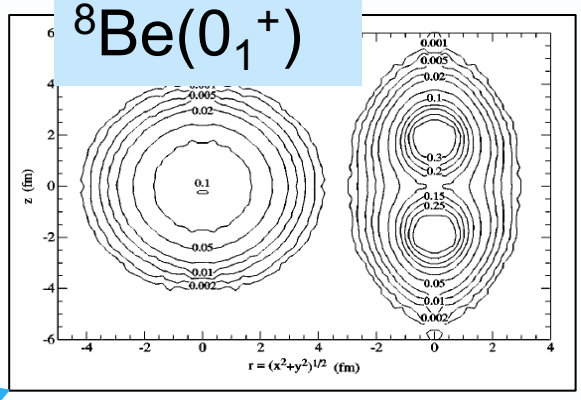
- Green's Function Monte Carlo (GFMC) [Wiringa et al. 2000]
- No Core Full Configuration (NCFC) :

  [Cockrel et al. 2012]
- Lattice EFT : Hoyle state [Epelbaum et al. 2012]
- *ab initio* Monte Carlo Shell Model (MCSM)

  This work -> clustering in Be and C isotopes

Molecular structure is added

$^8Be(0_1^+)$



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

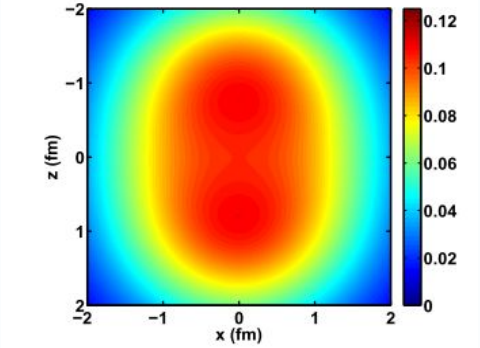
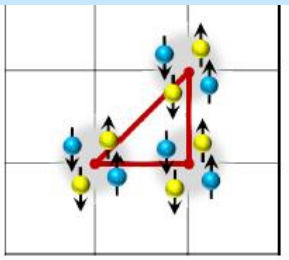


FIG. 12: (Color online) The $y = 0$ slice of the translationally-inv density for the same state is on the right. These densities were

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



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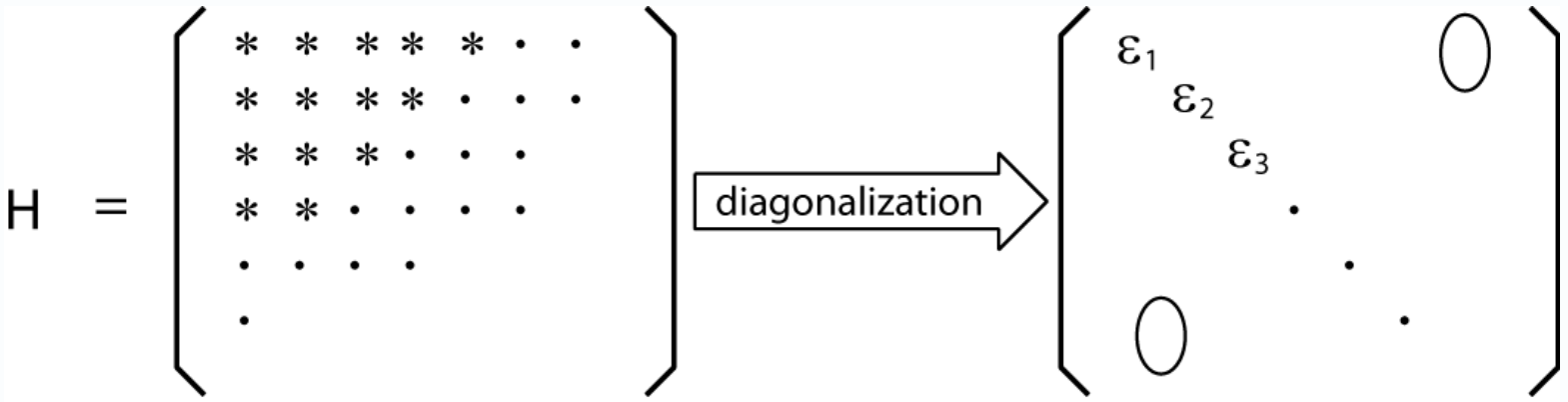
Two types of shell-model calculations

dim. <~ 10^{10}

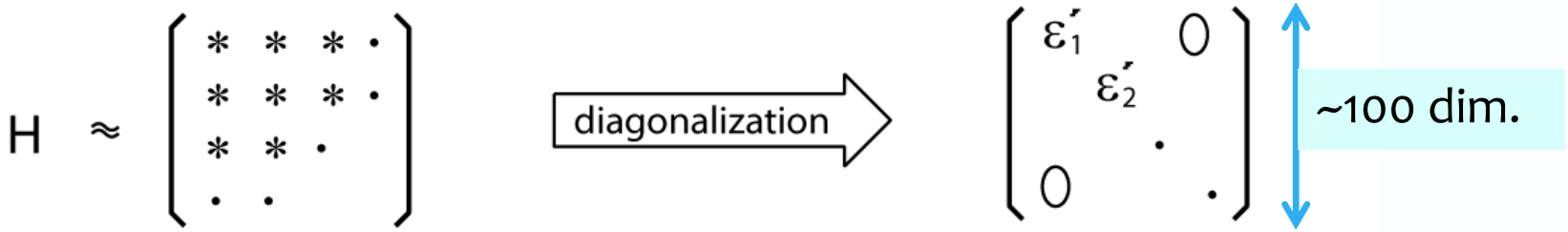


Conventional Shell Model

all Slater determinants

Direct diagonalization

For even bigger problem,



Monte Carlo Shell Model

bases important for a specific eigenstate

Selected

important basis vectors

Advanced Monte Carlo Shell Model (currently used)

N_B : number of basis vectors (dimension)

N_p : number of (active) particles

N_{sp} : number of single-particle states

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

amplitude

Projection op.

$$|\phi(D^{(n)})\rangle = \prod_{\alpha=1}^{N_p} \left(\sum_{i=1}^{N_{sp}} a_i^\dagger D_{i\alpha}^{(n)} \right) |-\rangle$$

n-th basis vector (Slater determinant)

Stochastically "deformed" single-particle state

$$E(D) = \langle \Psi(D) | H | \Psi(D) \rangle$$

Minimize $E(D)$ as a function of D utilizing qMC and conjugate gradient methods

Step 1 : stochastic generation of candidates of the n-th MCSM basis vector

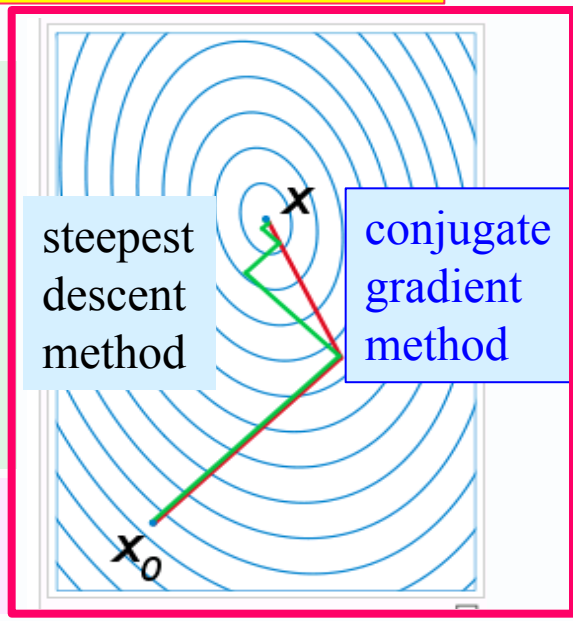
$$|\phi(\sigma)\rangle = \prod e^{\Delta\beta\, h(\sigma)} \cdot |\phi^{(0)}\rangle$$ *only theoretical background*

Shift randomly matrix elements of the matrix D.

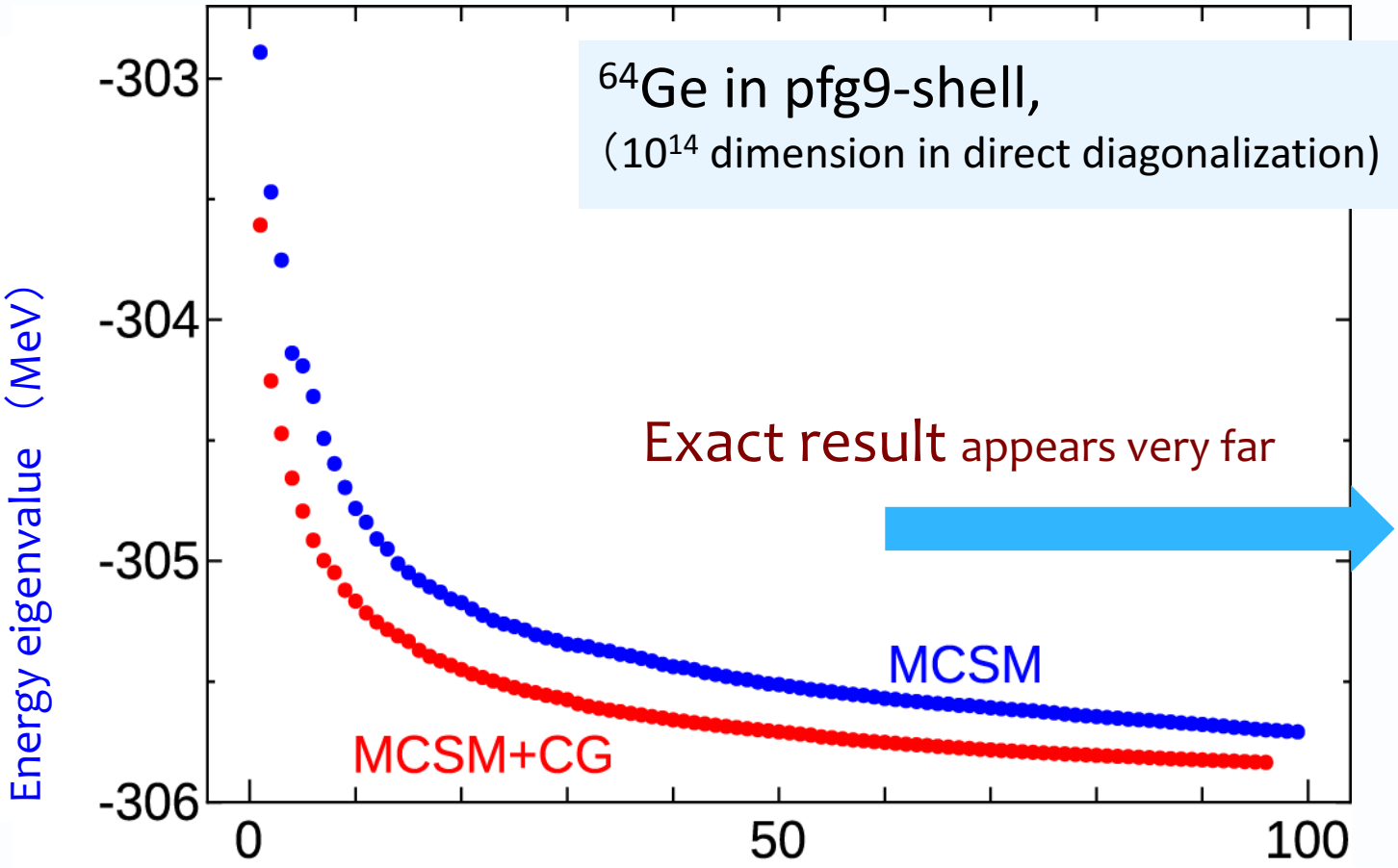
(The very initial one can be a Hartree-Fock state.)

Select the one producing the lowest $E(D)$ (rate < 0.1 %)

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



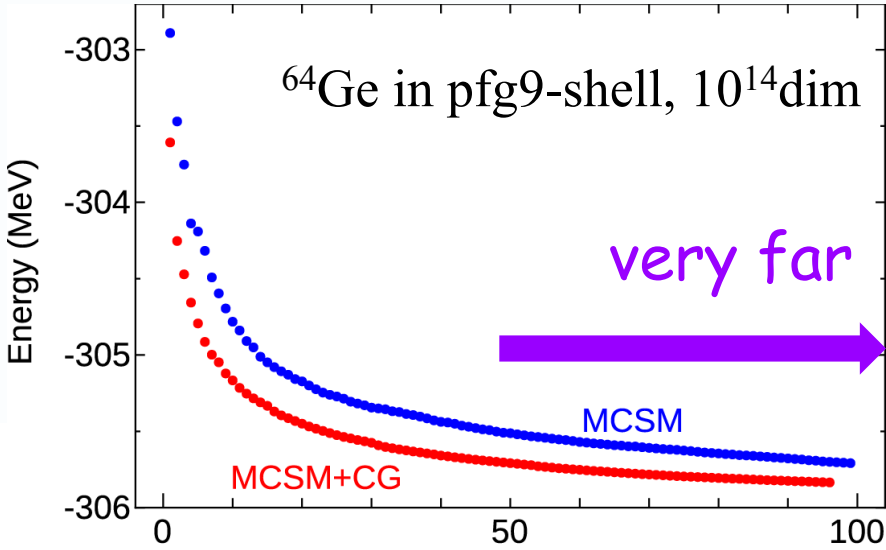
Example of MCSM calculation



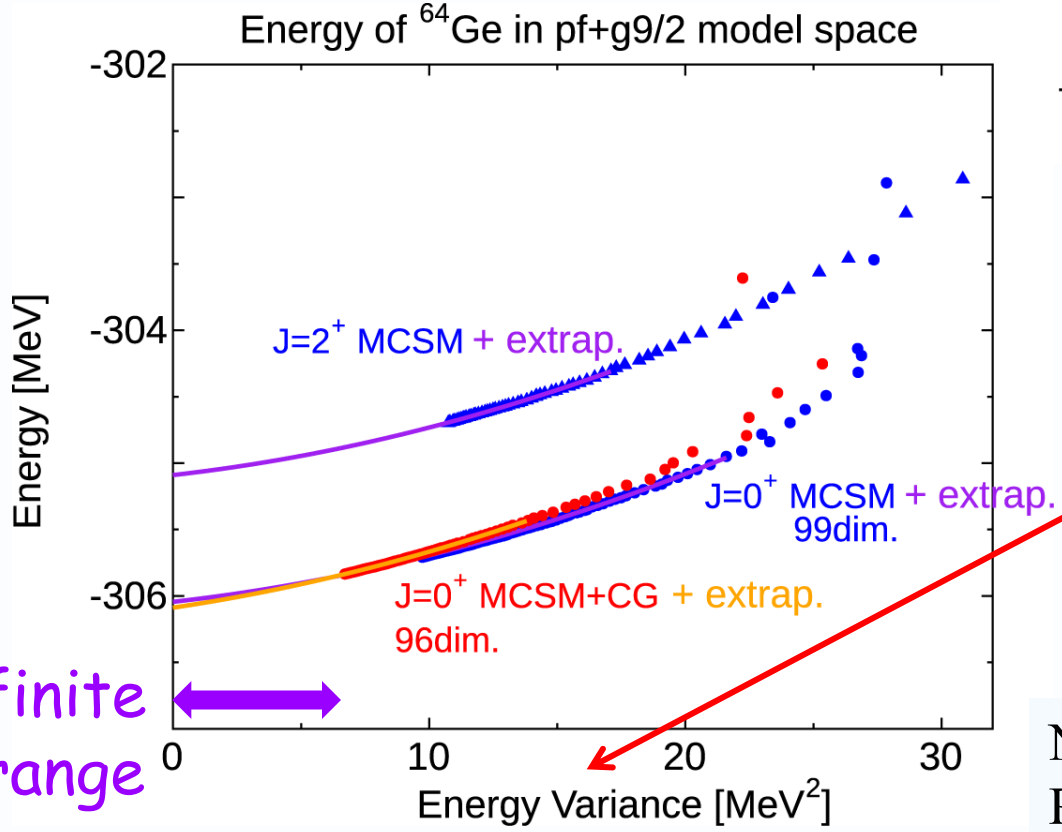
Numerous MC trials and CG optimization for each basis vector

Extrapolation by Energy Variance

employed in most of the calculations shown in this talk



Number of basis vectors
(deformed Slater determinants)



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

$$\langle H \rangle = E_0 + a\langle \Delta H^2 \rangle + b\langle \Delta H^2 \rangle^2 + \ldots$$

N. Shimizu, et al.,
Phys. Rev. C **82,** 061305(R) (2010).

MCSM (Monte Carlo Shell Model -*Advanced version*-)

1. Selection of important many-body basis vectors
   by quantum Monte-Carlo + diagonalization methods
   basis vectors : about 100 selected Slater determinants
   composed of "deformed" single-particle states
2. Variational refinement of basis vectors
   conjugate gradient method
3. Variance extrapolation method -> exact eigenvalues

+ innovations in algorithm and code (=> now moving to GPU)

K computer (in Kobe) 10 peta flops machine

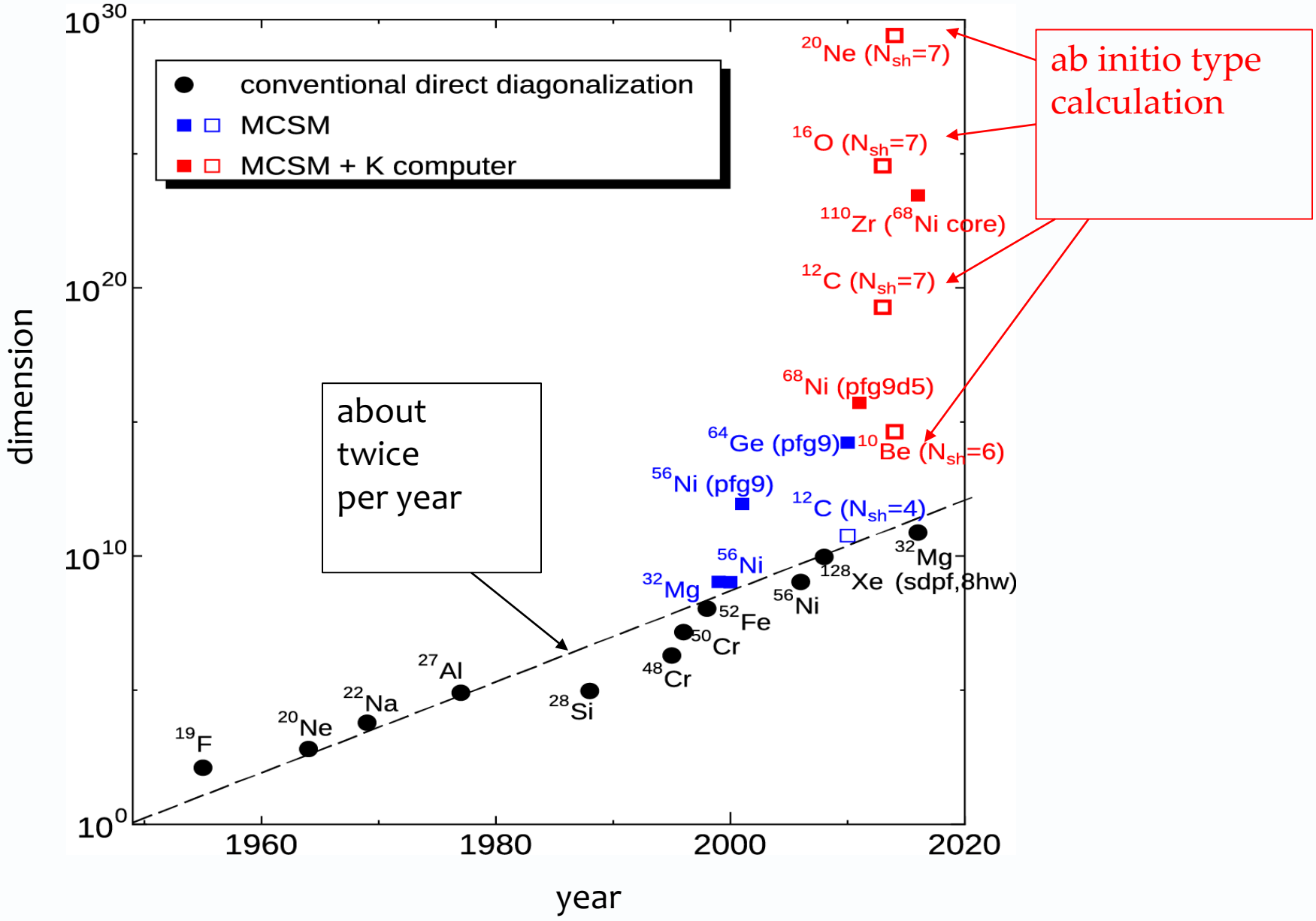
$\Rightarrow$ *Projection of basis vectors*

Rotation with three Euler angles

with about 50,000 mesh points

Example : 8^+ ^{68}Ni 7680 core x 14 h

Dimension of the shell-model many-body Hilbert space

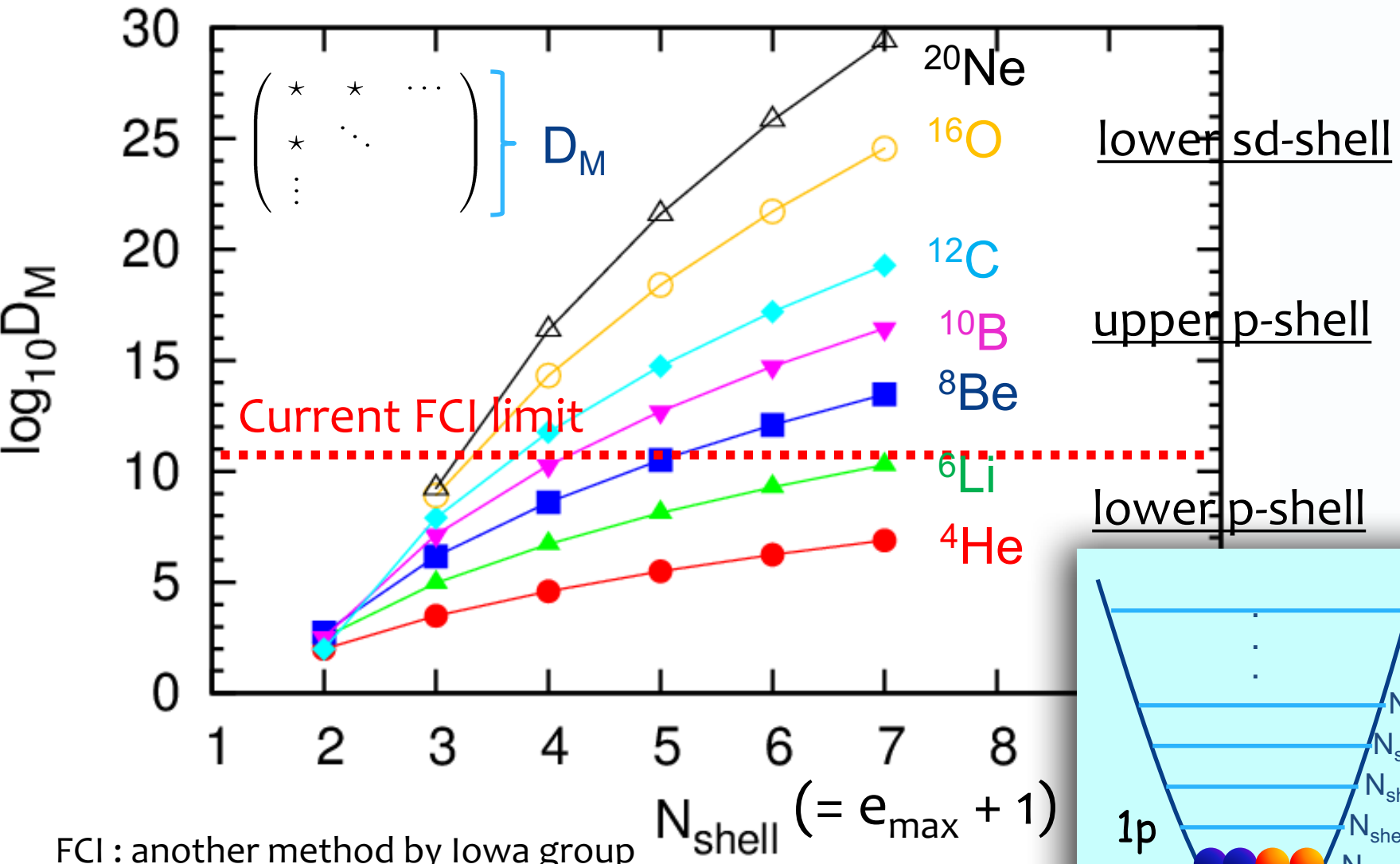


We apply this method to the no-core shell model.

→ *ab initio* MCSM

M-scheme dimension in N_{shell} truncation

No-core calculations

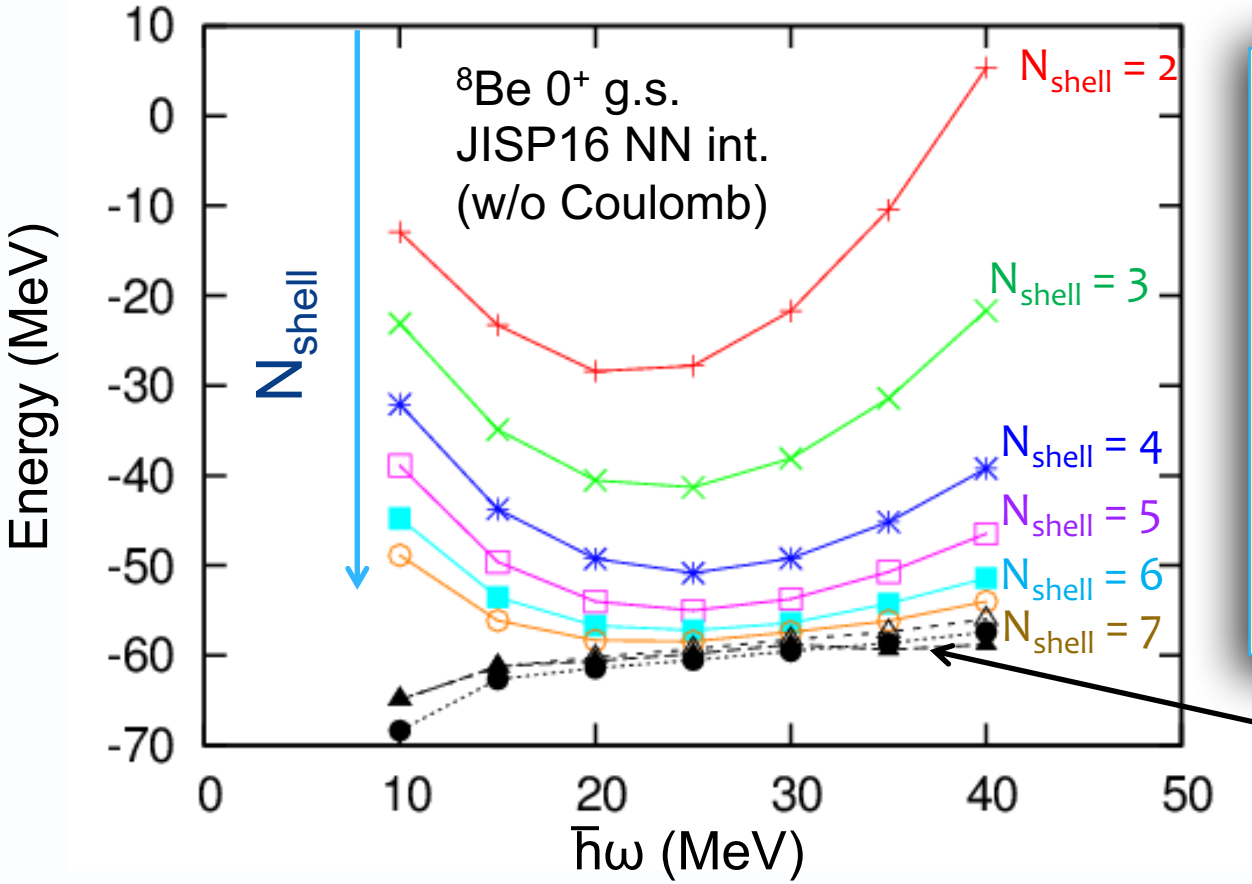


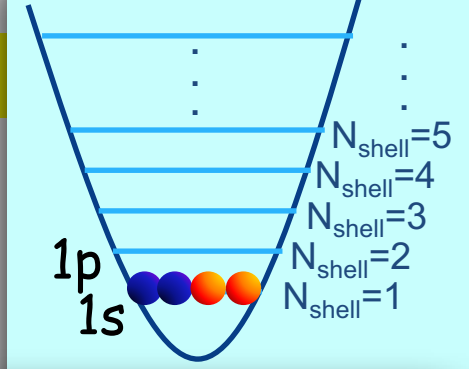
FCI : another method by Iowa group
~ conventional diagonalization

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

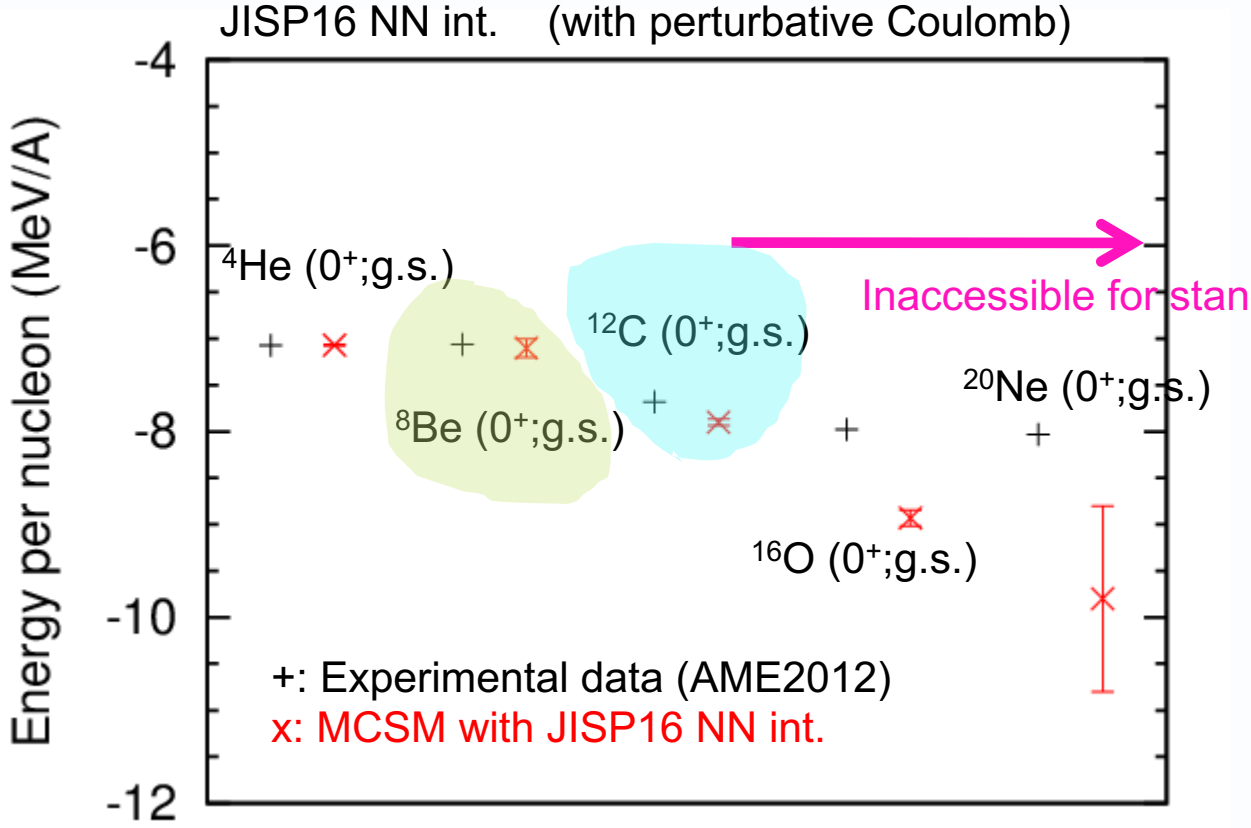
But, the eigenvalue in the infinite space should be independent of it, *i.e.*, flatness.

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)

Comparison of MCSM ground-state energies with experiment



MCSM results are obtained using K computer and extrapolated to infinite space with optimum choice of the harmonic oscillator parameter.
Coulomb interaction is included perturbatively.

MCSM results show good agreements with experimental data up to ^{12}C, slightly overbound for ^{16}O, and clearly overbound for ^{20}Ne.

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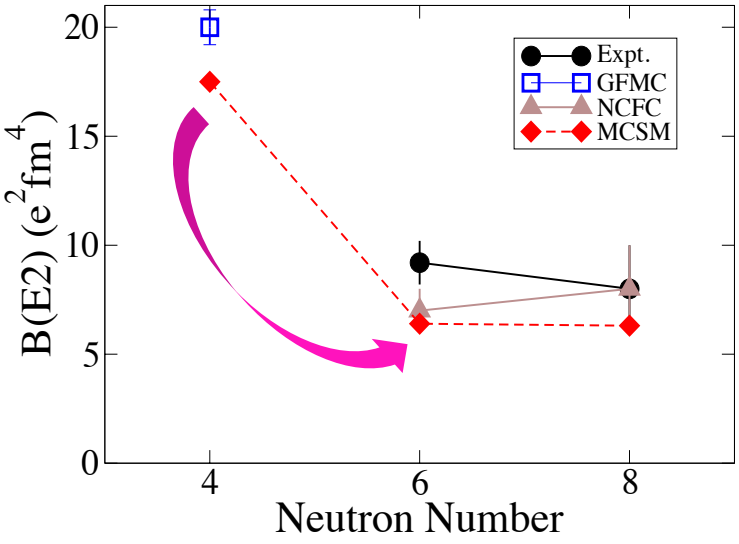
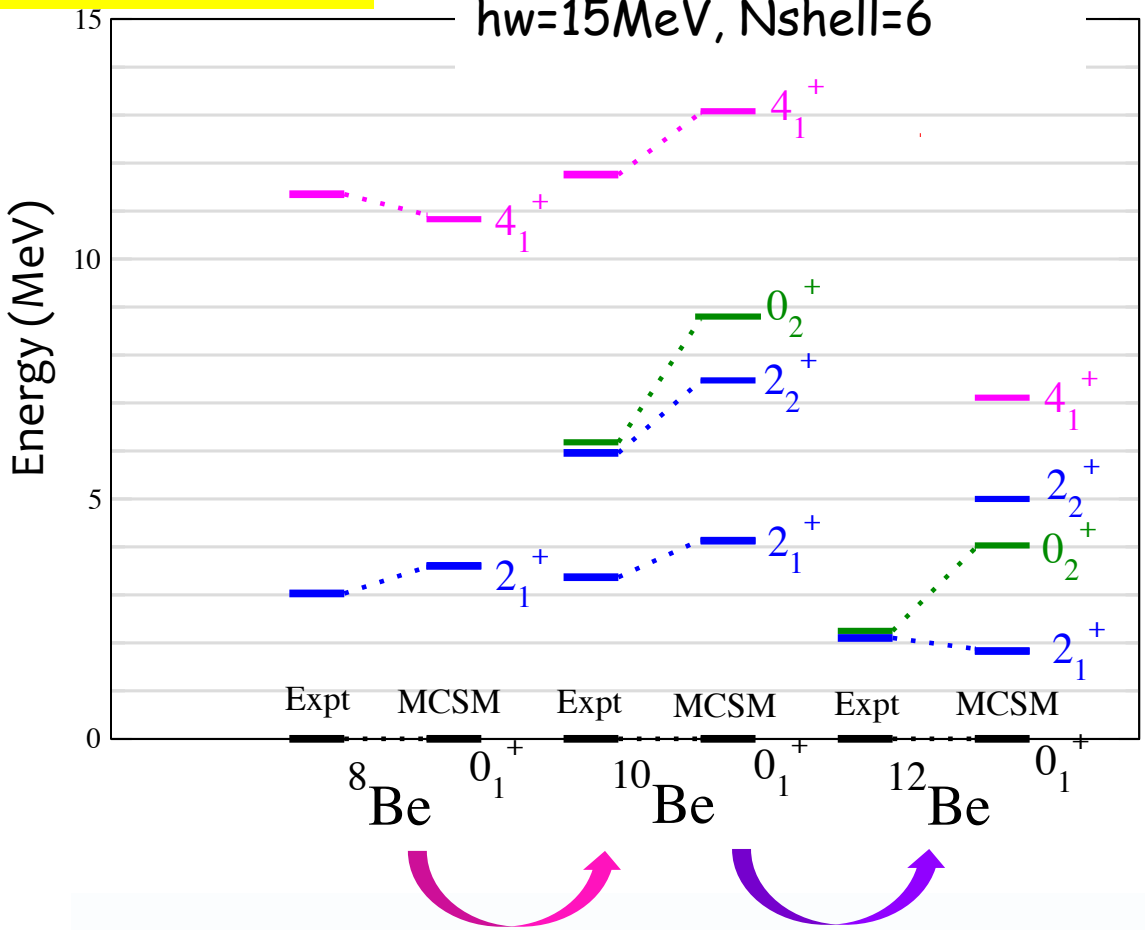
Levels and B(E2)'s of Be isotopes

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



calculated with
hw=15MeV, Nshell=6

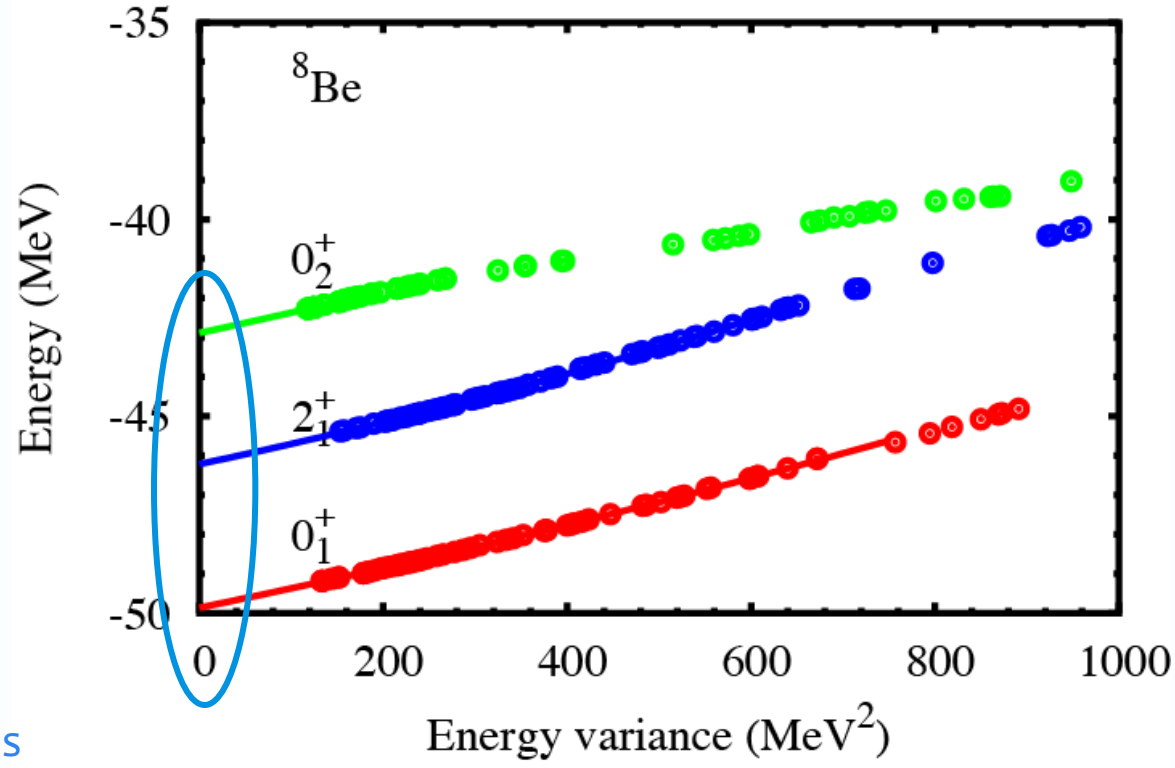


α-α distance smallest

enlarging of deformation (weaker E2 due to neutrons)

Exp : ^{8}Be, ^{10}Be : Tilley *et al.*, 2004
^{12}Be : Shimoura *et al.*, 2003

These energy levels are obtained by MCSM process including the variance extrapolation to the exact values.



exact values
for this model space

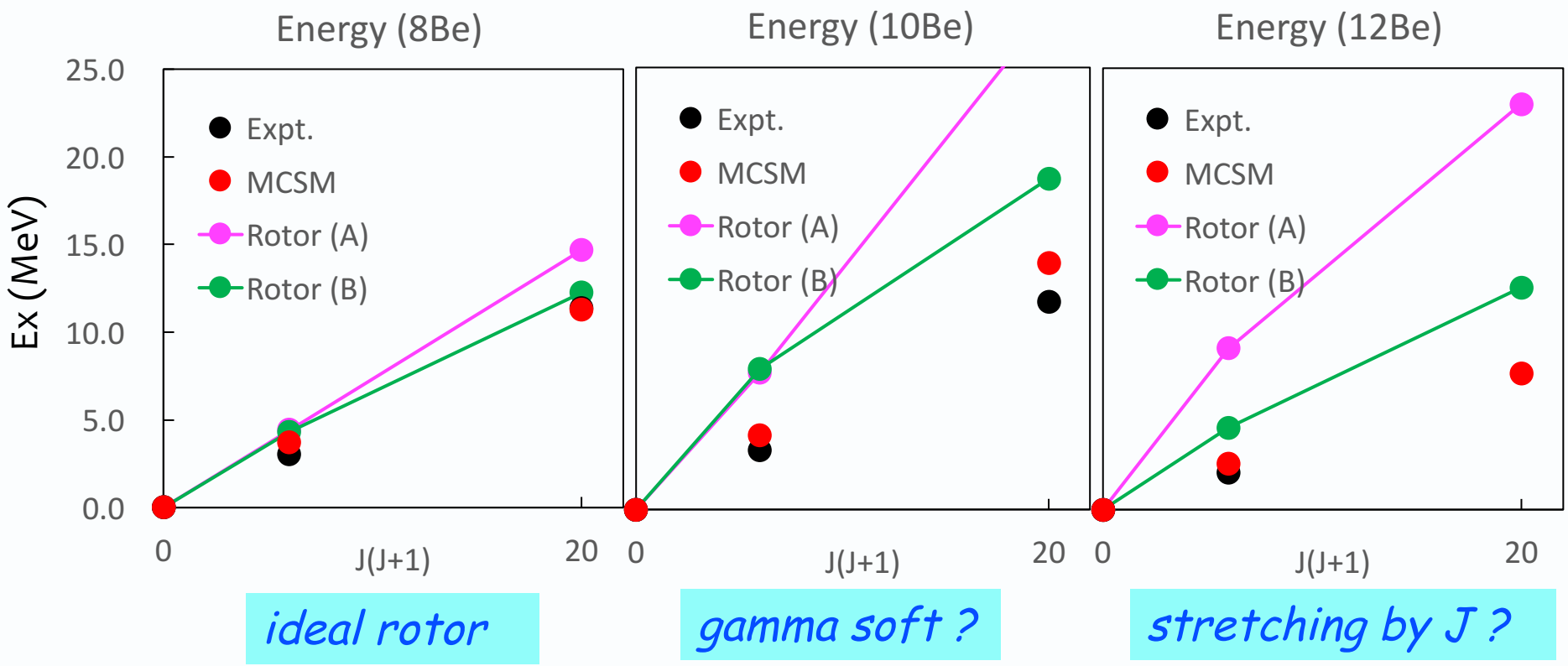
Variance : $\langle \Delta H^2 \rangle = \langle H^2 \rangle - \langle H \rangle^2$

$$\langle H \rangle = E_0 + a\langle \Delta H^2 \rangle + b\langle \Delta H^2 \rangle^2 + \ldots$$

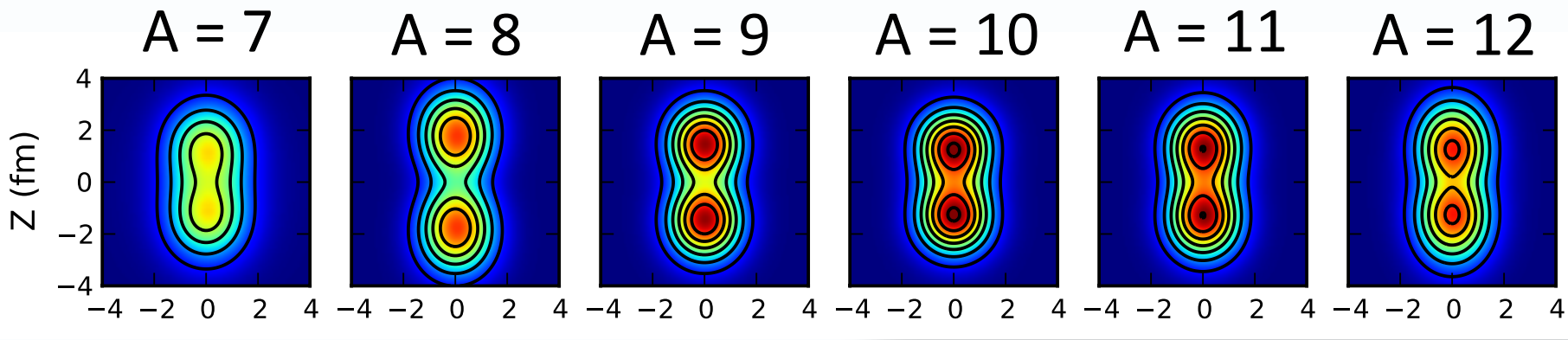
rotational levels

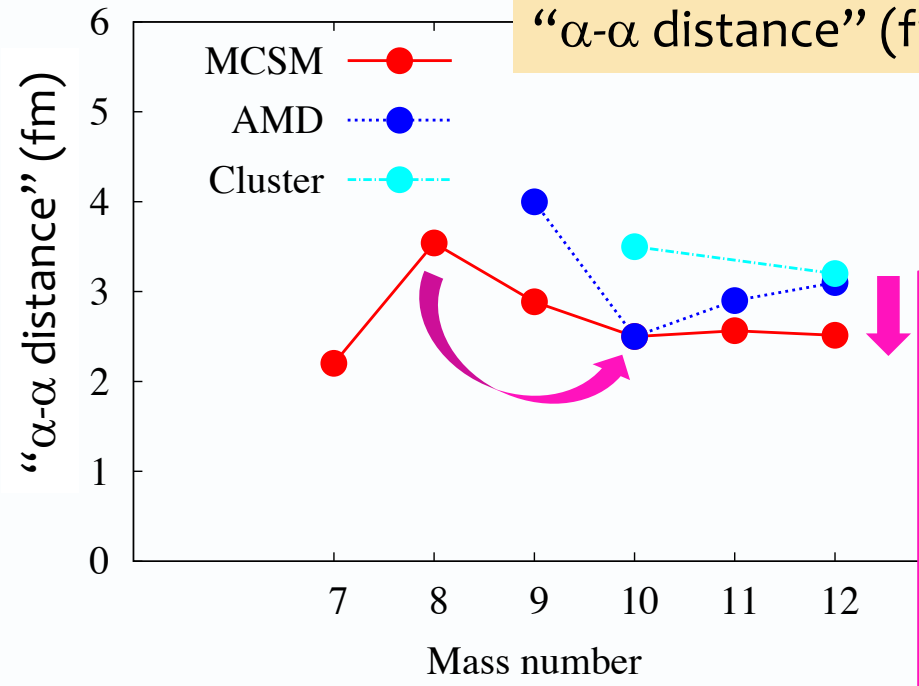
- experiment
- MCSM result (diagonalization)
- projection from MCSM basis vectors fixed for $J=0^+$
- projection from MCSM basis vectors fixed for $J=0^+$ with amplitudes re-optimized for each J

q moment axis alignment is made for ● and ●, and only $K=0^+$ components are included



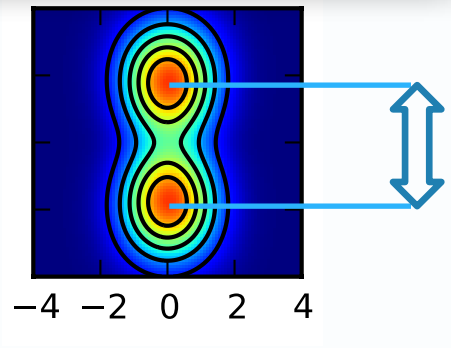
Evolution of α-clustering along the isotope chain





"α-α distance" (fm) :

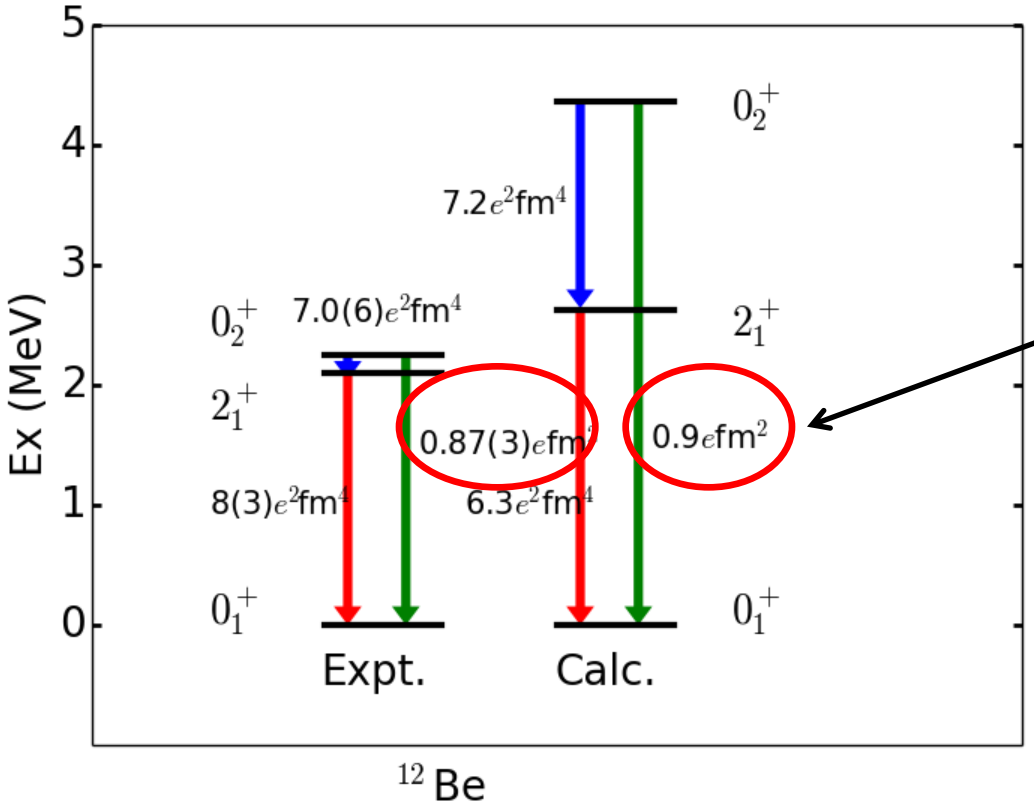
Definition:
Distance between the positions of each highest proton density



This effect may be due to more correlations incorporated in the MCSM calculation.

AMD: Y. Kanada-En'yo, Phys. Rev C68, 014319 (2003)
Cluster: M. Ito & K. Ikeda, Rep. Prog. Phys. 77, 096301 (2014)

*E*2 & *E*0 Transition strength of ^{12}Be



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

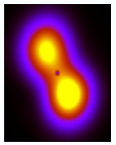
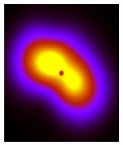
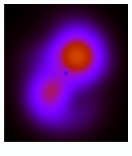
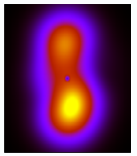
more relevant to molecular structure (to be discussed)

Expt.:

S. Shimoura, et al., Phys. Lett. B 654 87 (2007)

N. Imai, et al., Phys. Lett. B 673 179 (2009)

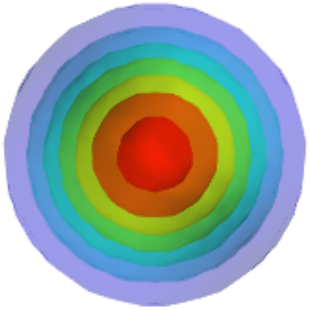
Intrinsic density of MCSM eigenstate

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

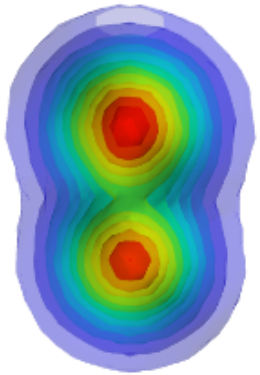
Angular-momentum projection

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

We need something like this.



^{8}Be 0^+ ground state



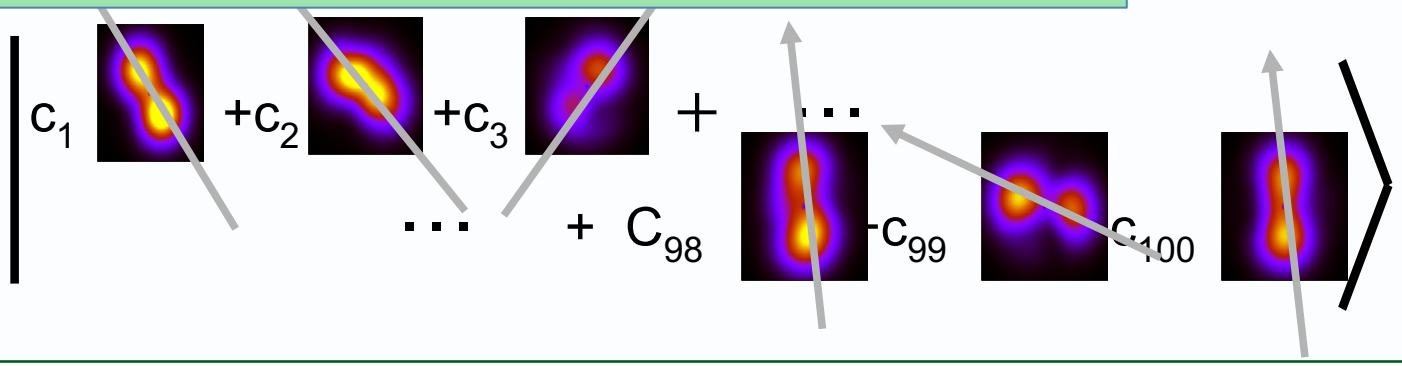
Laboratory frame

"Intrinsic" (body-fixed) frame

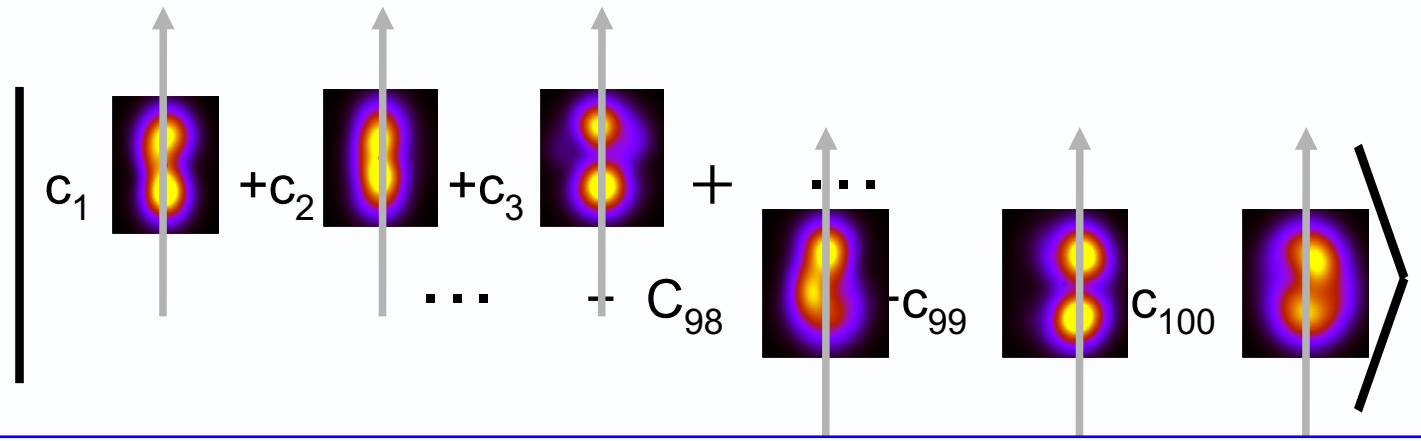
MCSM eigenstate : $\left|\Psi(D)\right\rangle = \sum_{n=1}^{N_B} c_i P^{J,\Pi} \left|\phi(D^{(n)})\right\rangle$

Deformed Slater determinant with three axes of ellipsoid

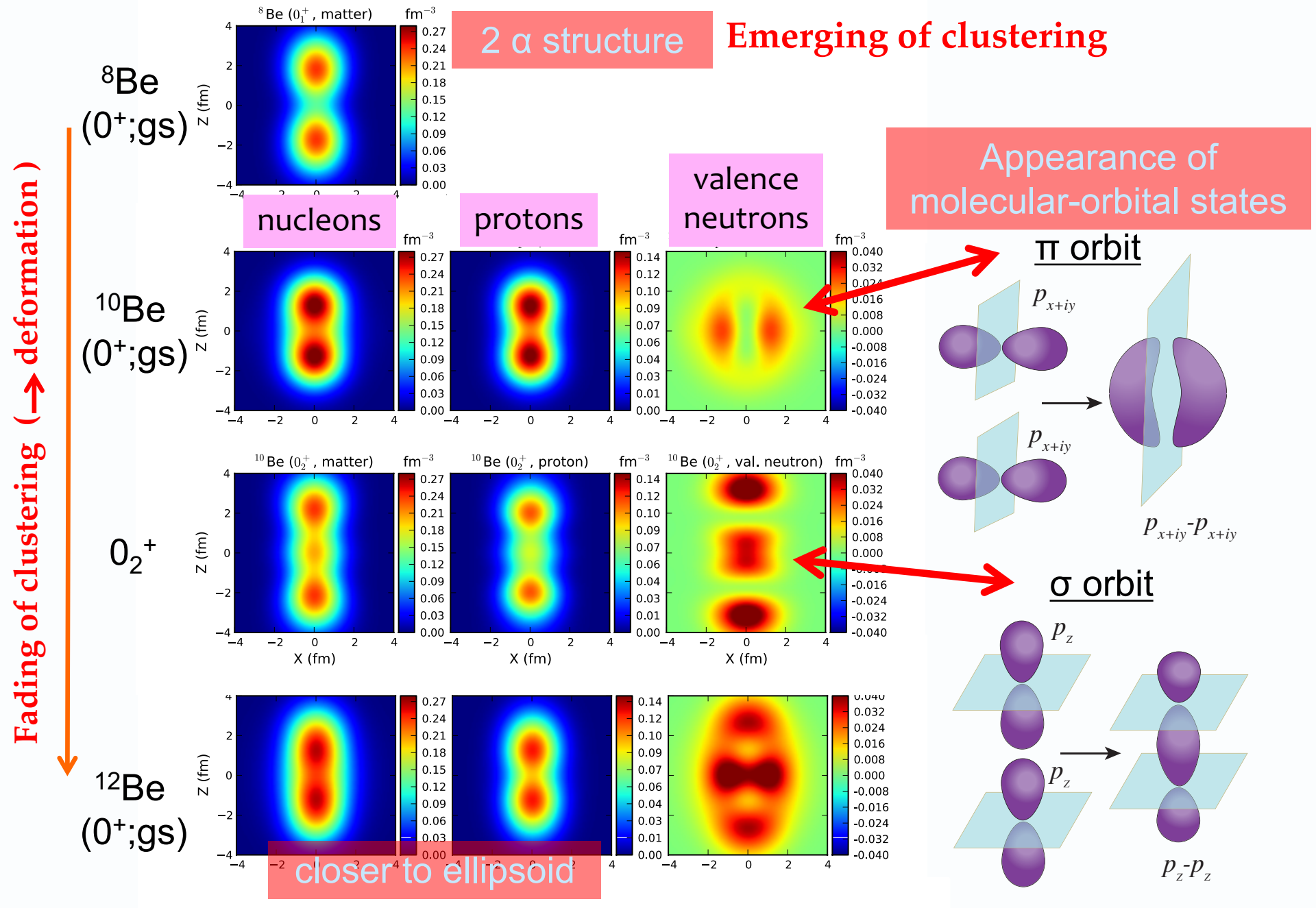
For J^π projected states, individual orientations are not relevant.

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

For "intrinsic state" with physical significance, all basis states are rotated so that three axes of the ellipsoid are aligned (as a first modelling).

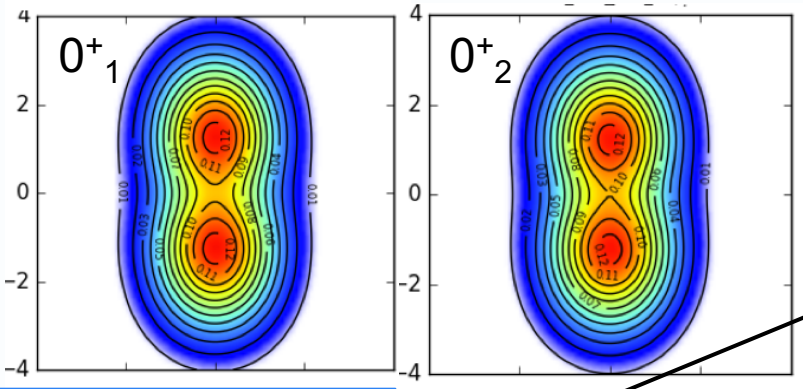
$\left|\Psi_{intr.}(D)\right\rangle =$ 

Cluster and Molecular structure of Be isotopes



Difference between 0^+_1 and 0^+_2 states of ^{12}Be

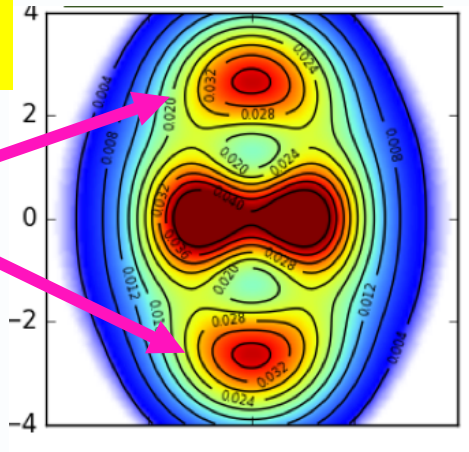
Proton intrinsic density (Q-moment aligned)



protons in two clusters are more separated

$\pi^4 + \pi^2\,\sigma^2$ configurations are mixed

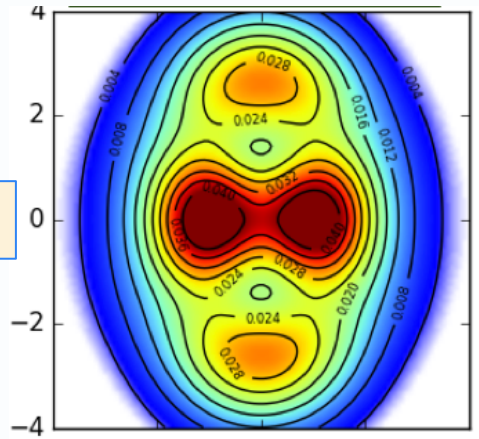
Neutron intrinsic density (Q-moment aligned)



0^+_1

more $\pi^2\,\sigma^2$

different mixings of π / σ orbit configurations



0^+_2

more π^4

A possible modelling ?

$$\psi(0^+_1) = \phi[\pi^4]\cos\theta + \phi[\pi^2\,\sigma^2]\sin\theta$$

$$\psi(0^+_2) = \phi[\pi^4]\sin\theta - \phi[\pi^2\,\sigma^2]\cos\theta$$

E0 transition

note: these two states may not be orthogonal

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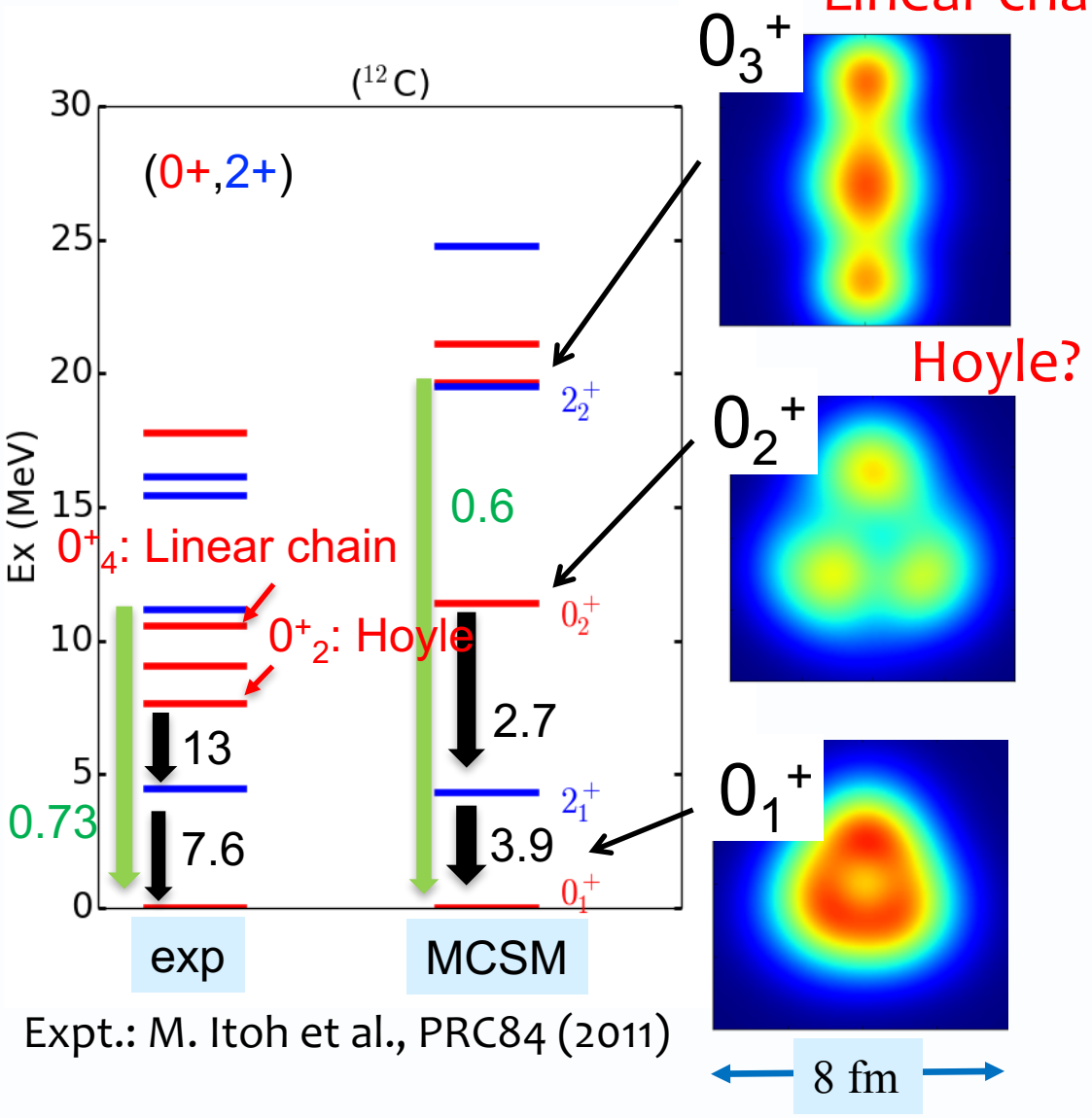
Energy level & transition strength of ^{12}C

Preliminary

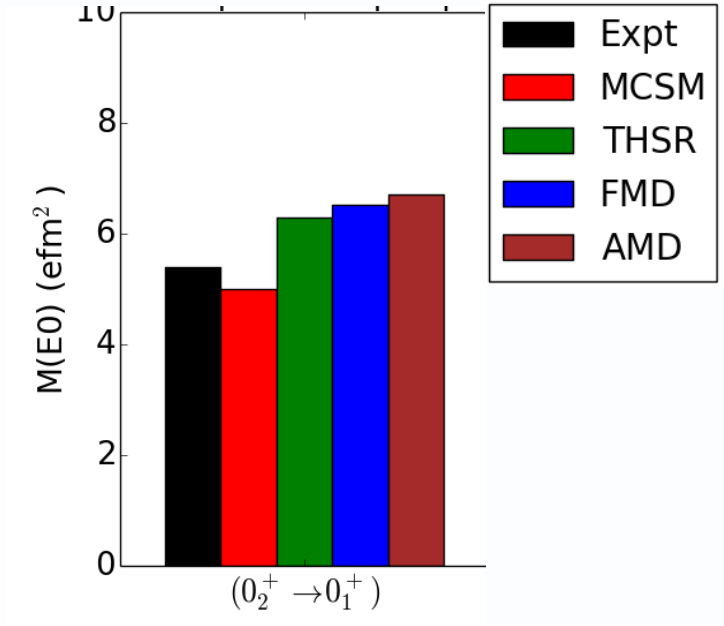


Expt.: M. Itoh et al., PRC84 (2011)

Linear chain?

Hoyle?

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



Expt.: P. Strehl 1970
THSR: Y. Funaki 2015
FMD: M. Chernykth 2007
AMD: Y. Kanada-En'yo 2007

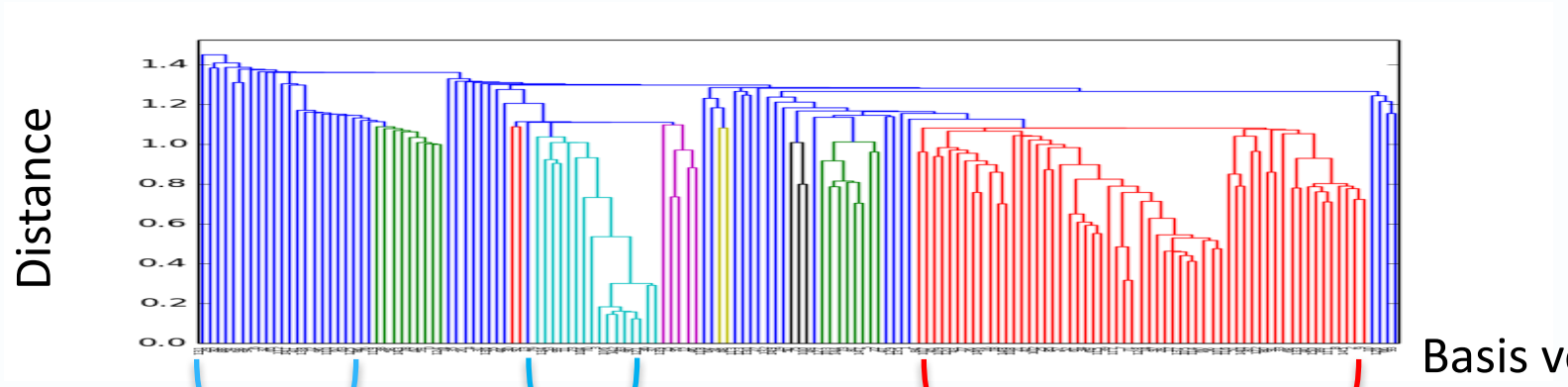
E_{gs} = -76.64 MeV (MCSM, JISP16, N_{shell} = 6, hw = 15 MeV)

Dendrogram of MCSM basis vectors for ^{12}C

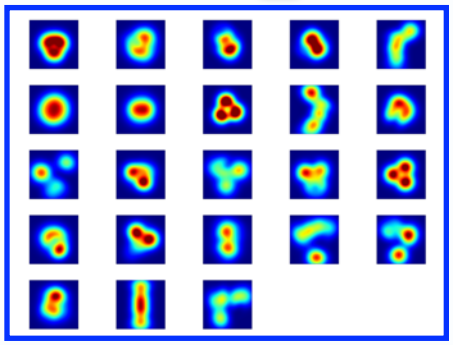
AI (Artificial Intelligence) : extraction of relevant information from "big data"

Dendrogram is used in "Cluster analysis": cluster structure extracted from a mass of different objects

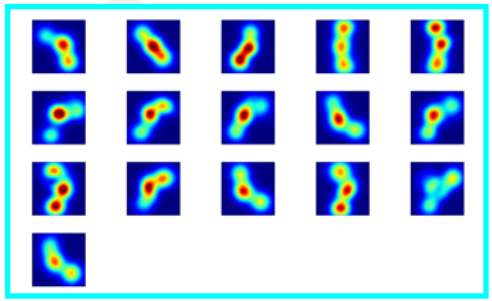
Basis vectors are divided into 16 groups (in this case)



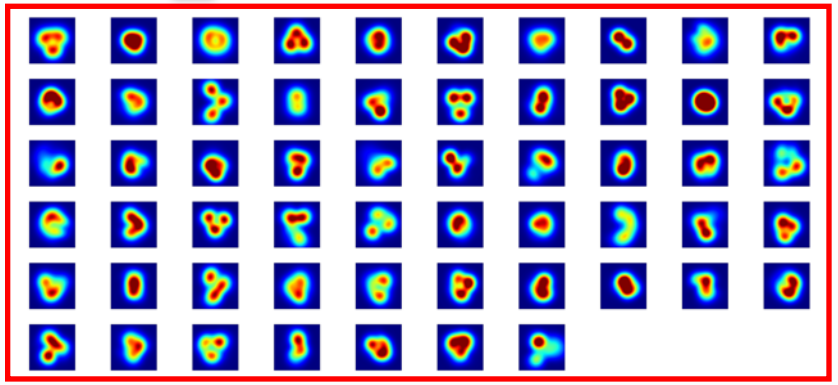
1st group



6th group



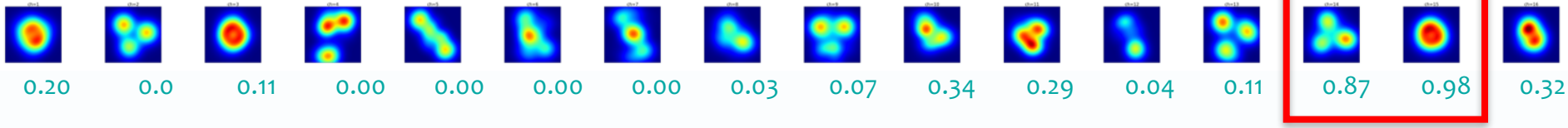
15th group



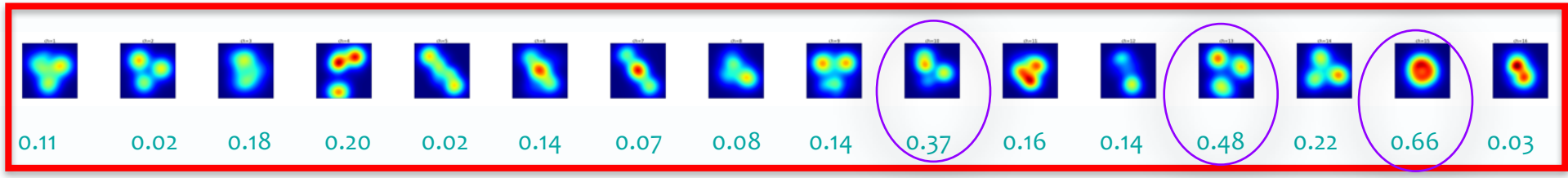
Overlap probability with the eigenstates : ^{12}C

There is non-orthogonality among the MCSM basis vectors.
Densities can be reduced due to cancellation among amplitudes.

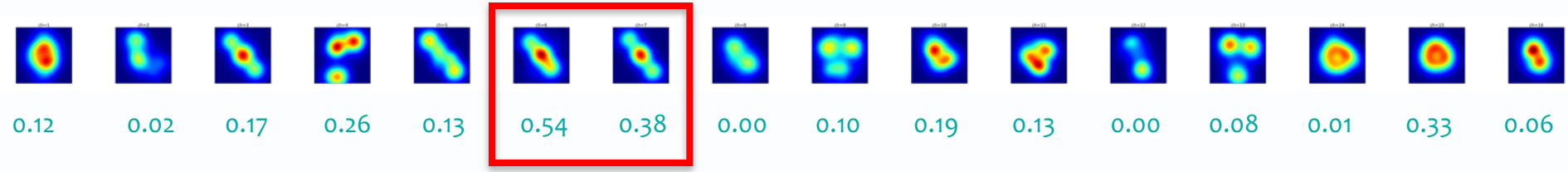
0^+_1 : Concentrated in 14th (3 clusters) & 15th (compact shape) groups



0^+_2 : Scattered among many categories (essence of Hoyle state ?)



0^+_3 : Concentration in 6th & 7th (linear shape) groups



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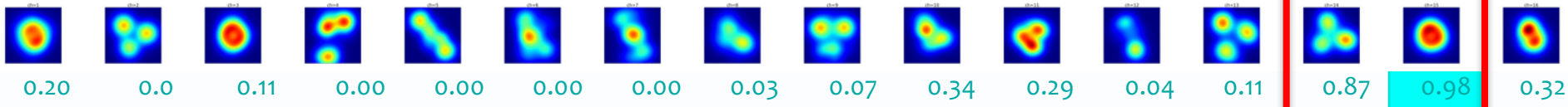
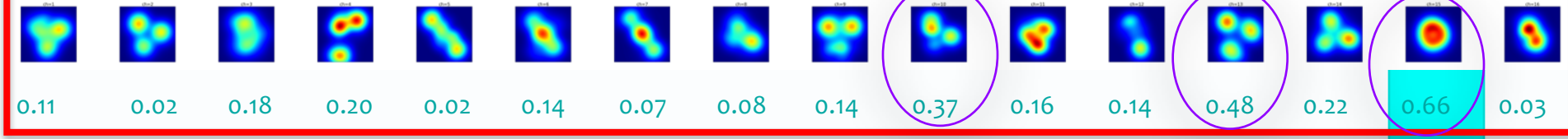
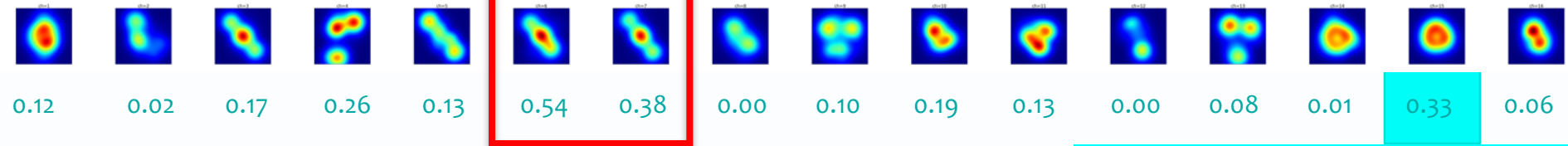


0^+_2 : Scattered among many categories (essence of Hoyle state ?)



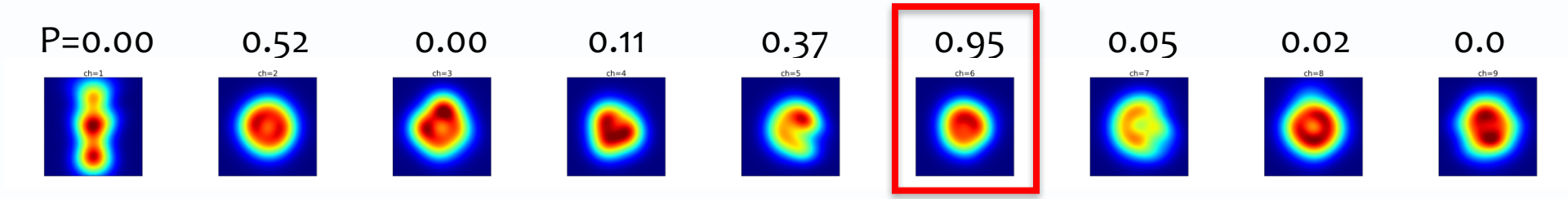
0^+_3 : Concentration in 6th & 7th (linear shape) groups



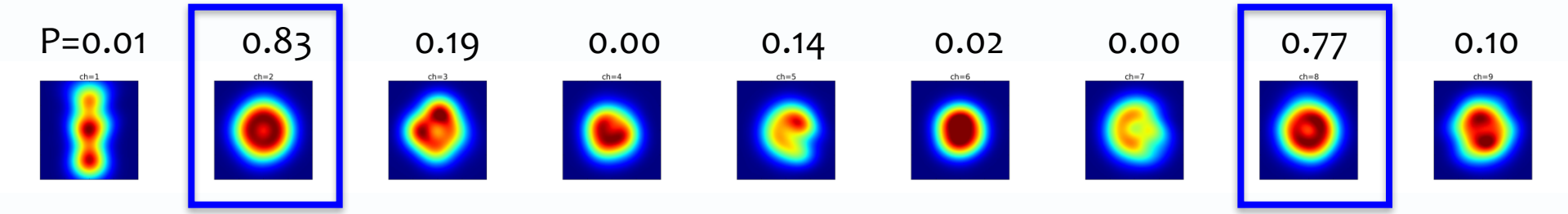
This "canonical" component is always present.

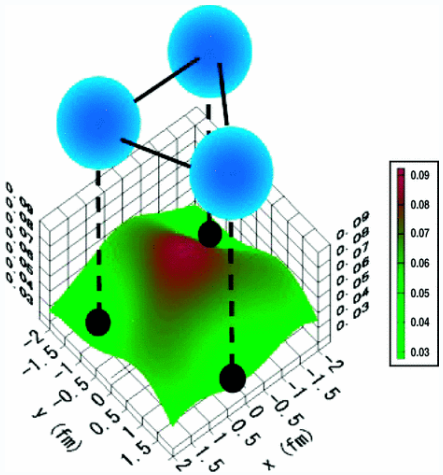
Overlap probability with the eigenstate : ^{14}C

- 0^+_1: shell-model like



- 0^+_2: less density at center





Relavance to the crystalization (equilateral-triangular shape) ?

N. Itagaki *et al.*, PRL92, 142501 (2004)

Summary

1. Ab initio MCSM is applied to Be and C isotopes with JISP16 interaction.

2. The emerging and evolution of the α clustering is seen without any assumption as a function of N as well as molecular structure.

3. Levels, E2, E0 and molecular properties of Be isotopes are described.

4. The intrinsic density profile is obtained by utilizing a unique feature (deformed Slater determinant) of MCSM.

5. The intrinsic shape of C is investigated in terms of the cluster analysis by the dendrogram. This is one of the AI techniques, and appears to be useful probably in many-body calculations with full of correlations. Various features of ^{12}C appear as a result of the calculation without any assumption, while mixings are always present.

6. Daejeon 16 interaction may improve the level scheme as JISP 16 may be at the edge of its applicability.

E N D

Thank you for your attention