TRIUMF Theory Workshop (Feb. 27 – Mar. 2, 2018)
Progress in Ab Initio Techniques in Nuclear Physics

# Recent advances in the no-core Monte Carlo shell model

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Supported by MEXT and JICFuS
Priority Issue 9 to be Tackled by Using Post K Computer "Elucidation of the Fundamental Laws and Evolution of the Universe"

TRIUMF

March 1, 2018

# Outline

- No-core Monte Carlo shell model (MCSM)
  - Introduction
  - Current status
- Cluster structure from no-core MCSM
  - Be isotopes
  - C isotopes
- Summary & future perspectives

# Monte Carlo shell model (MCSM)

## Standard shell model

$$\mathrm{H} = \begin{pmatrix} \star & \star & \star & \star & \star & \cdots \\ \star & \star & \star & \star & & \\ \star & \star & \star & & & \\ \star & \star & & \ddots & & \\ \star & & & & & \\ \vdots & & & & & \end{pmatrix} \Rightarrow \begin{pmatrix} E_0 & & & 0 \\ & E_1 & & \\ & & E_2 & \\ 0 & & & \ddots \end{pmatrix}$$

Diagonalization

Large sparse matrix $\sim \mathcal{O}(10^{10})$

# non-zero MEs $\sim \mathcal{O}(10^{13-14})$

- Importance truncation

T. Otsuka *et al*., Prog. Part. Nucl. Phys. 47, 319 (2001)

## Monte Carlo shell model

$$\mathrm{H} \sim \begin{pmatrix} \star & \star & \cdots \\ \star & \ddots & \\ \vdots & & \end{pmatrix} \Rightarrow \begin{pmatrix} E'_0 & & 0 \\ & E'_1 & \\ 0 & & \ddots \end{pmatrix}$$

Diagonalization

Important bases stochastically selected ~ O(100)

$$|\Psi(J,M,\pi)\rangle = \sum_i^{N_{basis}} f_i |\Phi_i(J,M,\pi)\rangle$$

$$|\Phi(J,M,\pi)\rangle = \sum_K g_K P^J_{MK} P^\pi |\phi\rangle$$

diagonalization

$$|\phi\rangle = \prod_i^A a_i^\dagger |-\rangle$$

← Deformed

$$a_i^\dagger = \sum_\alpha^{N_{sps}} c_\alpha^\dagger D_{\alpha i}$$

← Spherical

stochastic sampling & CG

# How to obtain ab-initio results from no-core MCSM

- Two steps of the extrapolation

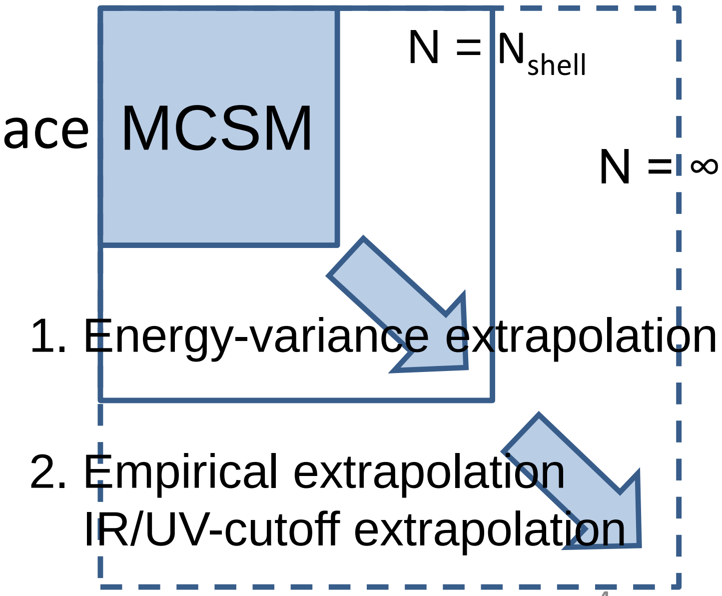
Same as in the MCSM w/ an inert core

1. Extrapolation of our MCSM (approx.) results to exact results in the fixed size of model space

Energy-variance extrapolation

N. Shimizu, Y. Utsuno, T. Mizusaki, T. Otsuka, T. Abe, & M. Honma, Phys. Rev. C82, 061305(R) (2010)

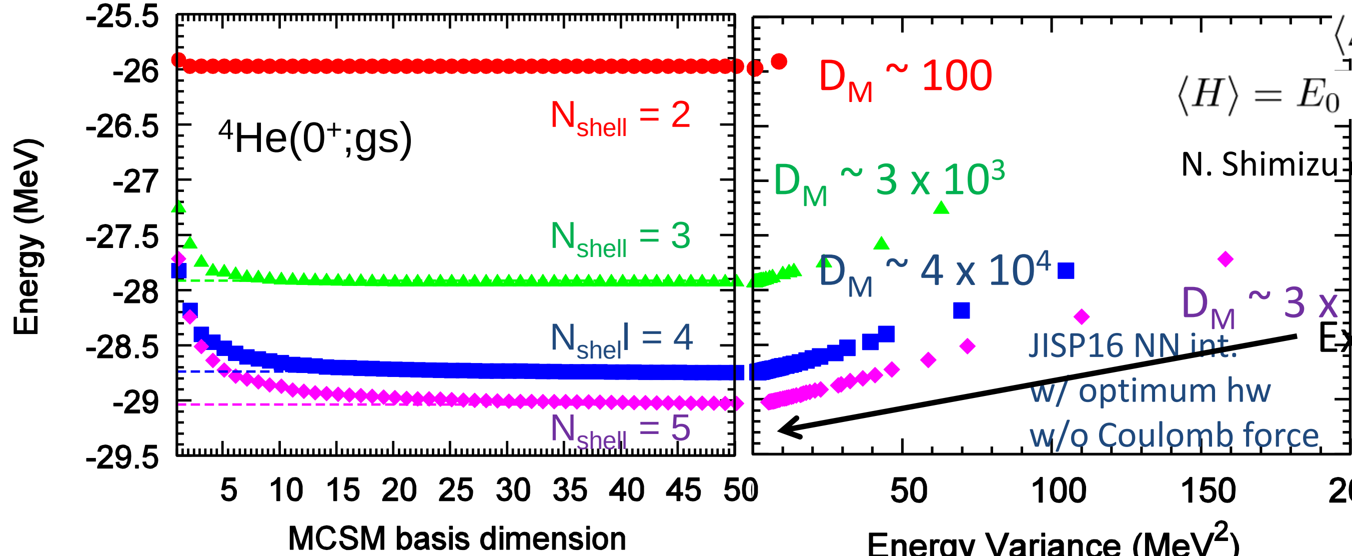
2. Extrapolation into the infinite model space
   - Empirical extrapolation w.r.t. $N_{shell}$
   - IR- & UV-cutoff extrapolations




→ Ab initio solution

# Extrapolations

- Extrapolation to FCI results (@ fixed size of basis space) <- Energy variance



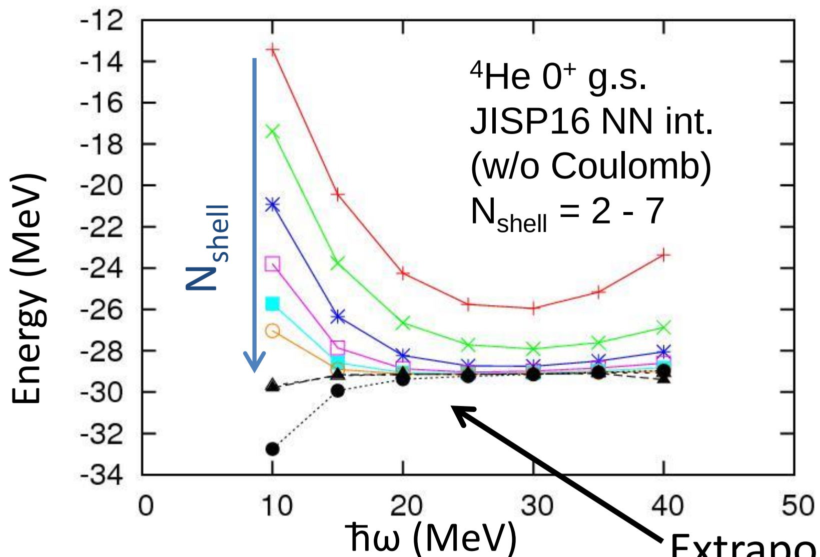

$$\langle \Delta H^2 \rangle = \langle H^2 \rangle - \langle H \rangle^2$$

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

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

Exact solution @ fixed $N_{shell}$

- Extrapolation to full ab initio solution (@ infinite size of basis space)



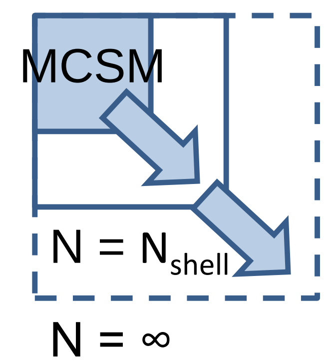

Extrapolations

( $N_{shell}$, ħω )

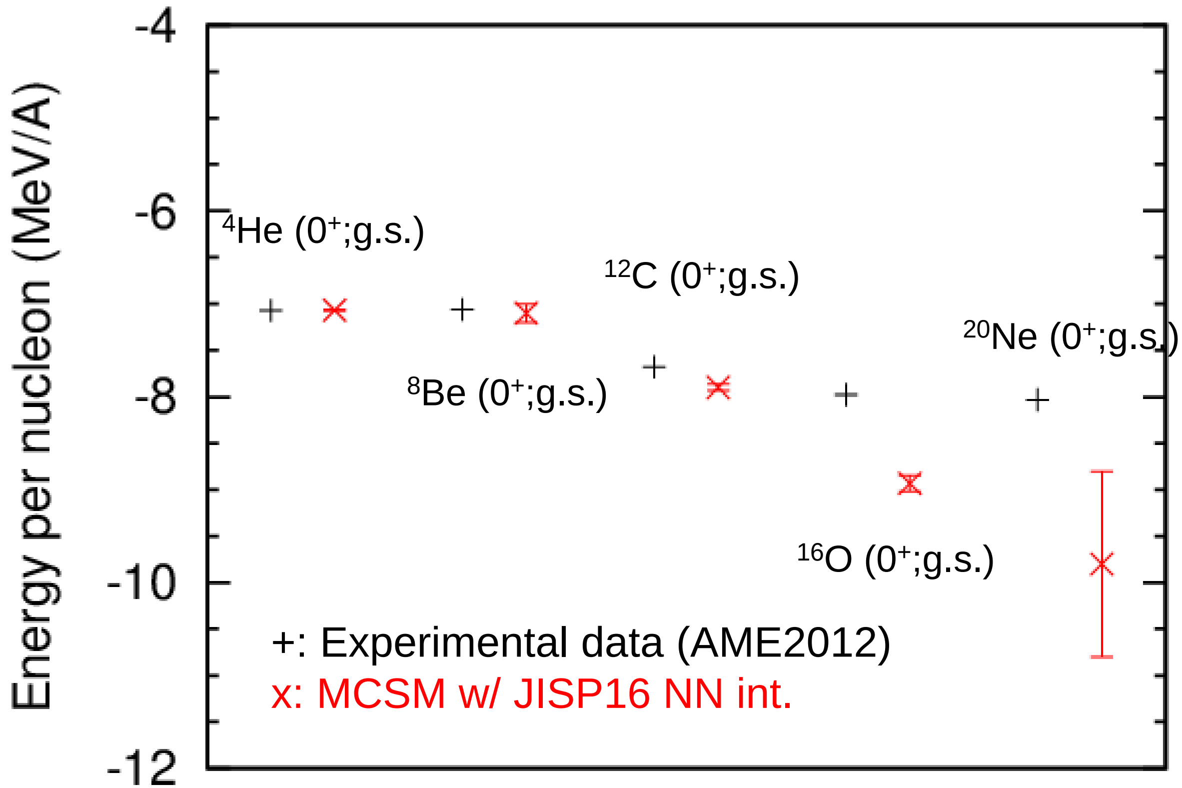
$$E(N) = E(N = \infty) + a \exp(-bN)$$

MCSM(traditional): -29.15(3) MeV
($N_{shell}$ = 3 - 7, ħw = 20 - 30 MeV)

c.f.) NCFC: -29.164(2) MeV
Extrapolated results to infinite $N_{max}$ space



# Comparison of MCSM results w/ experiments



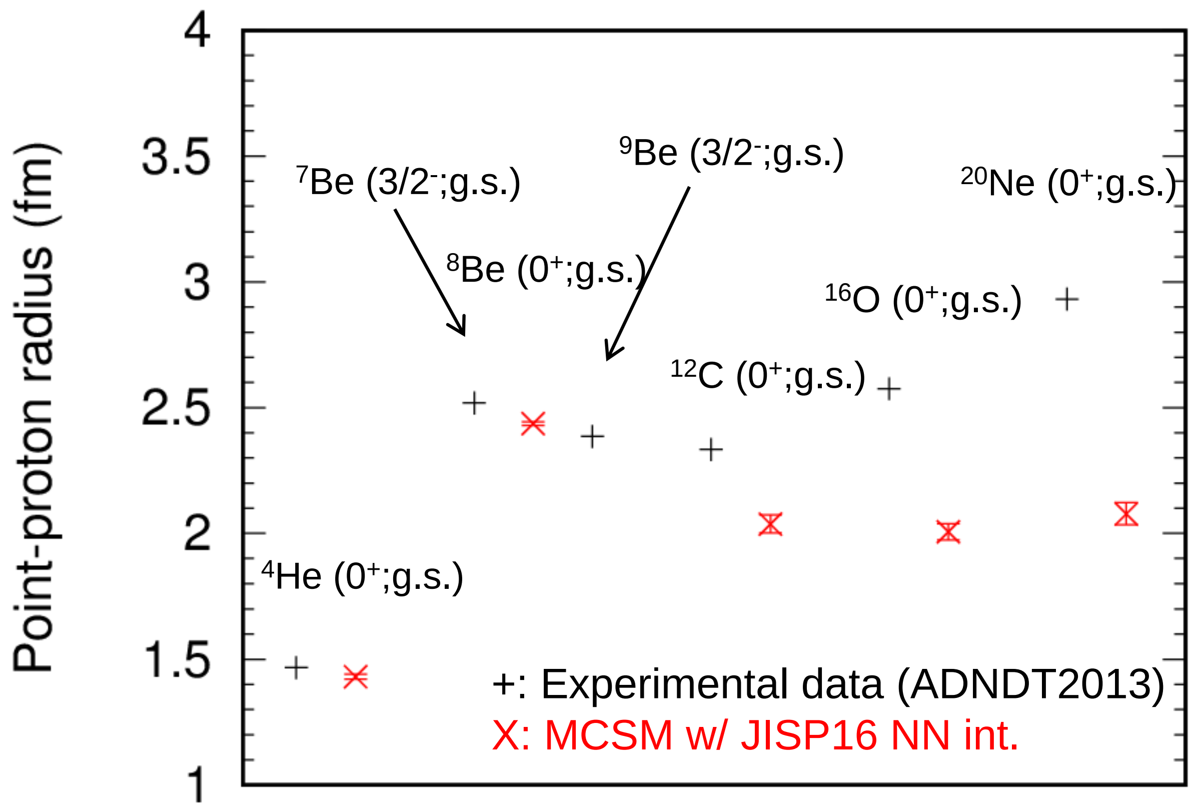

MCSM results are obtained using K computer by traditional extrapolation w/ optimum harmonic oscillator energies.

Coulomb interaction is included perturbatively.

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

→ Daejeon16, χEFT , …

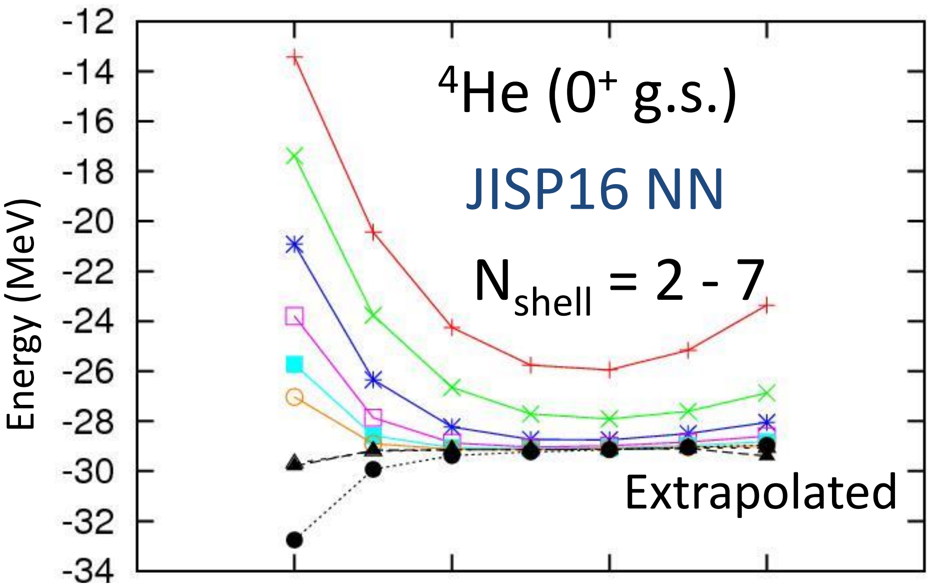
# Comparison of MCSM results w/ experiments




MCSM results are obtained using K computer around optimum harmonic oscillator energies for radii.

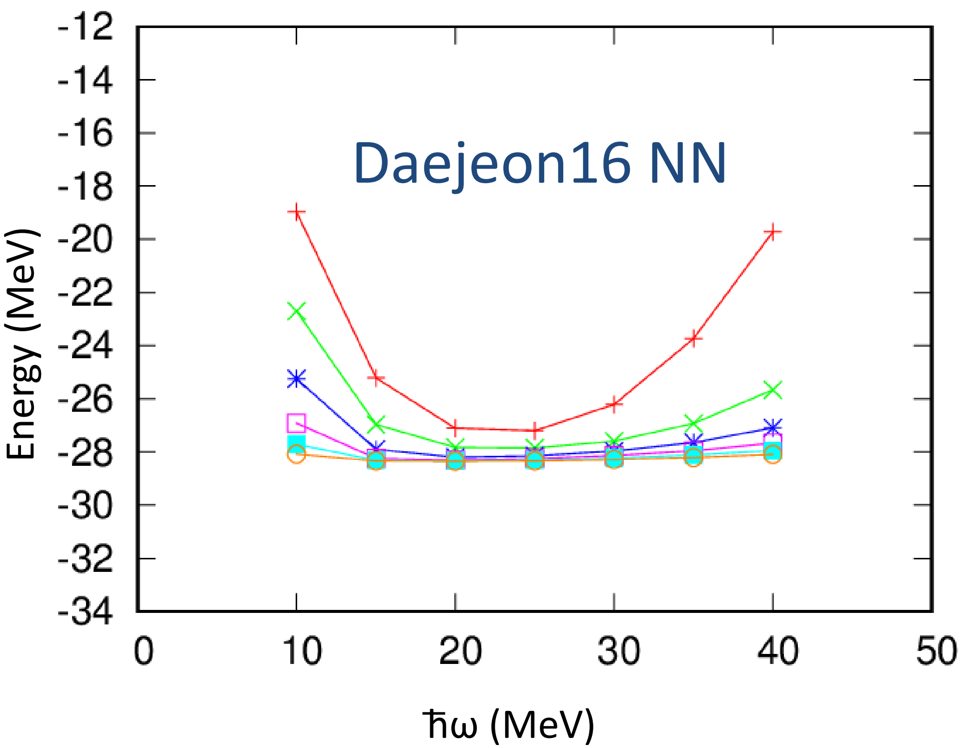
MCSM results show good agreements w/ experimental data up to $^{8}$Be, clearly smaller for heavier nuclei beyond $^{12}$C as A increases.

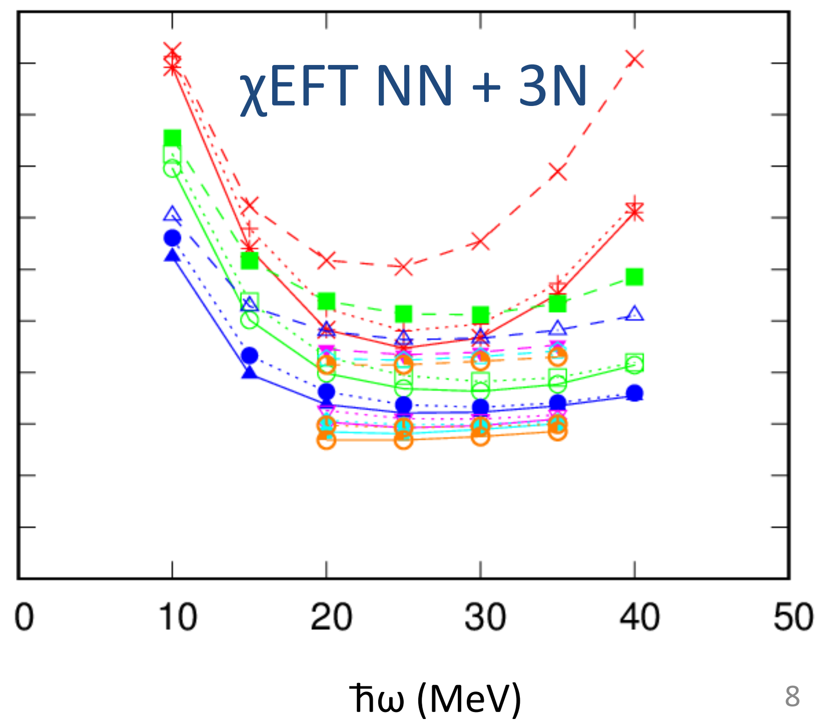
Preliminary




Work in progress ($^{12}$C, $^{16}$O, …)

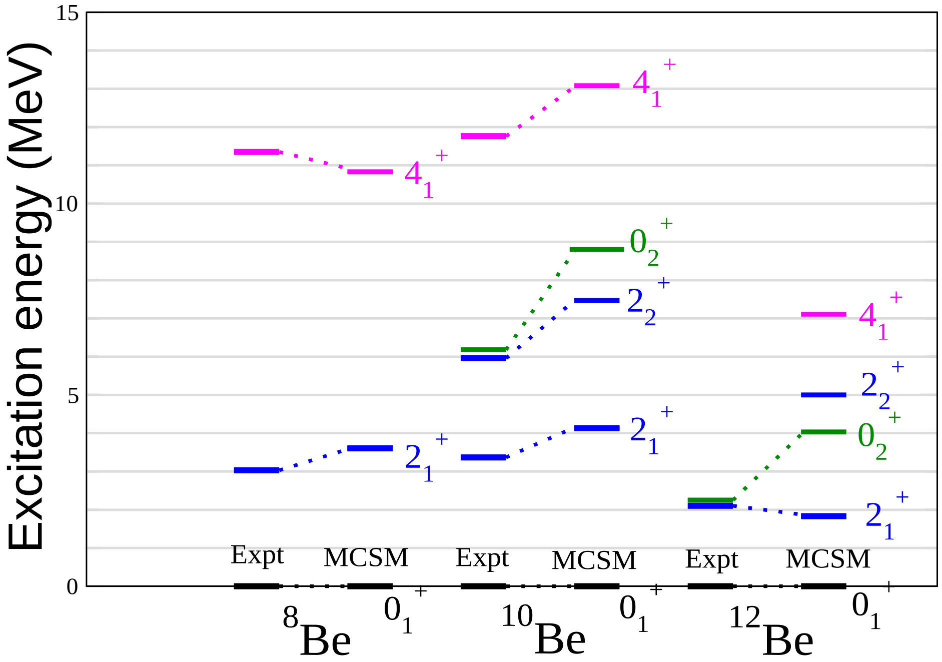
SRG-evolved χEFT int. (Λ = 2.0 fm$^{-1}$)
- NNonly
- NN + 3Nind(NO2B)
- NN + 3Nfull(NO2B)



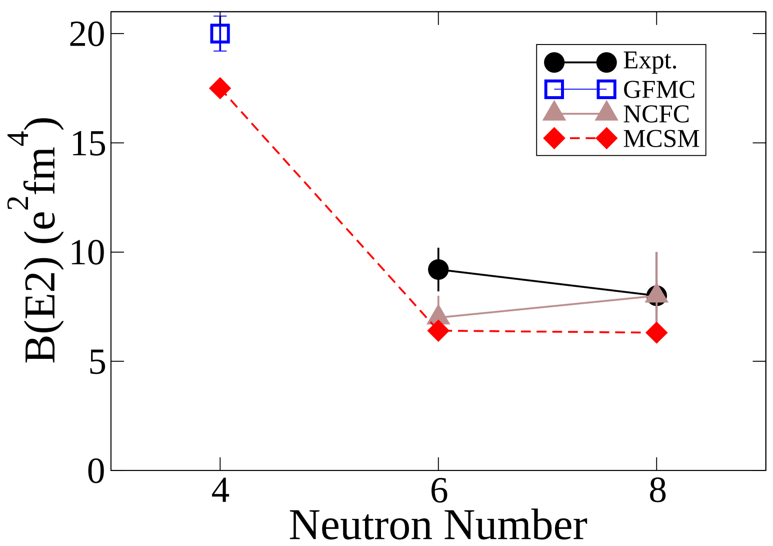
# Energy levels & E2 transition strengths of Be isotopes

- Excitation energies




Expt.: $^{8}$Be,$^{10}$Be (Tilley et al., 2004),
$^{12}$Be (Shimoura et al., 2003)
MCSM: JISP16 NN int., $N_{shell}$ = 6, hw = 15 MeV

- E2 transition strengths
$\underline{B(E2; 2^+_1 \rightarrow 0^+_1)}$

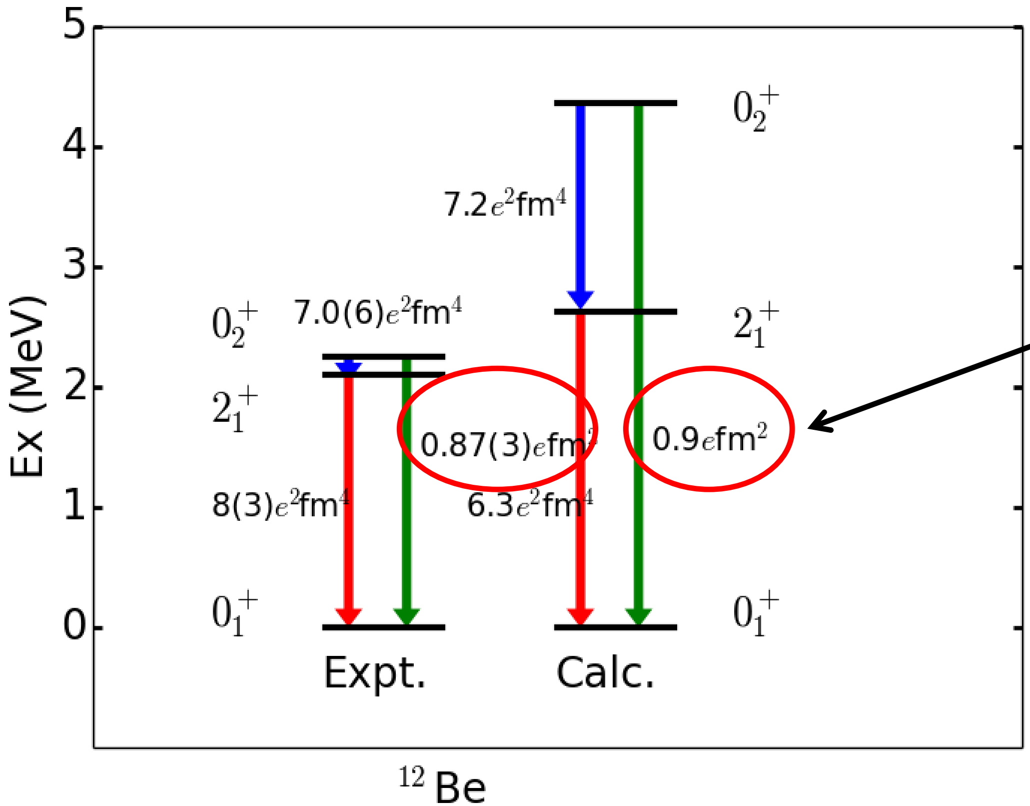



Expt.: $^{8}$Be Datar *et al*. 2013 + estimateby GFMC
$^{10}$Be McCutchan *et al*. 2009
$^{12}$Be Imai *et al*. 2009

Overall good agreement w/ experimental data

# $E2$ & $E0$ transition strength of $^{12}$Be

Preliminary



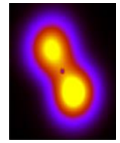
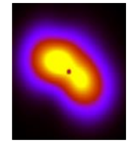
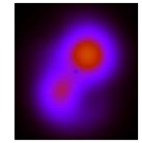
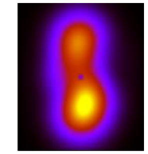

$B(E0; 0^+_2 \rightarrow 0^+_1)$

Expt.:

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

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

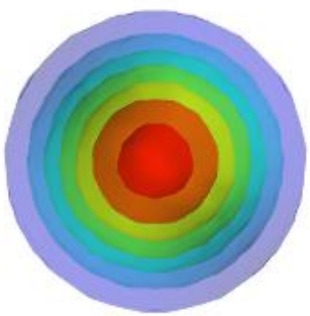
# Density distribution in MCSM

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

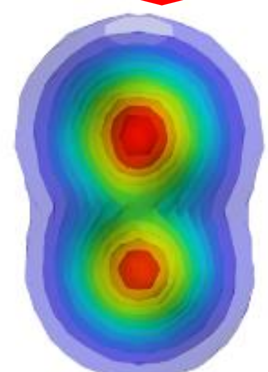
Angular-momentum projection

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

A way to construct an "intrinsic" density



$^8Be\ 0^+$ ground state



Laboratory frame

"Intrinsic" (body-fixed) frame

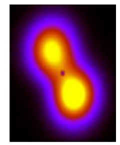
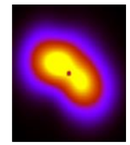
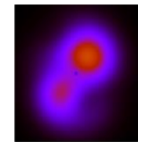
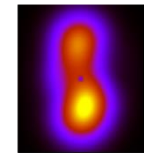
Densities in lab. & body-fixed frames can be constructed by MCSM

N. Shimizu, T. Abe, Y. Tsunoda, Y. Utsuno, T. Yoshida, T. Mizusaki, M. Honma, T. Otsuka,
Progress in Theoretical and Experimental Physics, 01A205 (2012)

# How to construct an “intrinsic” density from MCSM w.f.

- MCSM w.f. w/o spin & parity projections

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

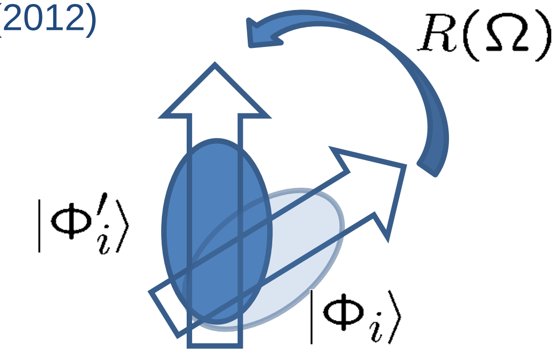
$c_1$  $+ c_2$  $+ c_3$  $+ c_4$  + …

- Possible ways to construct an “intrinsic” density
  - Rotation of each basis in terms of Q-moment
  - Rotation in terms of overlap btw bases
  - Rotation in terms of minimization of “intrinsic” energy
  - …

For a demonstration, we employ the way to construct an “intrinsic” density in terms of Q-moment.

# How to construct an "intrinsic" density from MCSM w.f.

N. Shimizu, T. Abe, Y. Tsunoda, Y. Utsuno, T. Yoshida, T. Mizusaki, M. Honma, T. Otsuka, Progress in Theoretical and Experimental Physics, 01A205 (2012)

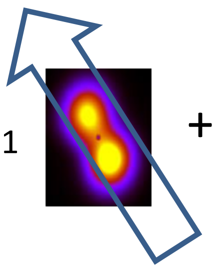
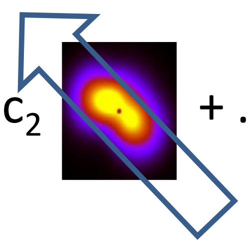
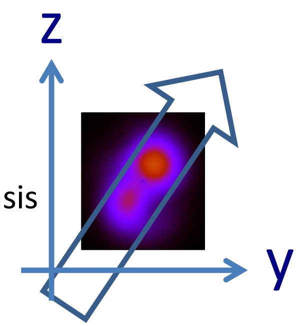



Rotation by diagonalizing Q-moment ($Q_{zz} > Q_{yy} > Q_{xx}$)

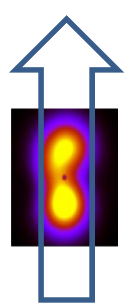
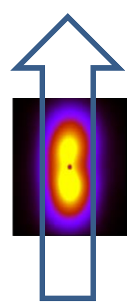
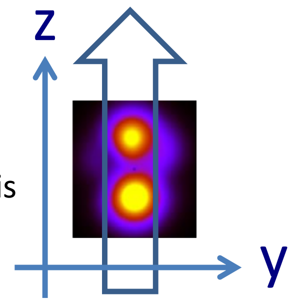
- MCSM wave function

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

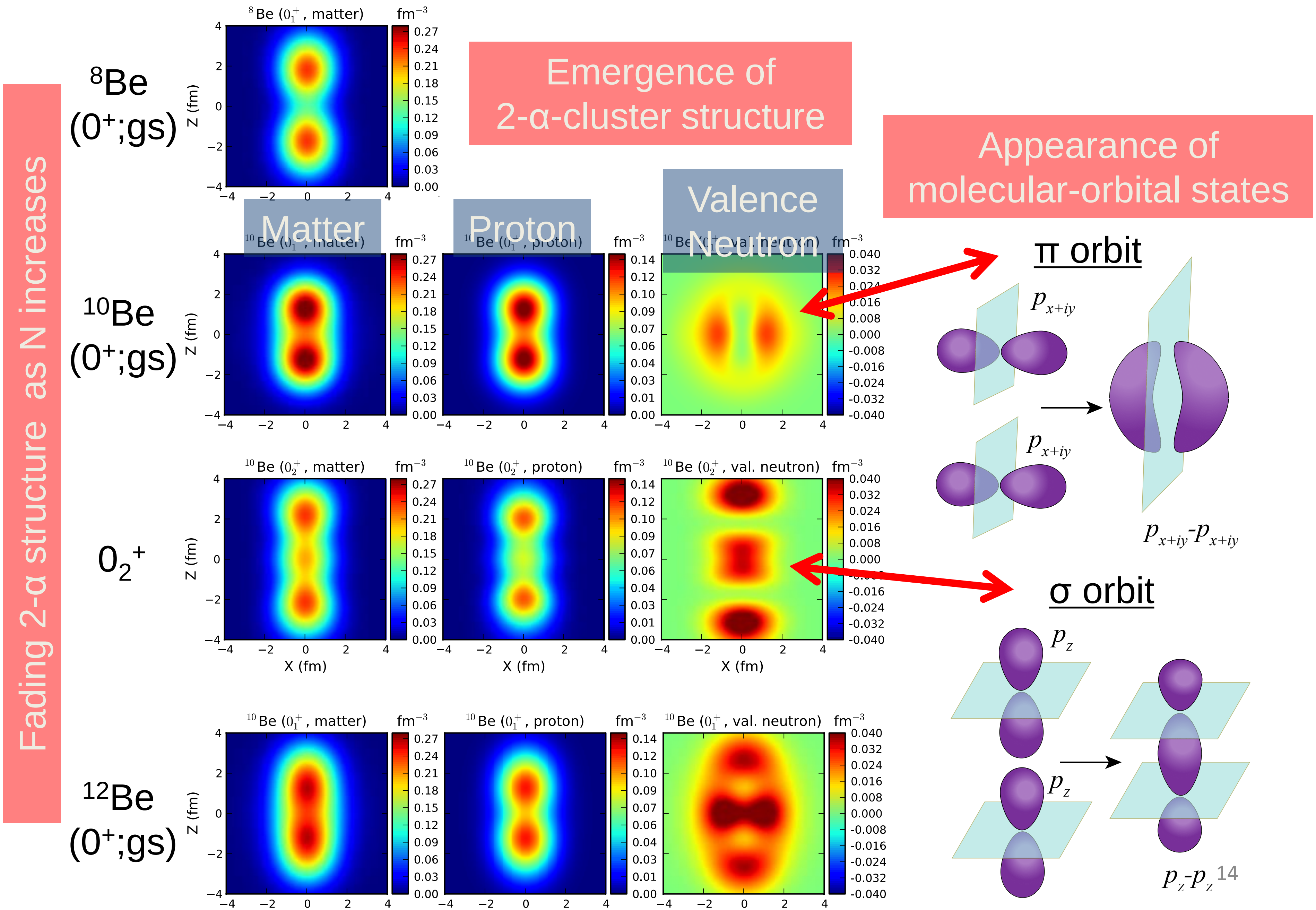
- Wave function w/o the projections

$$\sum_{i=1}^{N_{basis}} c_i |\Phi_i\rangle =$$ $c_1$  $+ c_2$  $+ \ldots + c_{Nbasis}$ 

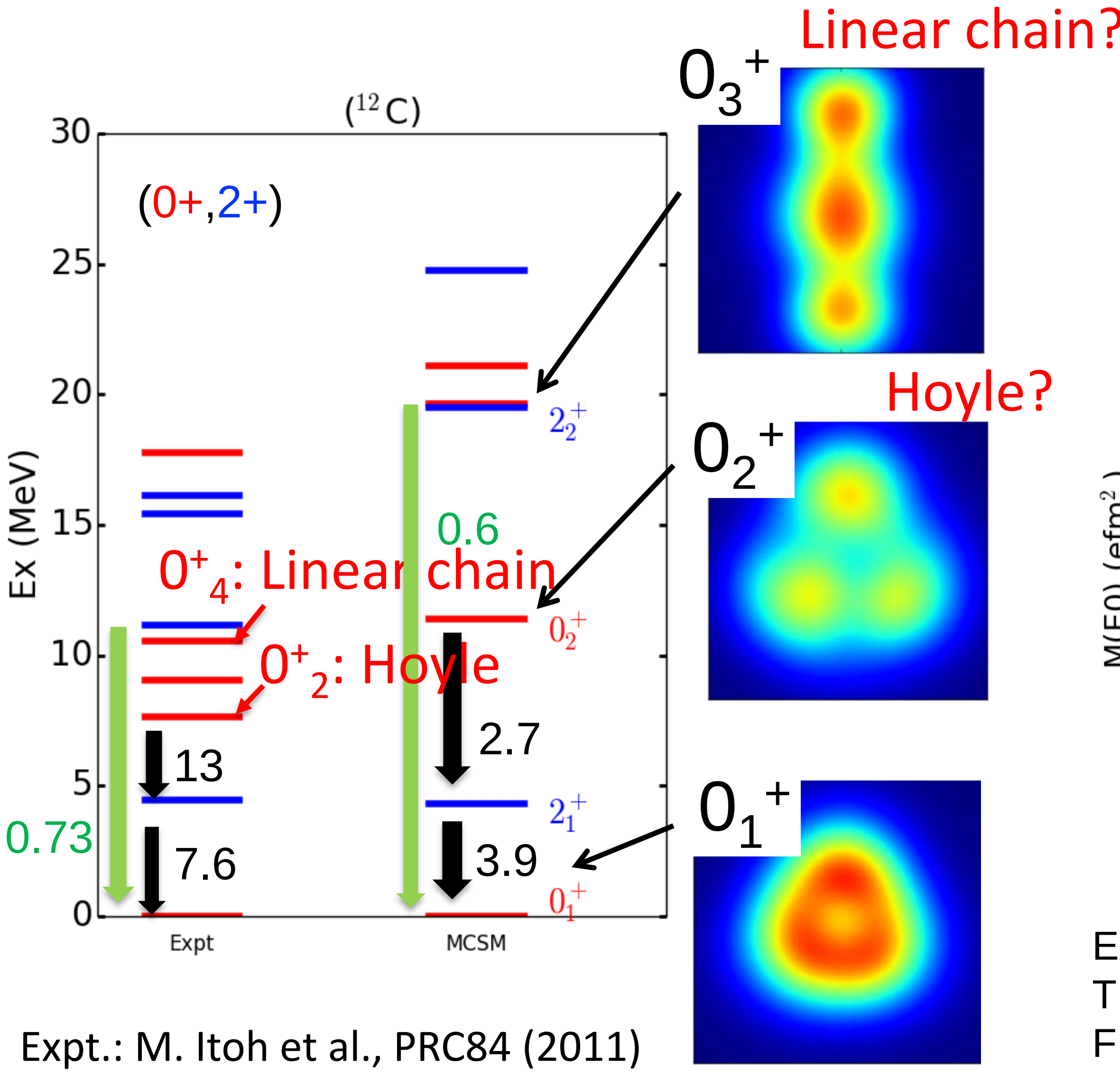

- Wave function w/o the projection w/ the alignment of Q-moment

$$\sum_{i=1}^{N_{basis}} c_i |\Phi'_i\rangle =$$ $c_1$  $+ c_2$  $+ \ldots + c_{Nbasis}$ 

# Density distribution of Be isotopes

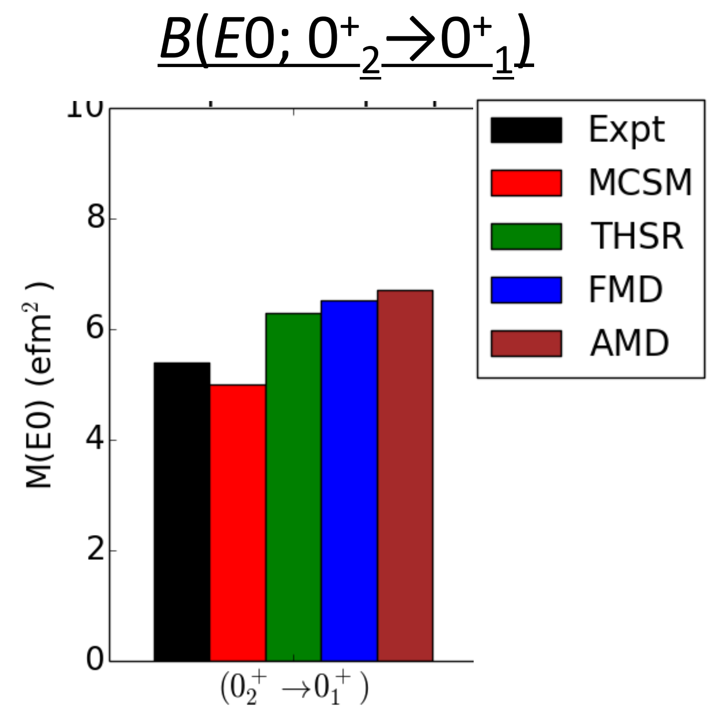


# Energy level & transition strength of $^{12}C$




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

Preliminary

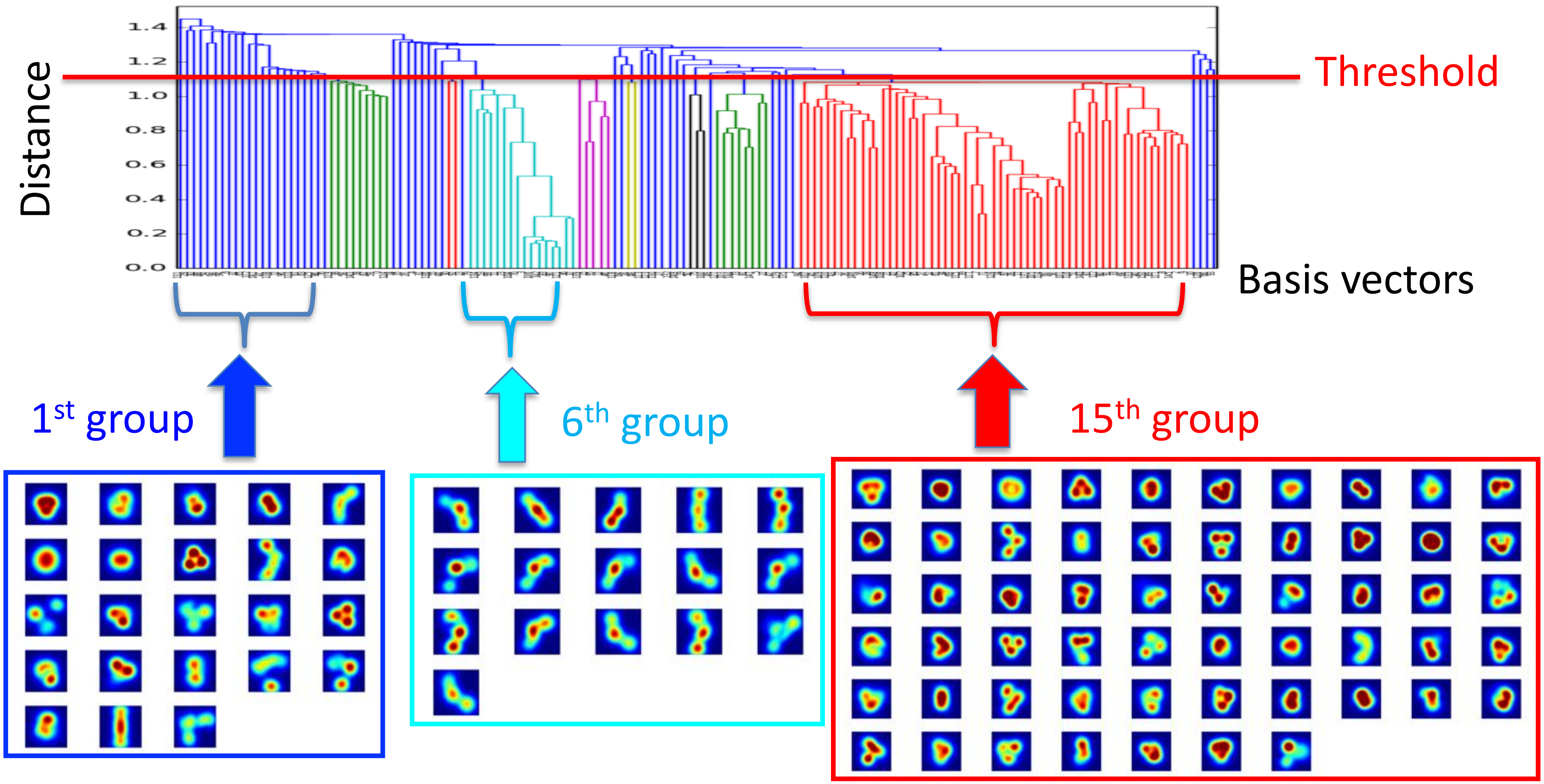



Expt.: P. Strehl 1970
THSR: Y. Funaki 2015
FMD: M. Chernykth 2007
AMD: Y. Kanada-En'yo 2007

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

# Closer look at density-distributions in $^{12}C$

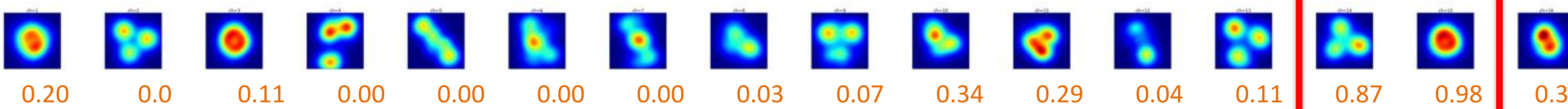
- Dendrogram in "Cluster analysis" of statistics
- Basis vectors are divided into 16 groups (in this case)



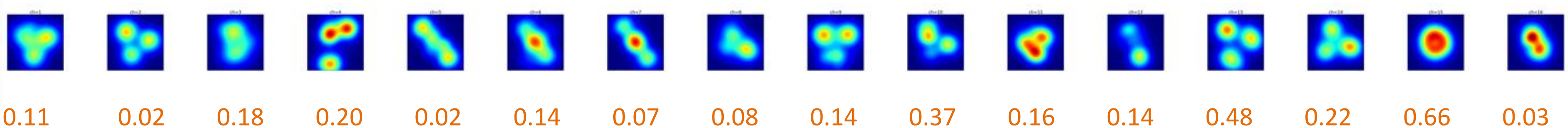
# Overlap probability in $^{12}C$

- Dendrogram in "Cluster analysis" of statistics
- Basis vectors are divided into 16 groups (in this case)

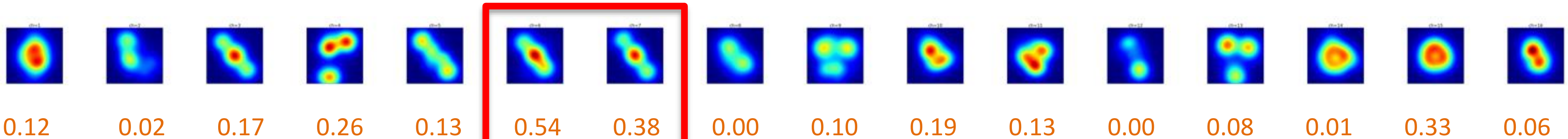
- $0^+_1$ : Concentrated in 14th (3 clusters) & 15th (compact shape) groups




- $0^+_2$ : Scattered among all groups → Gas-like state?



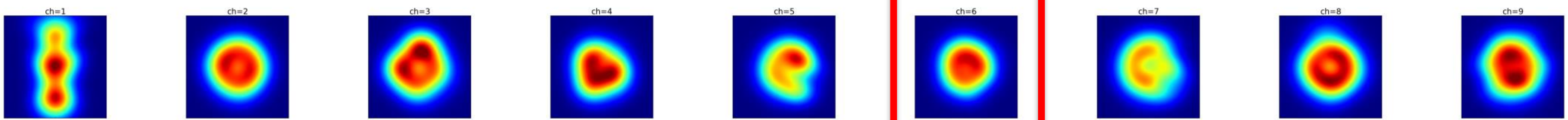

- $0^+_3$ : Concentrated in 6th & 7th (linear shape) groups



# Overlap probability in $^{14}$C

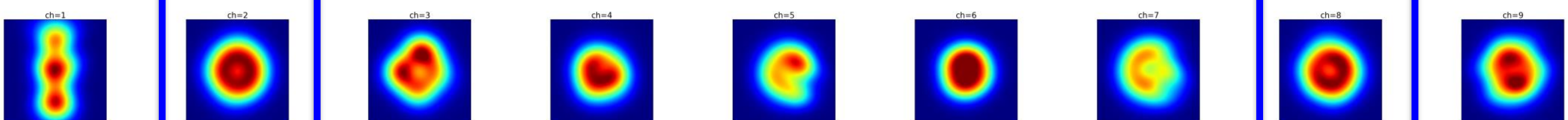
- $0^+_1$: shell-model like

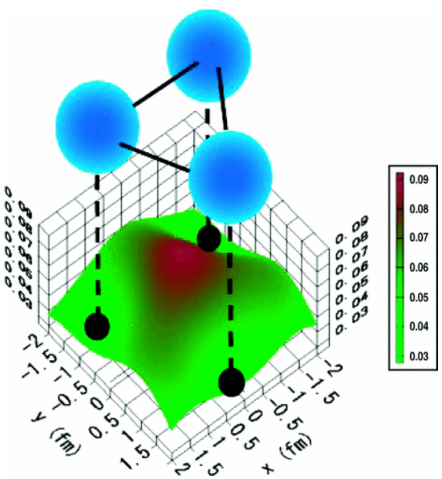
P=0.00 0.52 0.00 0.11 0.37 0.95 0.05 0.02 0.0



- $0^+_2$: less density at center

P=0.01 0.83 0.19 0.00 0.14 0.02 0.00 0.77 0.10






Equilateral-triangular shape
stabilized by excess neutrons?

Molecular orbit model:
N. Itagaki *et al.*, PRL92, 142501 (2004)

# Summary

- MCSM results for light nuclei (A<= 20) w/ a NN potential can be extrapolated to the infinite basis space to obtain ab initio solution.
  - JISP16 NN interaction gives good agreement w/ experimental data up to around $^{8}$Be.
  - Daejoen16 NN & SRG-evolved χEFT interactions are tested for $^{4}$He
- Cluster structure of Be & C isotopes can be visualized using MCSM wave functions.

# Future perspective

- Introduction of explicit 3NF effects in the no-core MCSM
- Heavier nuclei beyond $^{20}$Ne
- Quantitative analysis on cluster structure of Be & C isotopes

# Collaborators

- Takaharu Otsuka (RIKEN, Tokyo, Leuven, MSU)
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- Noritaka Shimizu (Tokyo)
- Tooru Yoshida (RIST)
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- James P Vary (Iowa State U)
- Pieter Maris (Iowa State U)
- Petr Navratil (TRIUMF)