International Conference “Nuclear Theory in the Supercomputing Era - 2018” (NTSE-2018)
October 29 – November 2, 2018

# No-core Monte Carlo shell model calculations with Daejeon16 NN interaction

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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”

Institute for Basic Science, Daejeon, Korea

November 2, 2018

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- Pieter Maris (Iowa State U)

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# Outline

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

# 1. No-core Monte Carlo shell model (MCSM)

- Introduction
- Current status

# "Ab initio" in low-energy nuclear structure physics

- Major challenge in nuclear physics

  - Nuclear structure & reactions directly from *ab-initio* calc. w/ nuclear forces

  - *ab-initio* approaches in nuclear structure calculations (A > 4):

    Light mass: Green's Function Monte Carlo, No-Core Shell Model (A ~ 12),

    Medium/heavy mass: Coupled Cluster (sub-shell closure +/- 1,2),

    Self-consistent Green's Function theory, IM-SRG, UMOA, Lattice EFT, …

- Solve the non-relativistic many-body Schroedinger eq. and obtain the eigenvalues and eigenvectors.

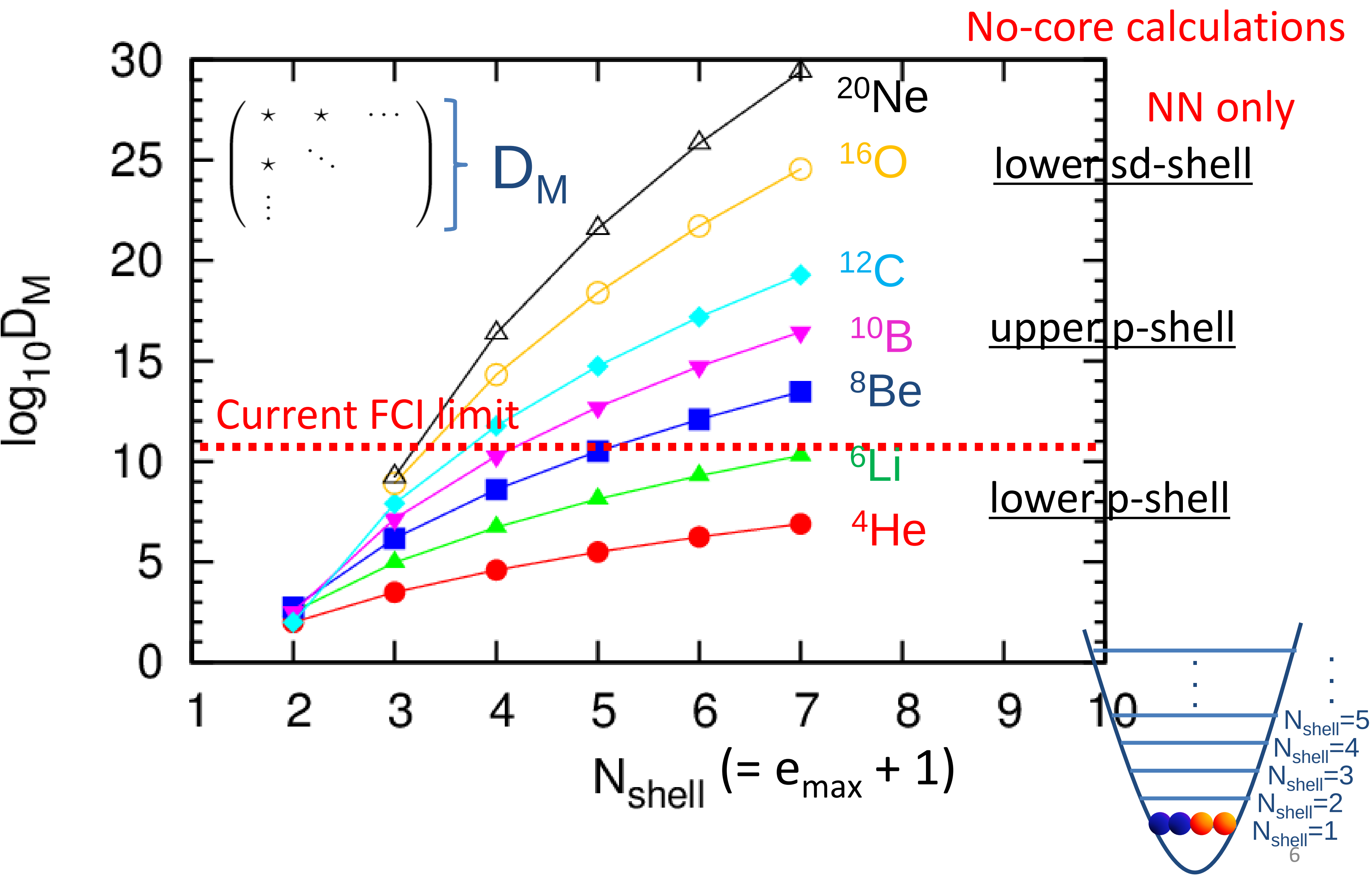
$$H|\Psi\rangle = E|\Psi\rangle$$

$$H = T + V_{\rm NN} + V_{\rm 3N} + \cdots + V_{\rm Coulomb}$$

  – Ab initio: All nucleons are active, and Hamiltonian consists of realistic NN (+ 3N + …) potentials.

→ Computationally demanding → Monte Carlo shell model (MCSM)

# M-scheme dimension in $N_{shell}$ truncation



# Monte Carlo shell model (MCSM)

## Standard shell model

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

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

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

Diagonalization

Important bases stochastically selected ~ O(100)

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

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

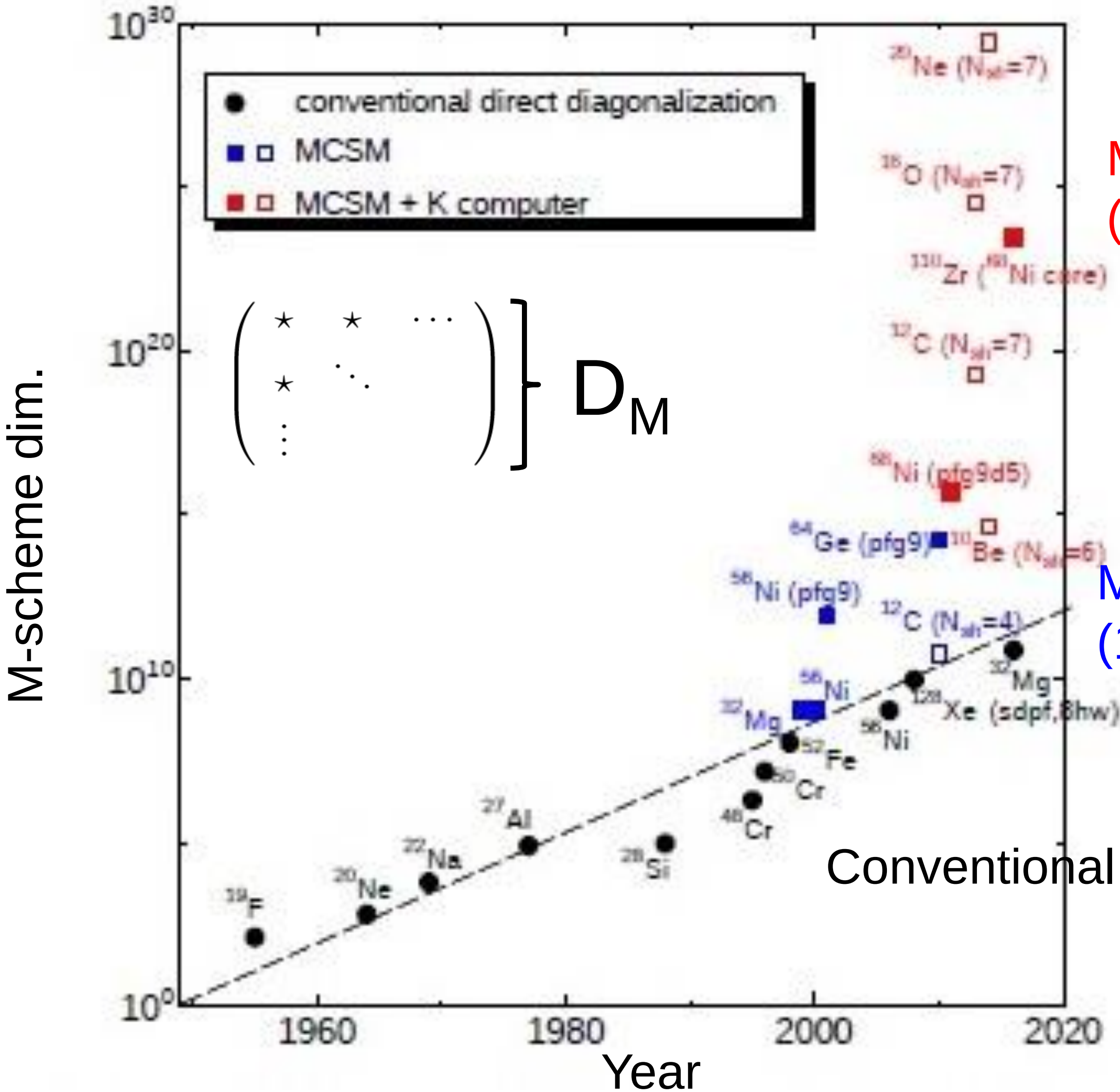
diagonalization

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

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

stochastic sampling & CG method

# Historical evolution/development of the MCSM




MCSM
($2^{nd}$ generation: 2010 - )

MCSM
($1^{st}$ generation: 1990's - 2010)

Conventional Shell Model

N. Shimizu et al., Phys. Scr. 92, 063001 (2017).

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

- Two steps of the extrapolation

Same as in the MCSM w/ an inert core

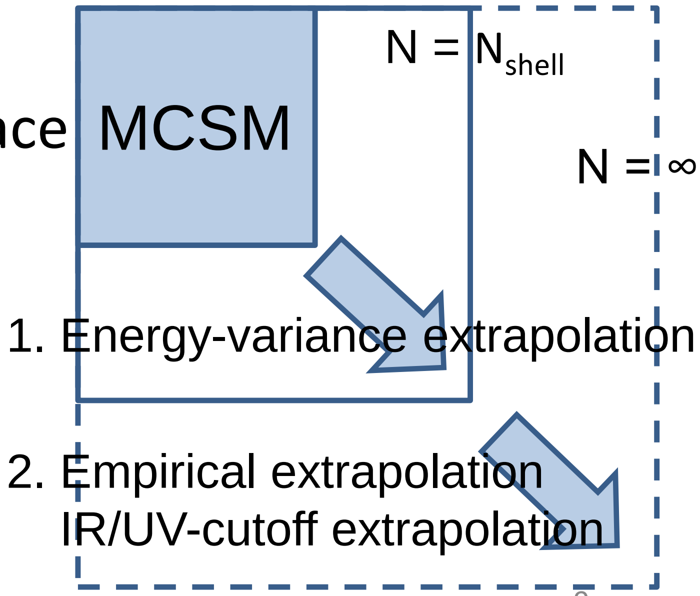
1. Extrapolation of our MCSM (approx.) results to exact results in the fixed size of model space

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

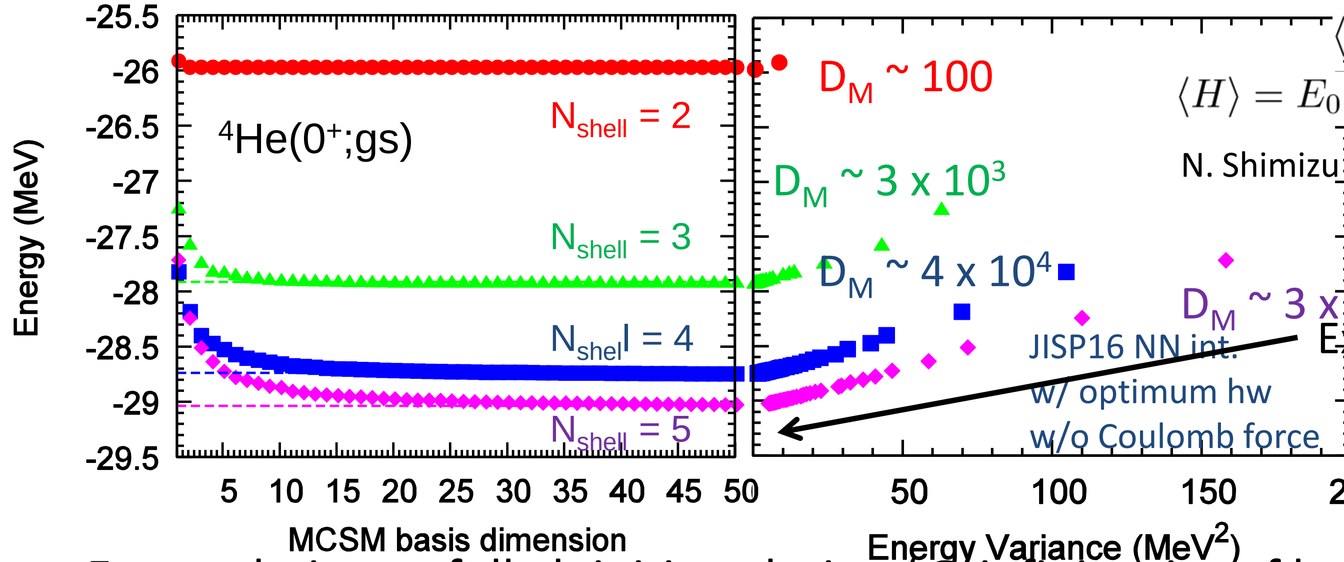
- Empirical extrapolation w.r.t. $N_{shell}$
- IR- & UV-cutoff extrapolations




→ Ab initio solution

# Extrapolations

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



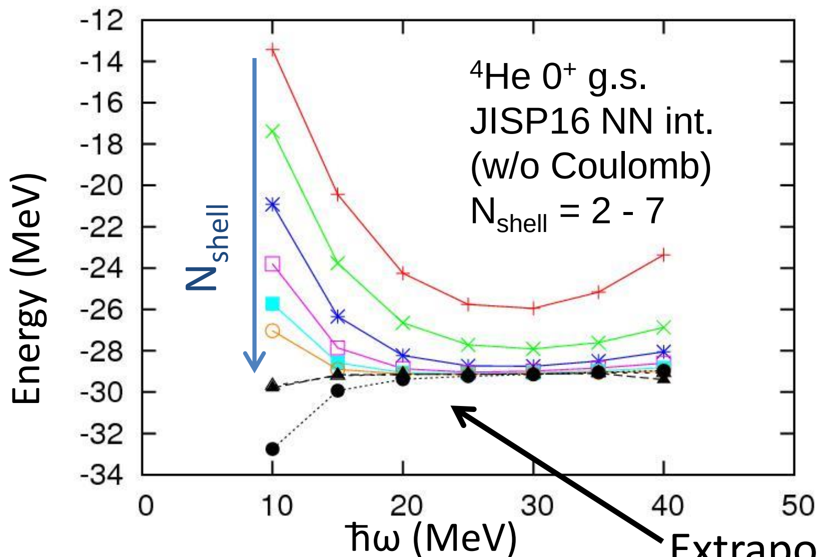

$$\langle \Delta H^2 \rangle = \langle H^2 \rangle - \langle H \rangle^2$$

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

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

Exact solution @ fixed $N_{shell}$

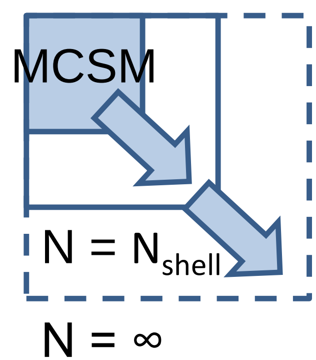
- Extrapolation to full ab initio solution (@ infinite size of basis space)




Extrapolations

( $N_{shell}$, ħω )

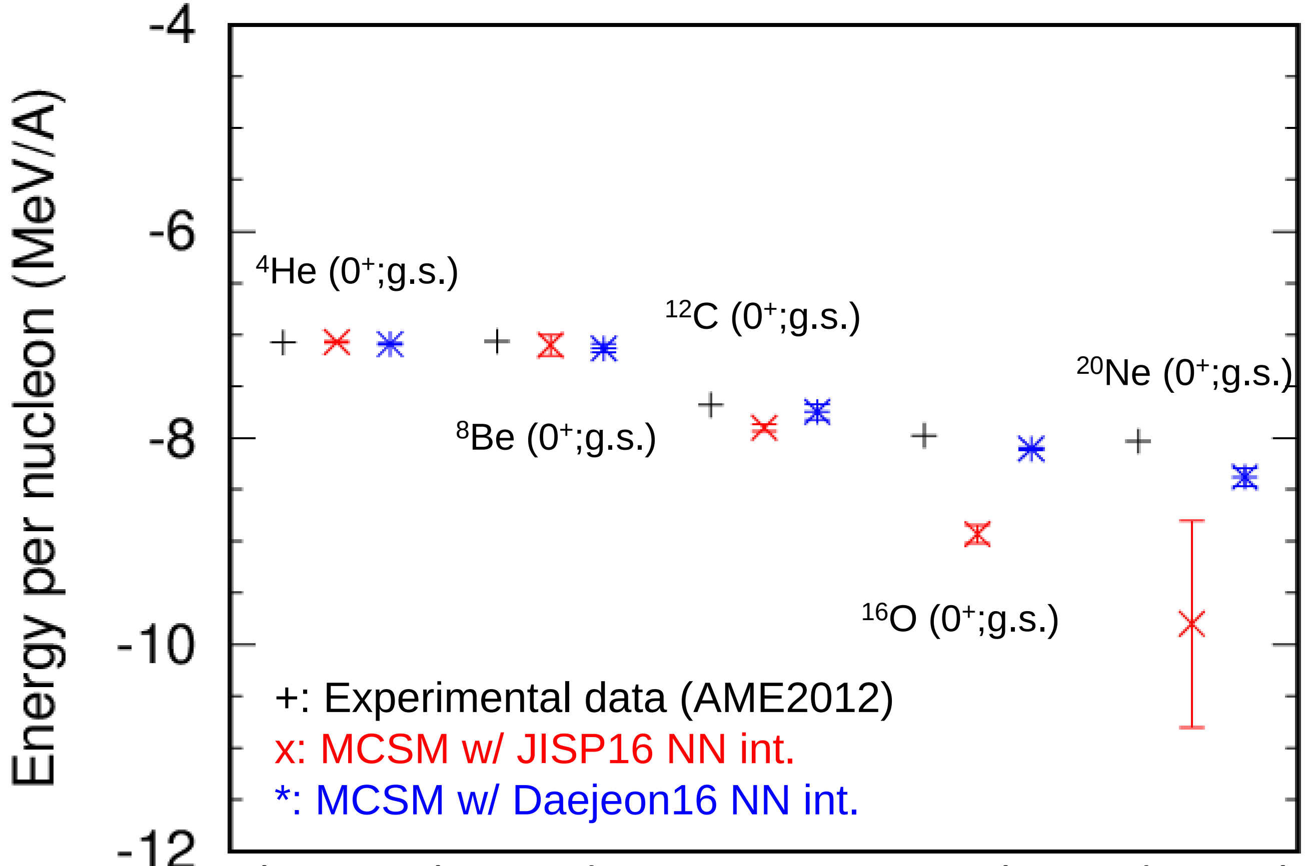
$$E(N) = E(N = \infty) + a \exp(-bN)$$




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



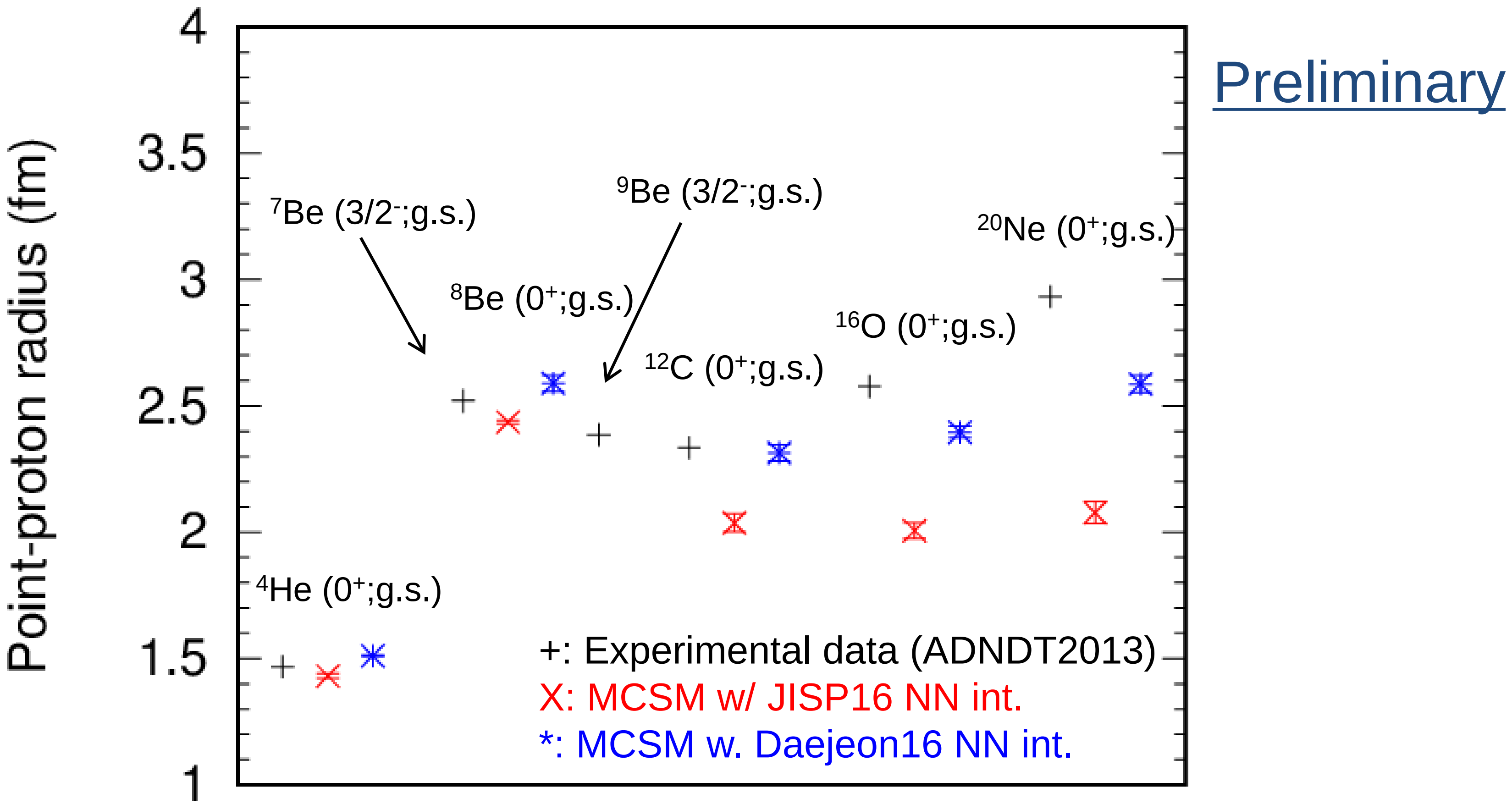

Preliminary

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

JISP16 results show good agreements w/ experimental data up to $^{12}C$, slightly overbound for $^{16}O$, and clearly overbound for $^{20}Ne$.

Daejeon16 results show good agreements w/ experimental data up to $^{20}Ne$.
(Energy-variance extrapolation has not been done yet)

# Comparison of MCSM results w/ experiments



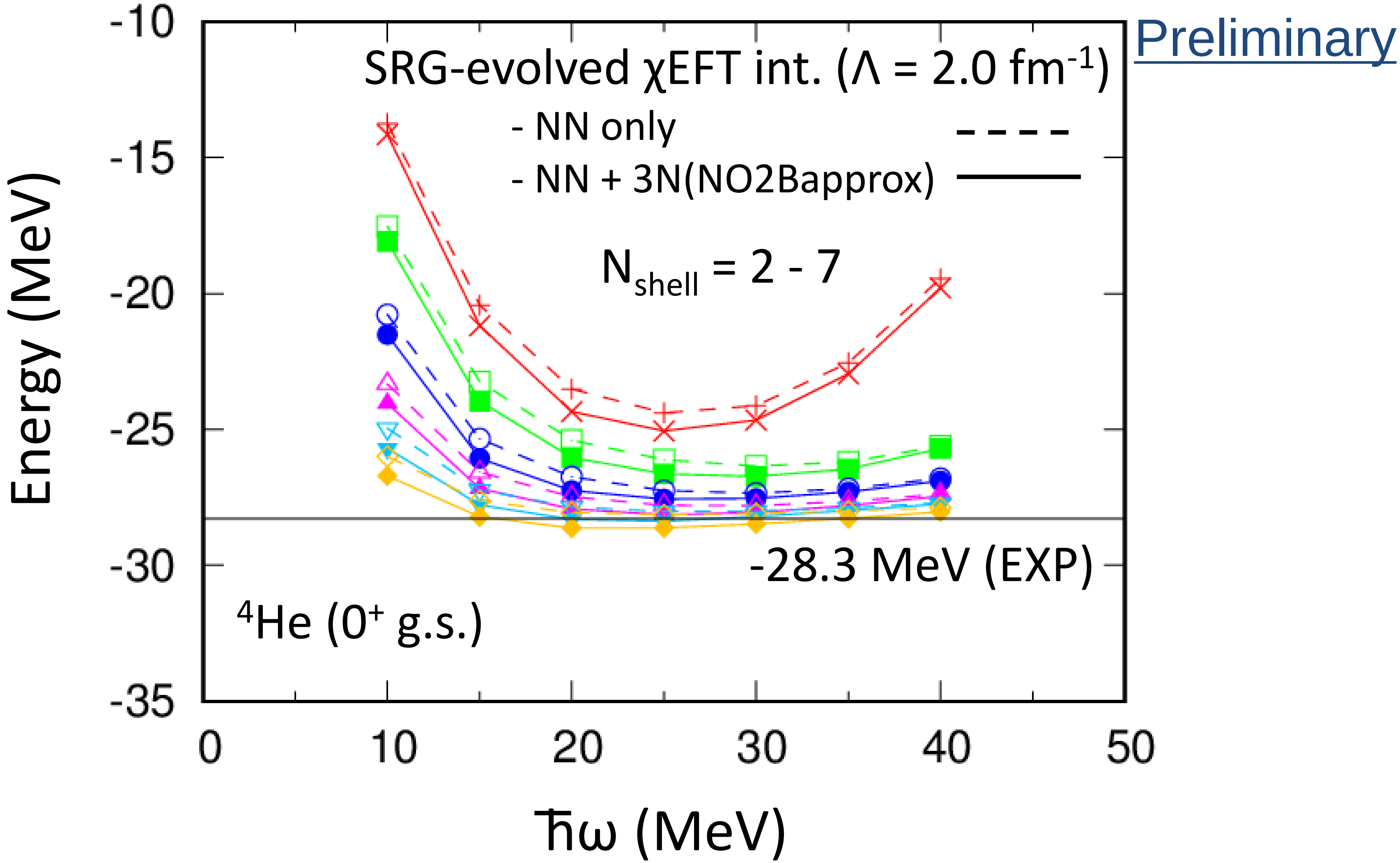

MCSM results are obtained using K computer around optimum harmonic oscillator energies for radii.

JISP16 results show good agreements w/ experimental data up to $^{8}$Be, clearly smaller for heavier nuclei beyond $^{12}$C as A increases.

Daejeon16 results show larger radii than JISP16 ones (Energy-variance extrapolation has not been done yet)

# Test of chiral 3N int. for closed-shell nuclei

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

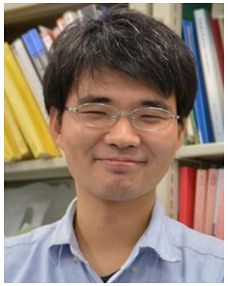



→ NC-MCSM calc. for Open-shell nuclei

# 2. Cluster structure from no-core MCSM

- Be isotopes
- C isotopes

# Cluster structure of Be & C isotopes



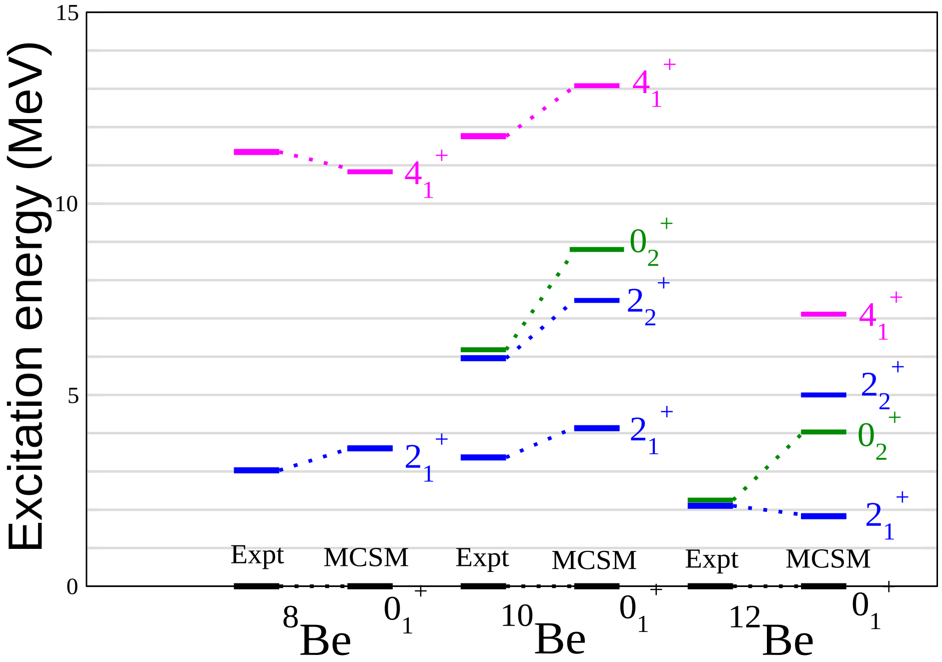
T. Yoshida (RIST)

Remarks

- Size of model space & HO frequency are fixed.
  - $N_{shell}$ = 6, hw = 15 MeV
  - Not quantitative discussion, but qualitative
  - Most of the results are preliminary.
- Starting from a realistic NN potential (JISP16)

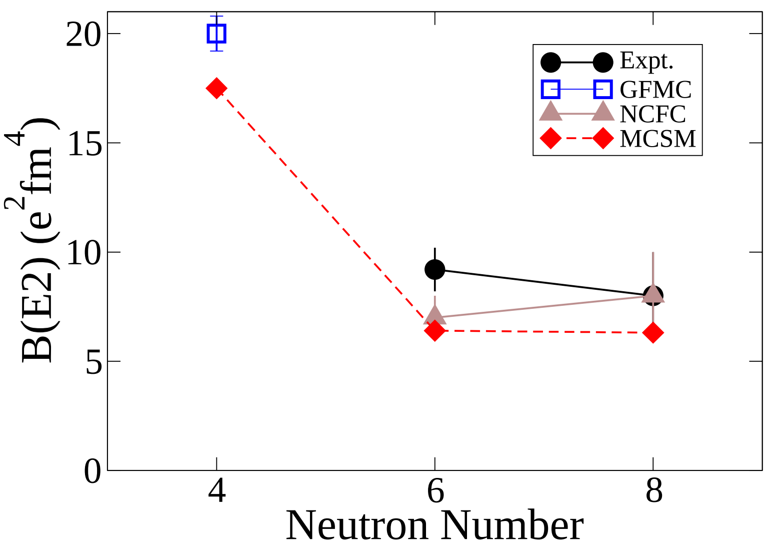
# Energy levels & E2 transition strengths of Be isotopes

- Excitation energies




- E2 transition strengths

$\underline{B(E2; 2^+_1 \to 0^+_1)}$



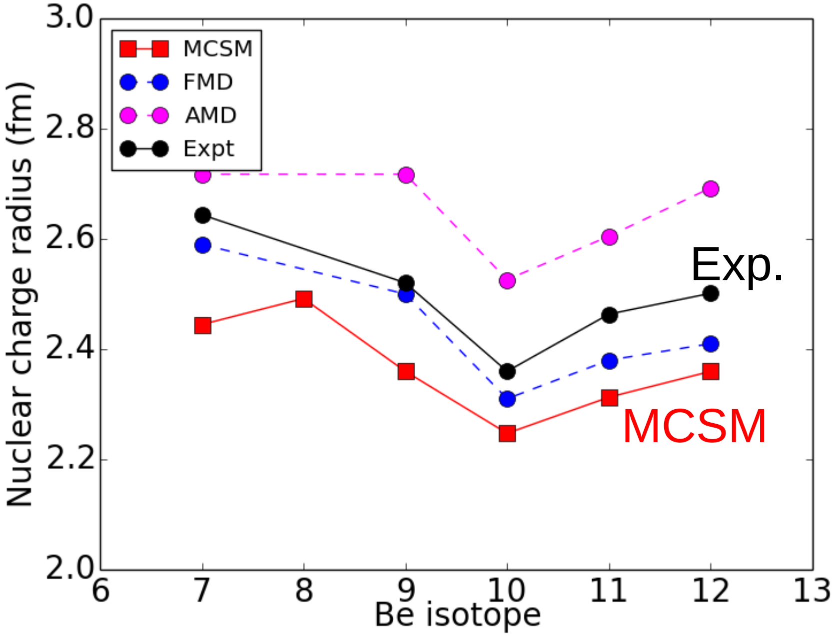

Expt.: $^{8}$Be,$^{10}$Be (Tilley et al., 2004),
$^{12}$Be (Shimoura et al., 2003)
MCSM: JISP16 NN int., $N_{shell}$ = 6, hw = 15 MeV

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

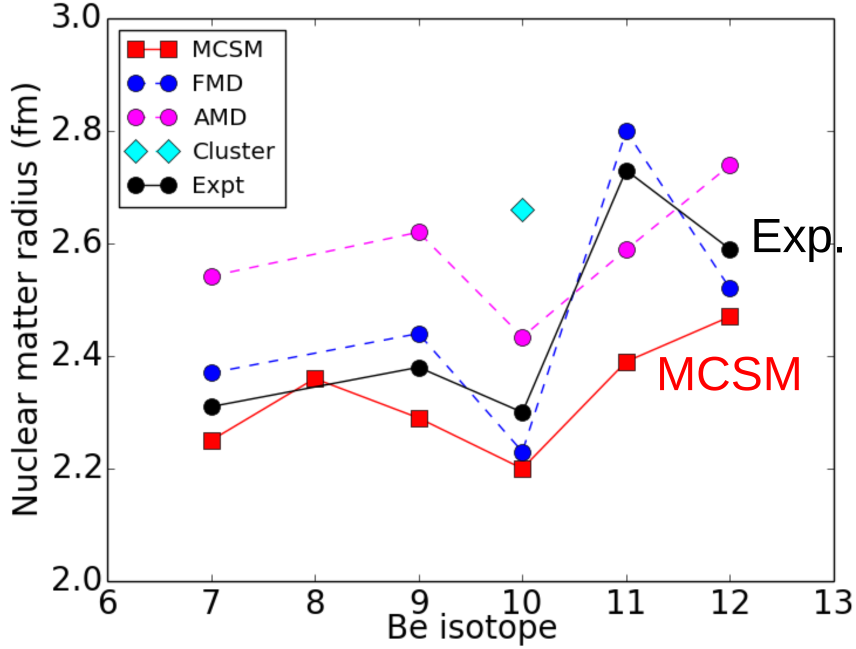
Overall good agreement w/ experimental data

# Radii of Be isotopes

## Point-proton radius




## Matter radius

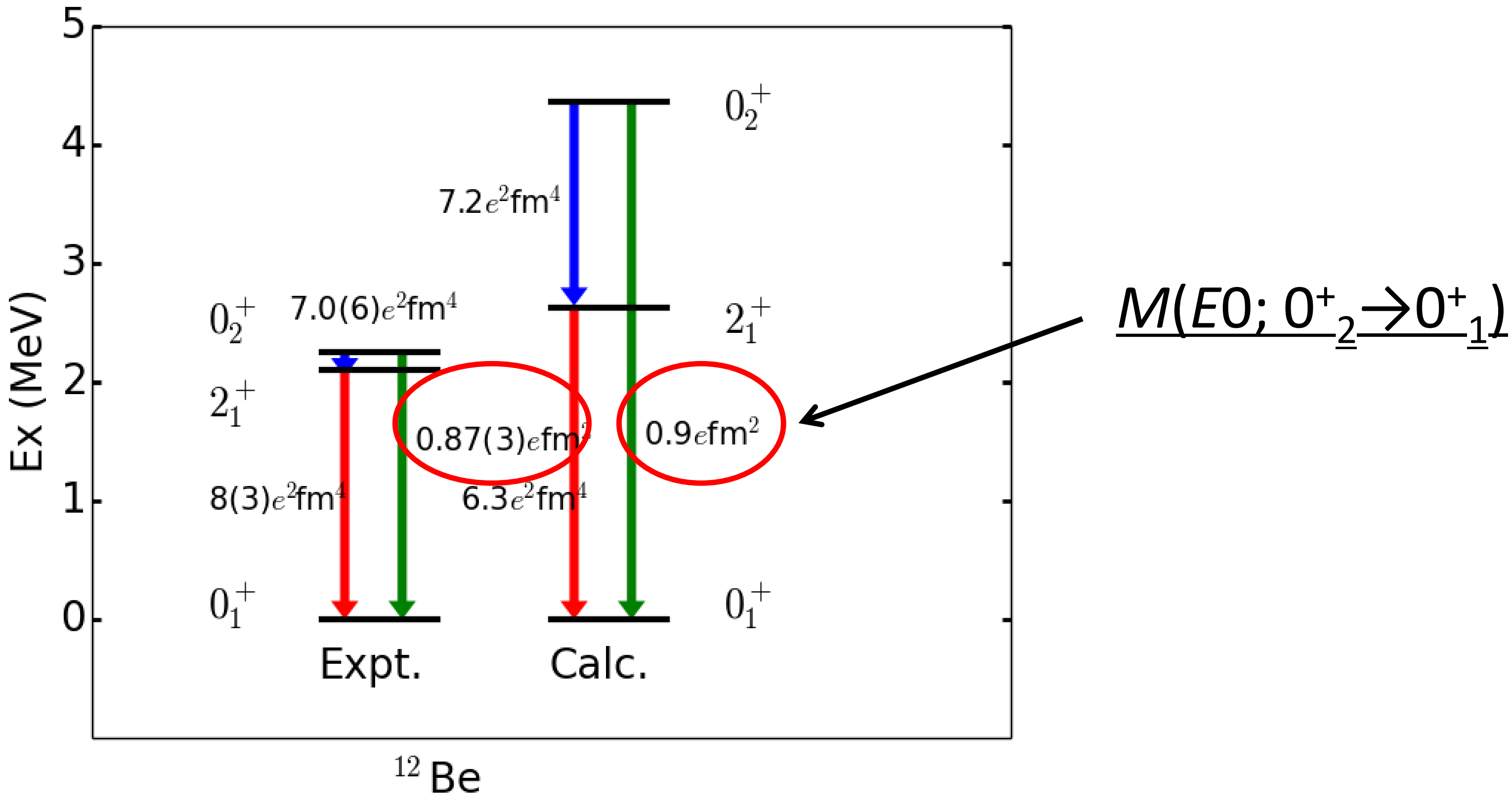



Rather good agreement w/ overall trend, except for $^{11}$Be neutron halo

MCSM < Expt., FMD < AMD, Cluster model

Expt., FMD: F. Ajzenberg-Selove, NPA 506, 1 (1990), A. Krieger et al., PRL 108, 142501 (2012)
AMD : Y. Kanada-En'yo, PRC91, 014315 (2015)
Cluster: M. Ito & K. Ikeda, Rep. Prog. Phys. 77, 096301 (2014)

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




Expt.:

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

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

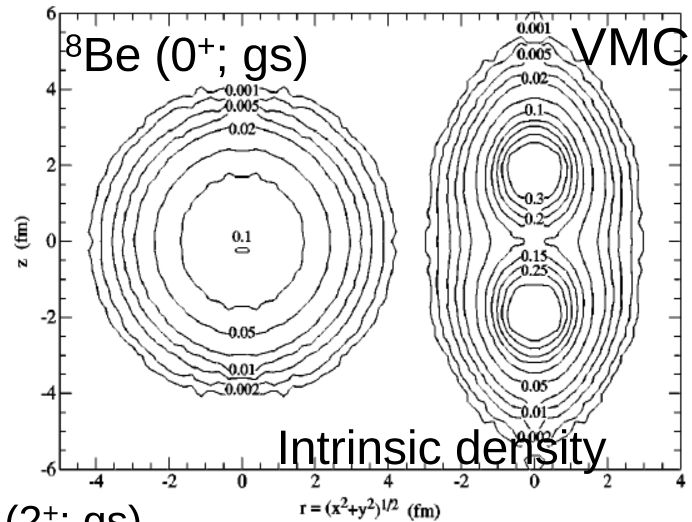
# Density distribution from ab initio calc.

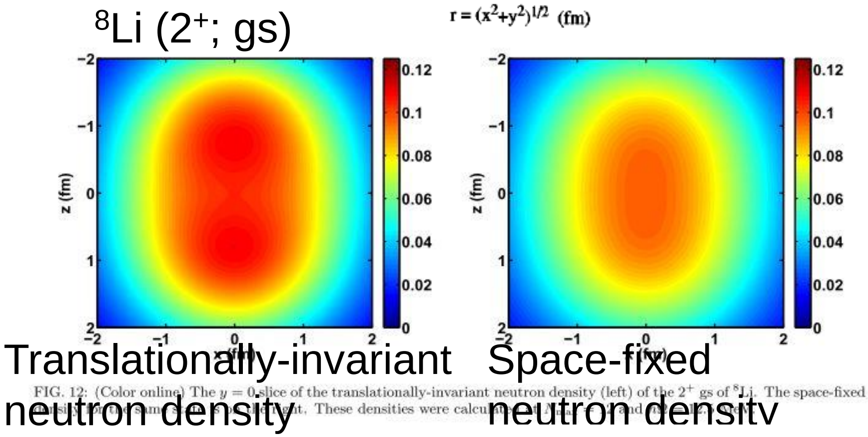
- Green's function Monte Carlo (GFMC)
  - "Intrinsic" density is constructed by aligning the moment of inertia among samples
  R. B. Wiringa, S. C. Pieper, J. Carlson, & V. R. Pandharipande, Phys. Rev. C62, 014001 (2000)

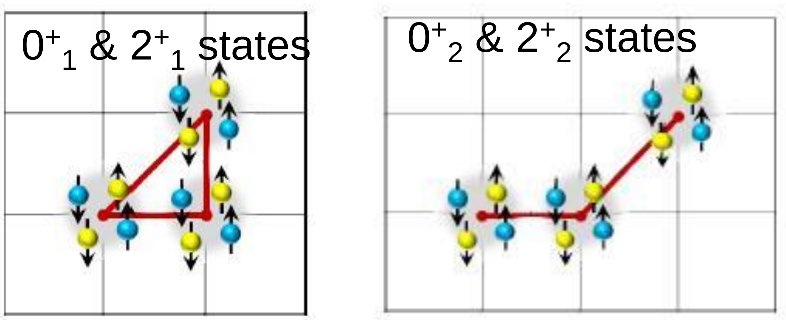
- No-core full configuration (NCFC)
  - Translationally-invariant density is obtained by deconvoluting the intrinsic & CM w.f.
  C. Cockrell J. P. Vary & P. Maris, Phys. Rev. C86, 034325 (2012)

- Lattice EFT
  - Triangle structure of carbon-12
  E. Epelbaum, H. Krebs, T. A. Lahde, D. Lee, & U.-G. Meissner, Phys. Rev. Lett. 109, 252501 (2012), …

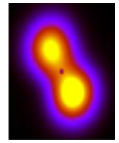
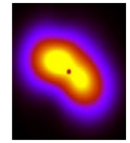
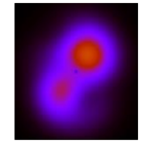
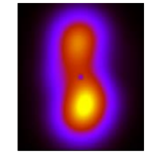
- FMD
  H. Feldmeier, Nucl. Phys. A515, 147 (1990), …



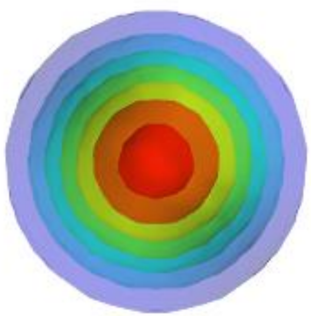
# Density distribution in MCSM

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

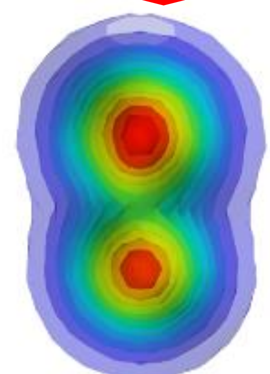
Angular-momentum projection

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

A way to construct
an "intrinsic" density



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



Laboratory frame

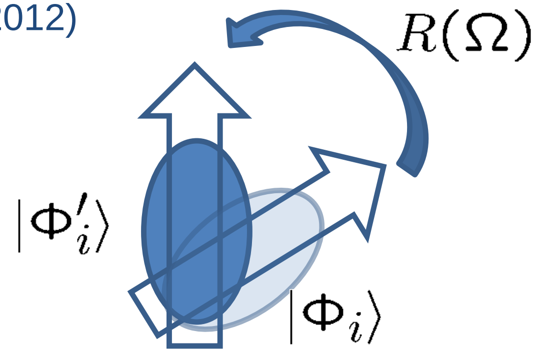
"Intrinsic" (body-fixed) frame

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.

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



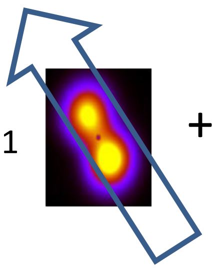

Rotation by diagonalizing Q-moment ($Q_{zz} > Q_{yy} > Q_{xx}$)

- MCSM wave function

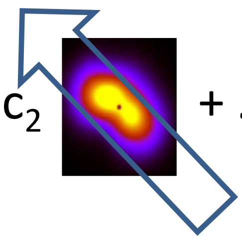
$$|\Psi\rangle = \sum_{i=1}^{N_{basis}} c_i P^J P^\pi |\Phi_i\rangle$$

- Wave function w/o the projections

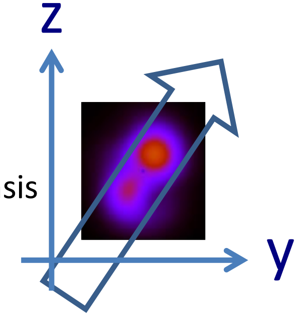
$$\sum_{i=1}^{N_{basis}} c_i |\Phi_i\rangle =$$ $c_1$



$+ c_2$

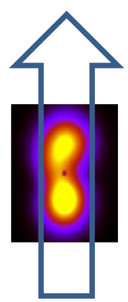


$+ \ldots + c_{Nbasis}$

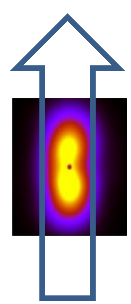



- Wave function w/o the projection w/ the alignment of Q-moment

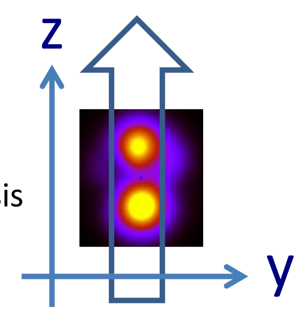
$$\sum_{i=1}^{N_{basis}} c_i |\Phi'_i\rangle =$$ $c_1$



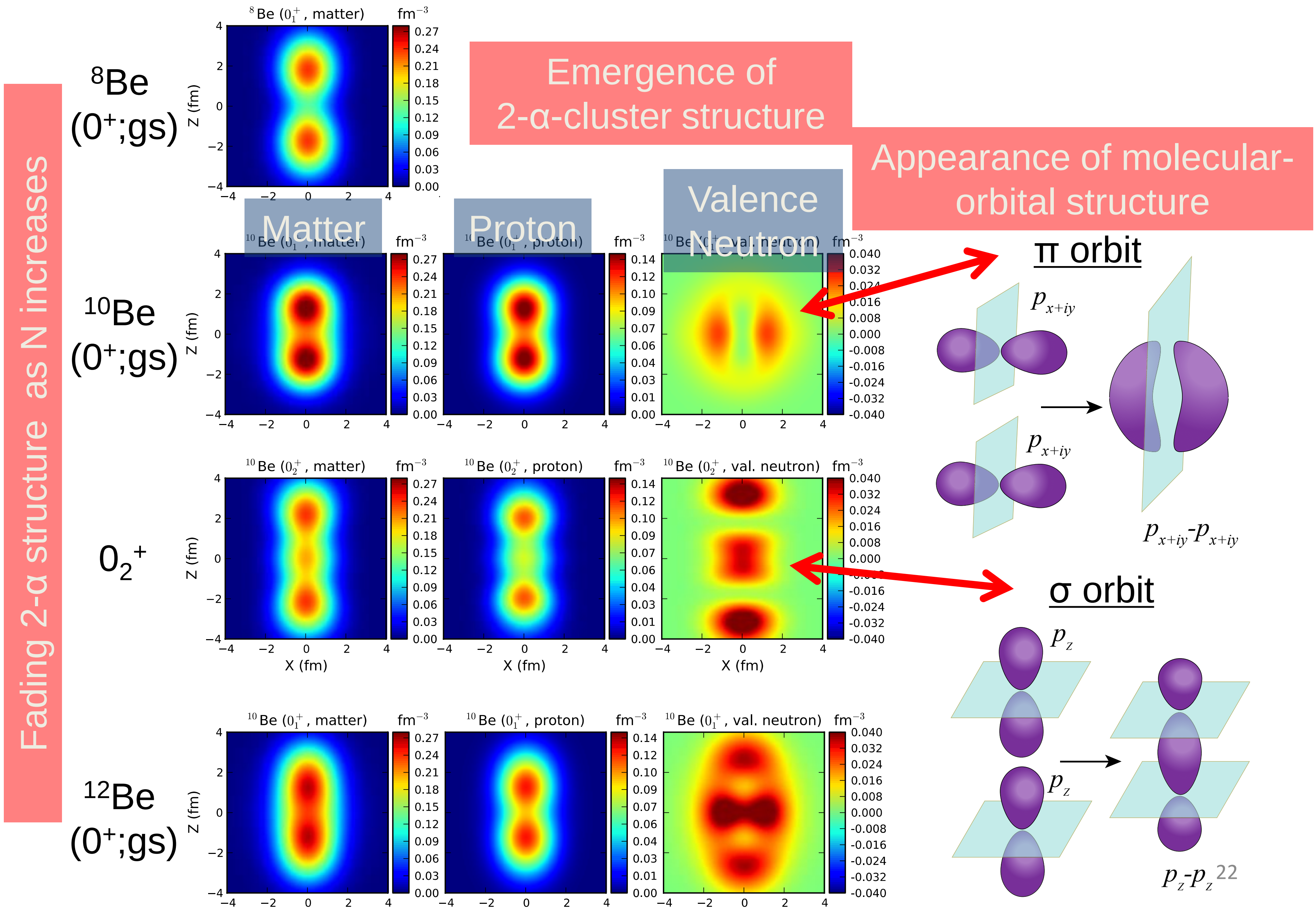
$+ c_2$



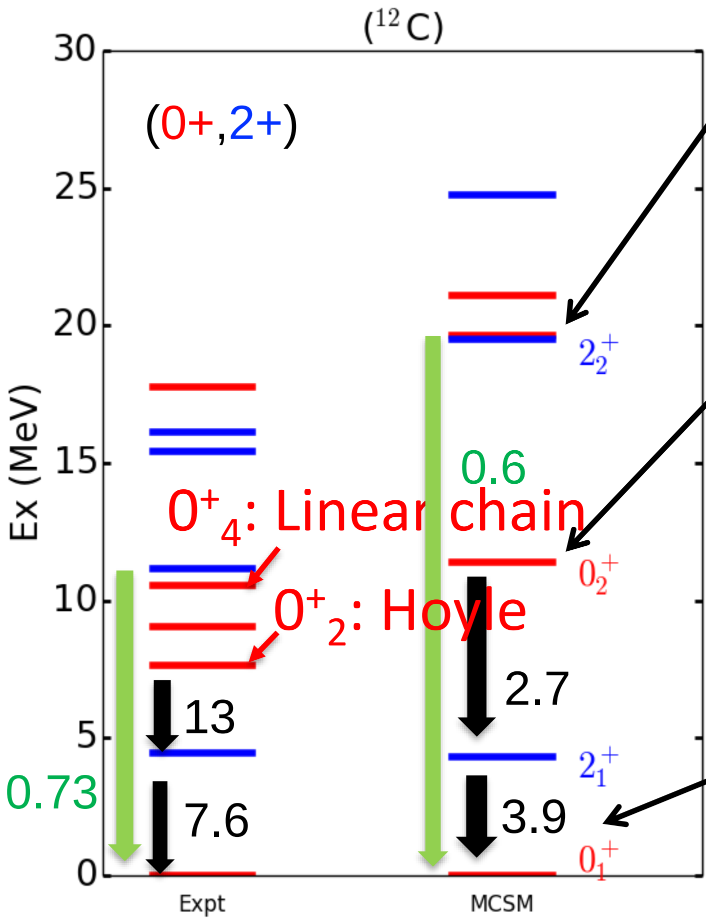
$+ \ldots + c_{Nbasis}$

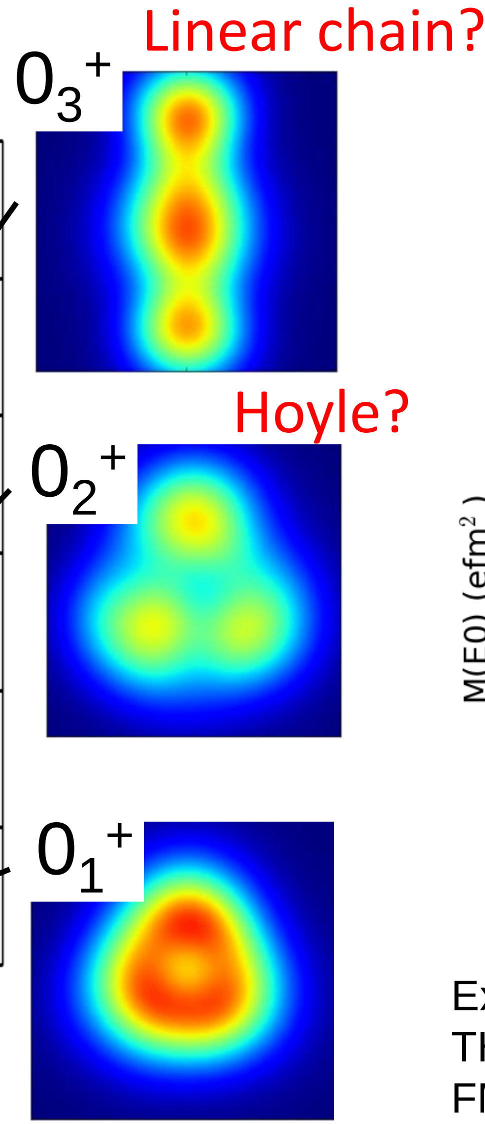


# Density distribution of Be isotopes

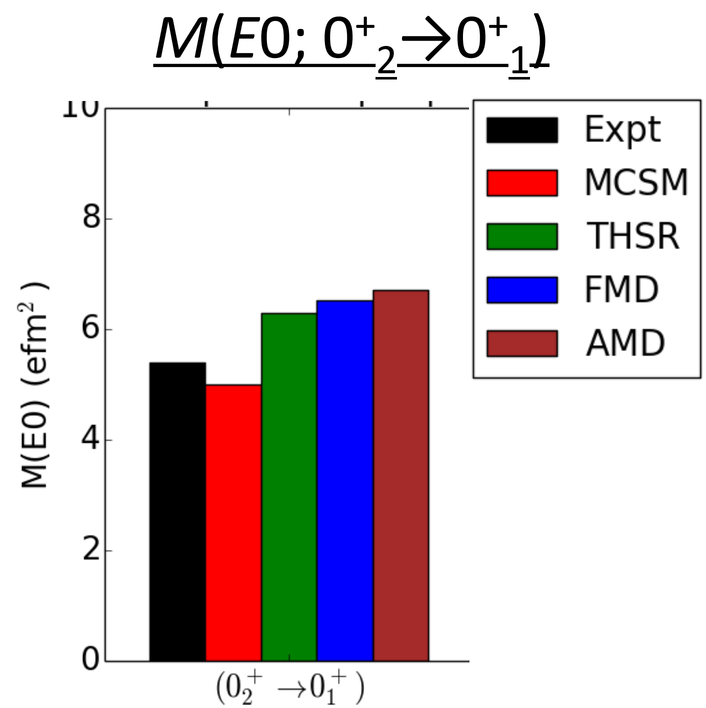


# Energy level & transition strength of $^{12}C$




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

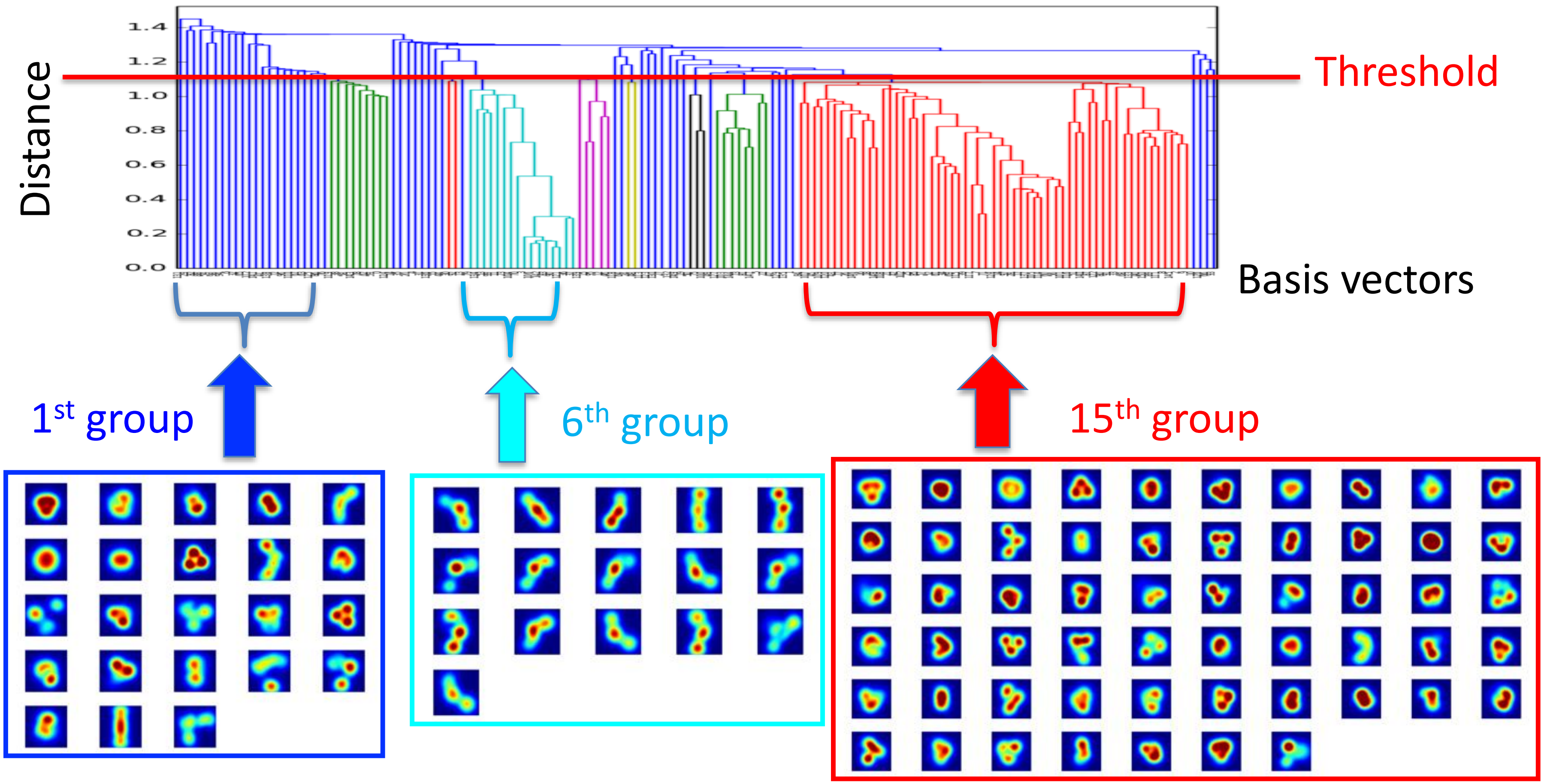



Expt.: P. Strehl 1970
THSR: Y. Funaki 2015
FMD: M. Chernykth 2007
AMD: Y. Kanada-En'yo 2007

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

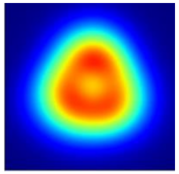
# Closer look at density distributions in $^{12}C$

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

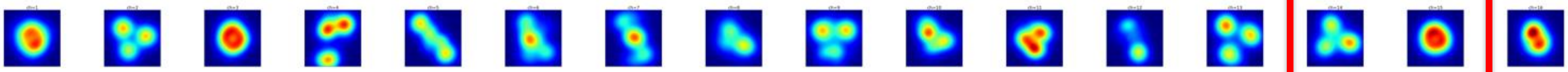


# Overlap probability in $^{12}C$

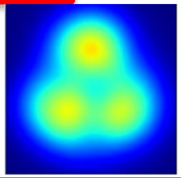
- Dendrogram in “Cluster analysis” of statistics
- Basis vectors are divided into 16 groups (in this case)



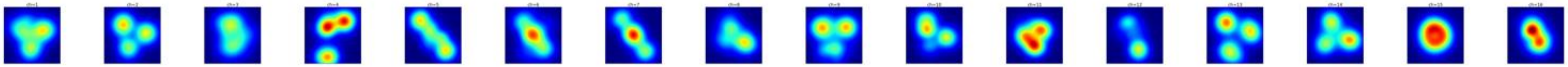
- $\underline{0^+_1}$ : Concentrated in 14th (3 clusters) & 15th (compact shape) groups



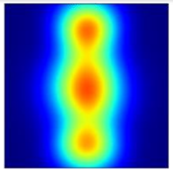
| #1 | #2 | #3 | #4 | #5 | #6 | #7 | #8 | #9 | #10 | #11 | #12 | #13 | #14 | #15 | #16 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.20 | 0.0 | 0.11 | 0.00 | 0.00 | 0.00 | 0.00 | 0.03 | 0.07 | 0.34 | 0.29 | 0.04 | 0.11 | 0.87 | 0.98 | 0.32 |



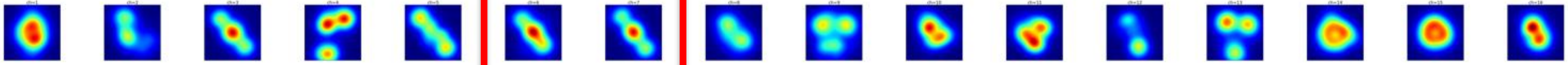
- $\underline{0^+_2}$ : Scattered among all groups → Gas-like state?



| #1 | #2 | #3 | #4 | #5 | #6 | #7 | #8 | #9 | #10 | #11 | #12 | #13 | #14 | #15 | #16 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.11 | 0.02 | 0.18 | 0.20 | 0.02 | 0.14 | 0.07 | 0.08 | 0.14 | 0.37 | 0.16 | 0.14 | 0.48 | 0.22 | 0.66 | 0.03 |



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



| #1 | #2 | #3 | #4 | #5 | #6 | #7 | #8 | #9 | #10 | #11 | #12 | #13 | #14 | #15 | #16 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.12 | 0.02 | 0.17 | 0.26 | 0.13 | 0.54 | 0.38 | 0.00 | 0.10 | 0.19 | 0.13 | 0.00 | 0.08 | 0.01 | 0.33 | 0.06 |

# 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.
  - Daejoen16 NN interaction gives better agreement w. experimental data than those by JISP16 (preliminary, need energy-variance extrapolation).
- Cluster structure of Be & C isotopes can be visualized using MCSM wave functions.

# Future perspective

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