TRIUMF Theory Workshop (Feb. 26 – Mar. 1, 2019)
Progress in Ab Initio Techniques in Nuclear Physics

Alpha-cluster structure from no-core Monte Carlo shell model

Takashi Abe (U of Tokyo)

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, 2019

“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, IM-SRG,

  Self-consistent Green’s Function theory, Lattice EFT, UMOA, …

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

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

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

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

→ Computationally demanding → Monte Carlo shell model (MCSM)

Monte Carlo shell model (MCSM)

Standard shell model

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

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

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

Diagonalization

Important bases stochastically selected ~ O(100)

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

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

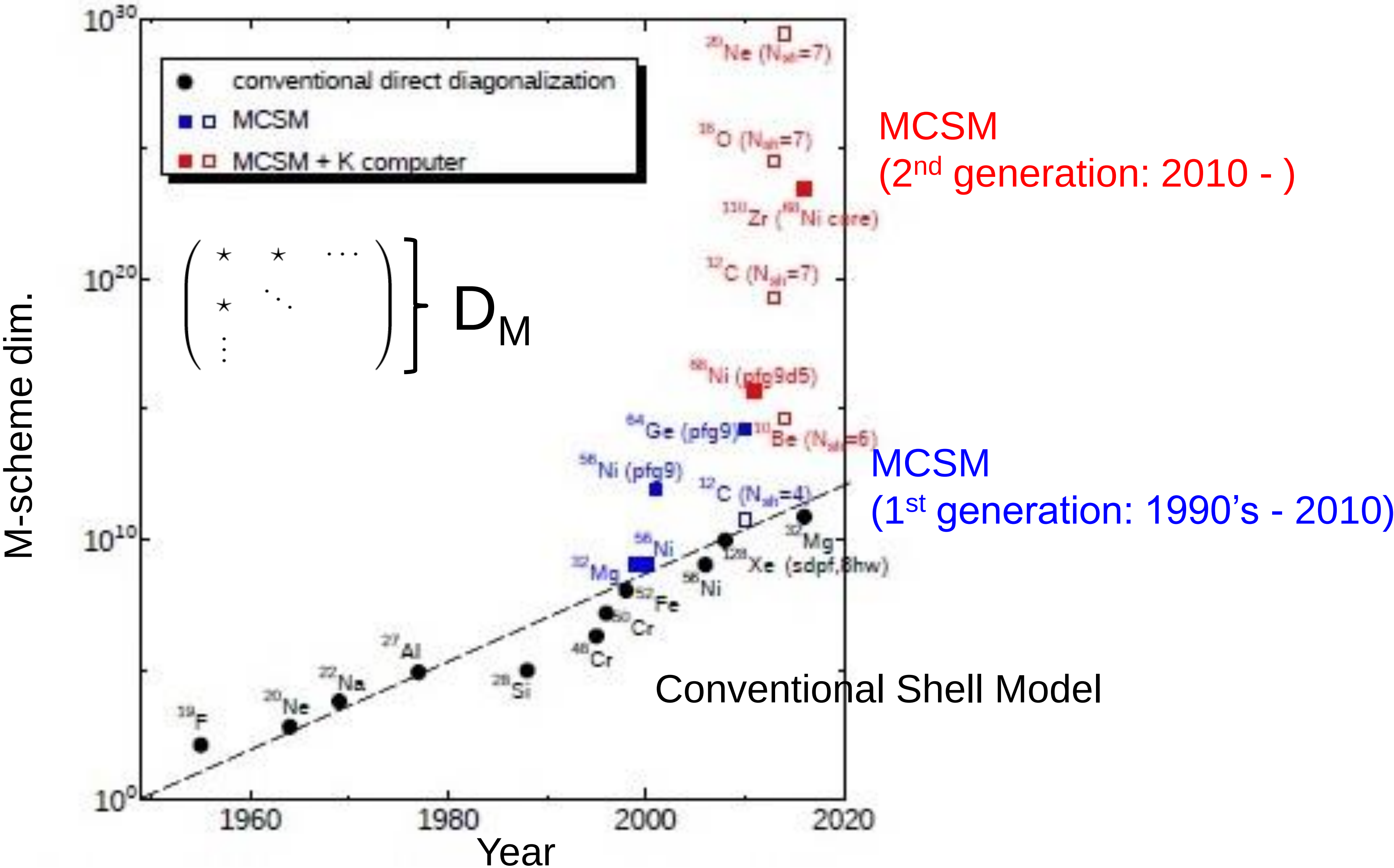
diagonalization

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



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

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

- Two steps of the extrapolation

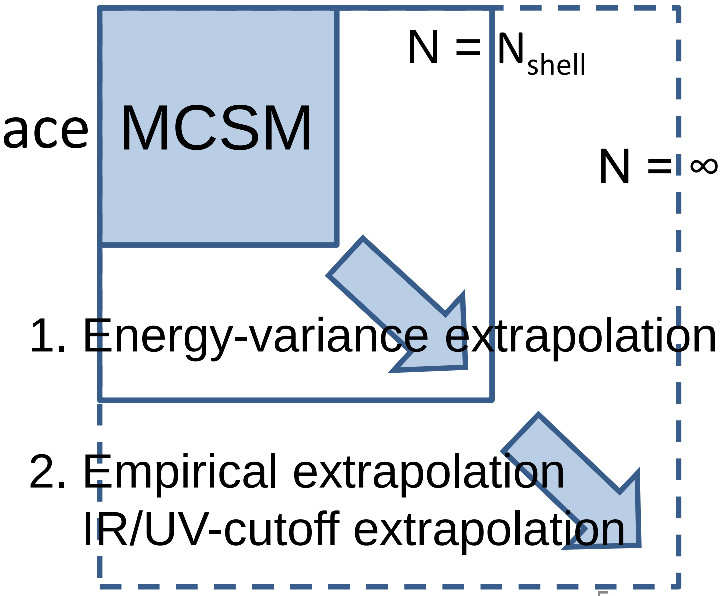
Same as in the MCSM w/ an inert core

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)

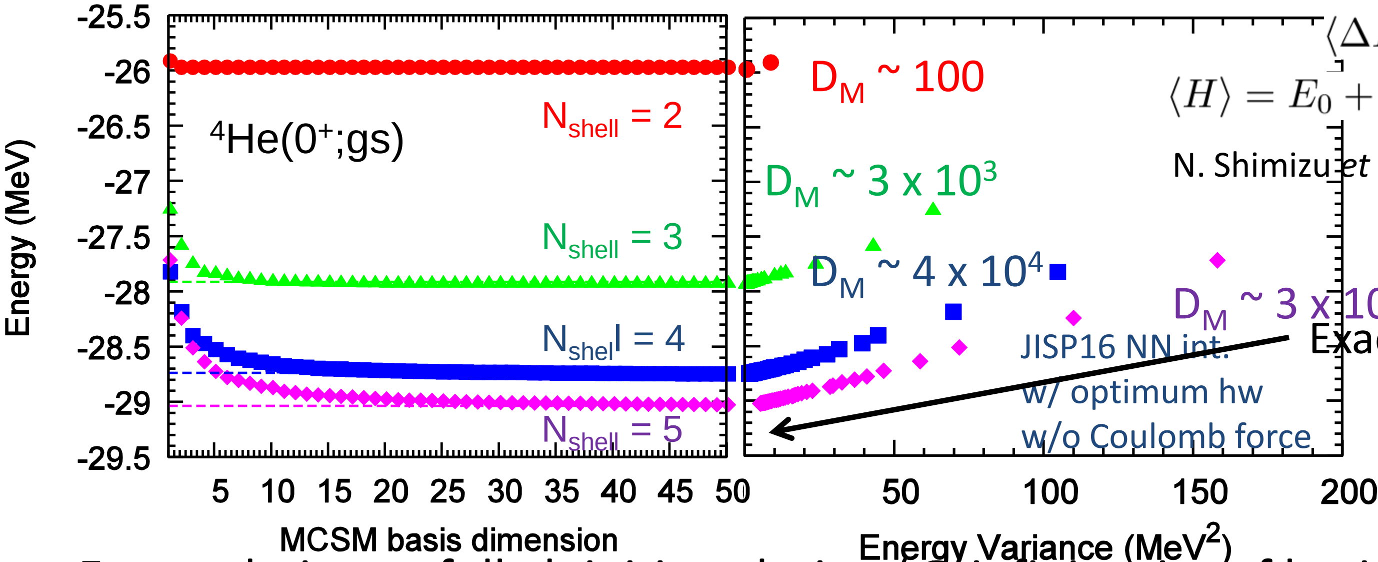
2. Extrapolation into the infinite model space
   - Empirical extrapolation w.r.t. N_{shell}
   - IR- & UV-cutoff extrapolations



→ Ab initio solution

Extrapolations

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



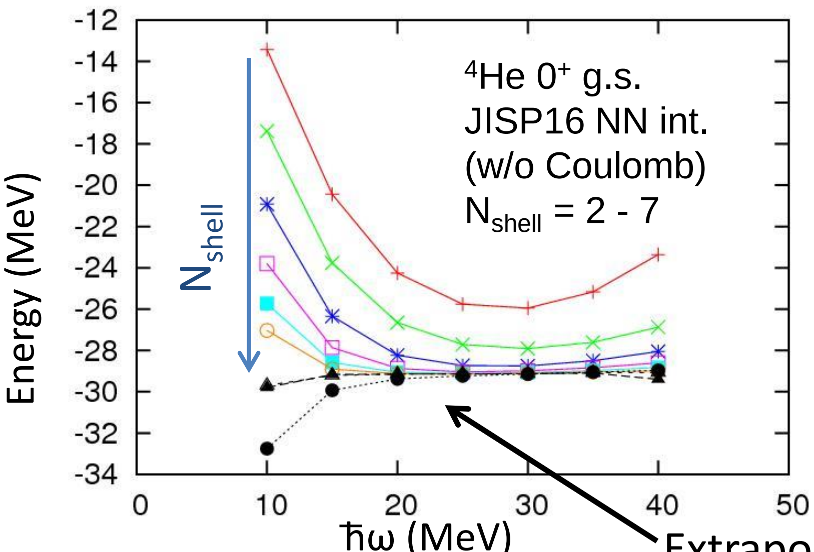
$$\langle \Delta H^2 \rangle = \langle H^2 \rangle - \langle H \rangle^2$$

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

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

Exact solution @ fixed N_{shell}

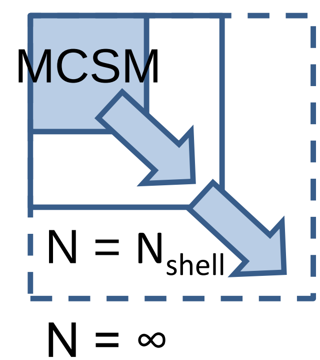
- Extrapolation to full ab initio solution (@ infinite size of basis space)



Extrapolations

(N_{shell}, ħω)

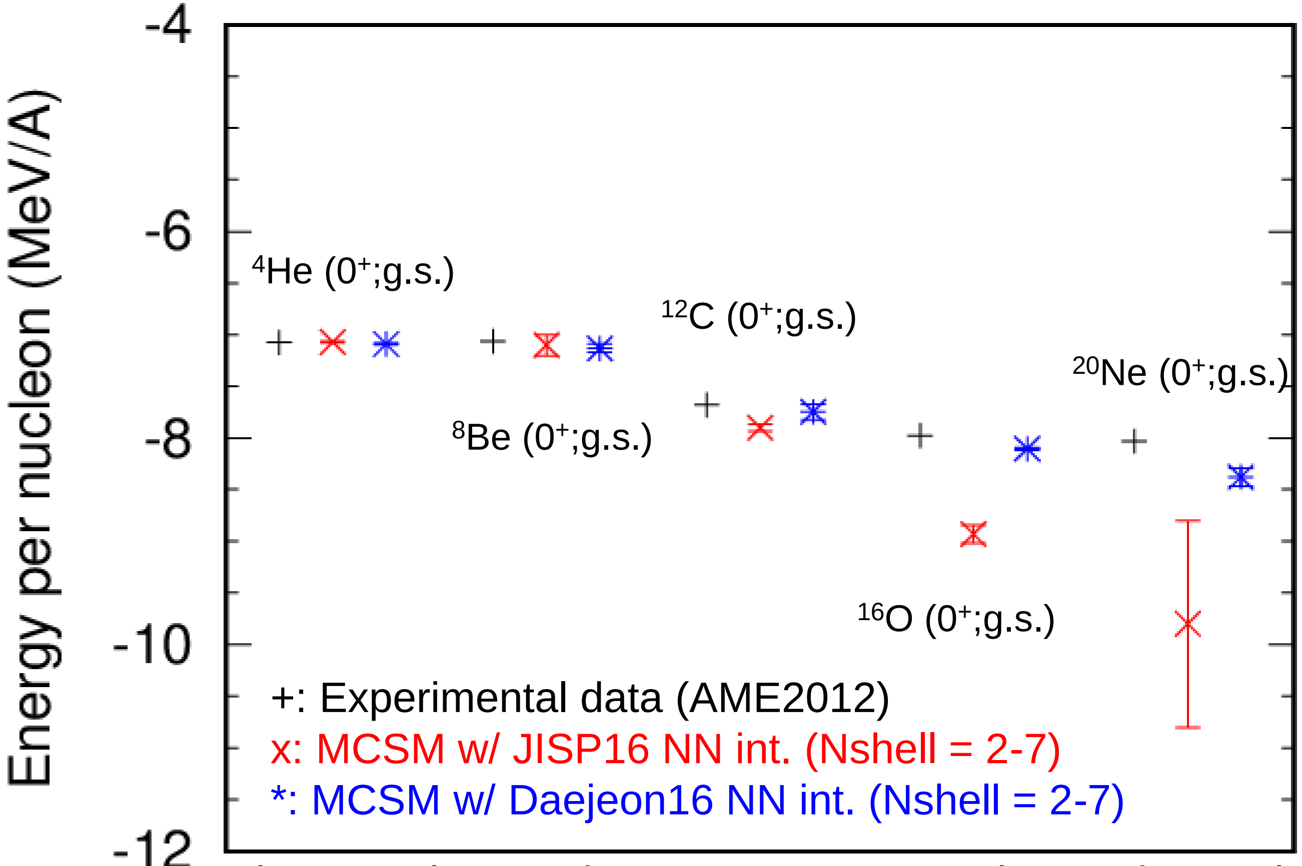
$$E(N) = E(N = \infty) + a \exp(-bN)$$



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



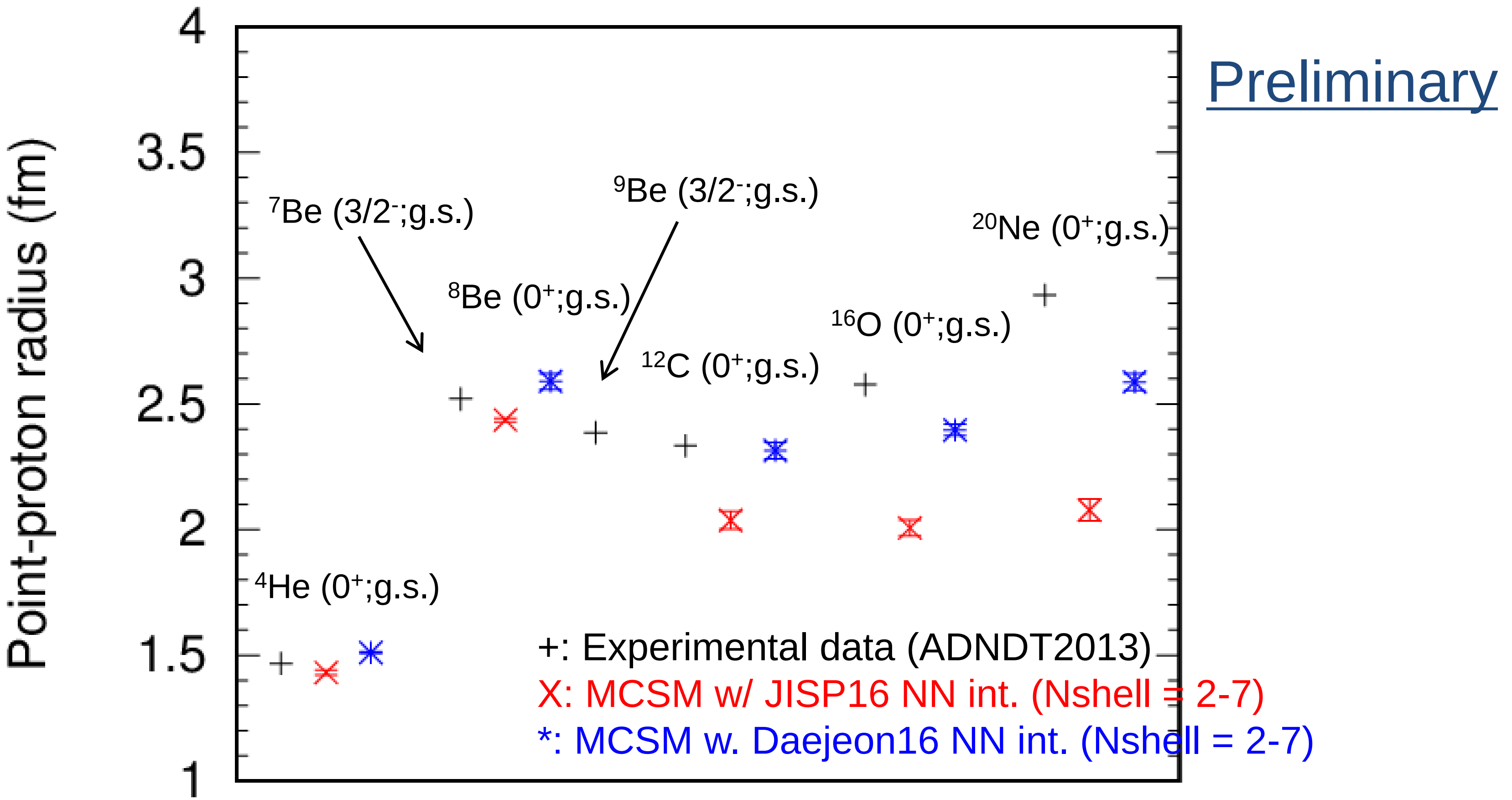
Preliminary

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.

Comparison of MCSM results w/ experiments



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

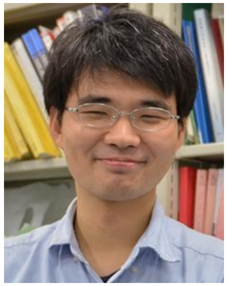
JISP16 results show good agreements w/ experimental data up to ^{8}Be, clearly smaller for heavier nuclei beyond ^{12}C as A increases.

Daejeon16 results show larger radii than JISP16 ones.

G.S. energies & excitation spectra of Be isotopes

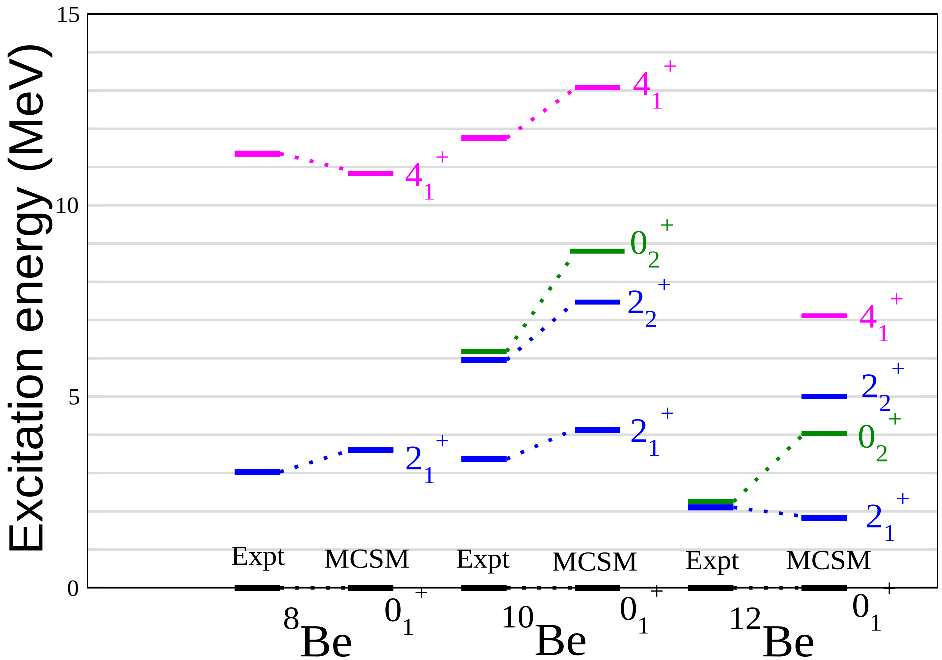
- Ground-state energies

	MCSM (MeV)	Expt (MeV)
^{8}Be (0^+)	-49.95	-56.499
^{10}Be (0^+)	-53.4	-64.98
^{12}Be (0^+)	-49.93	-68.65



T. Yoshida (RIST)

- Excitation energies



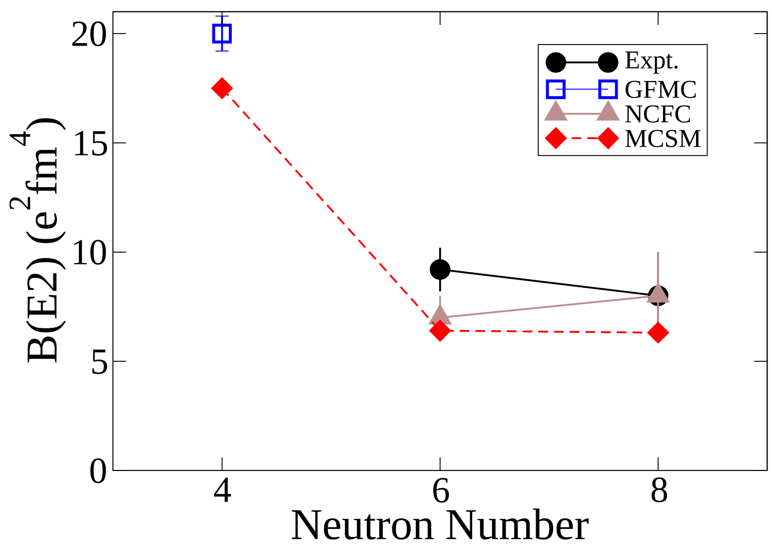
JISP16 NN
N_{shell} = 6, hw = 15 MeV

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 & E0 transition strengths of Be isotopes

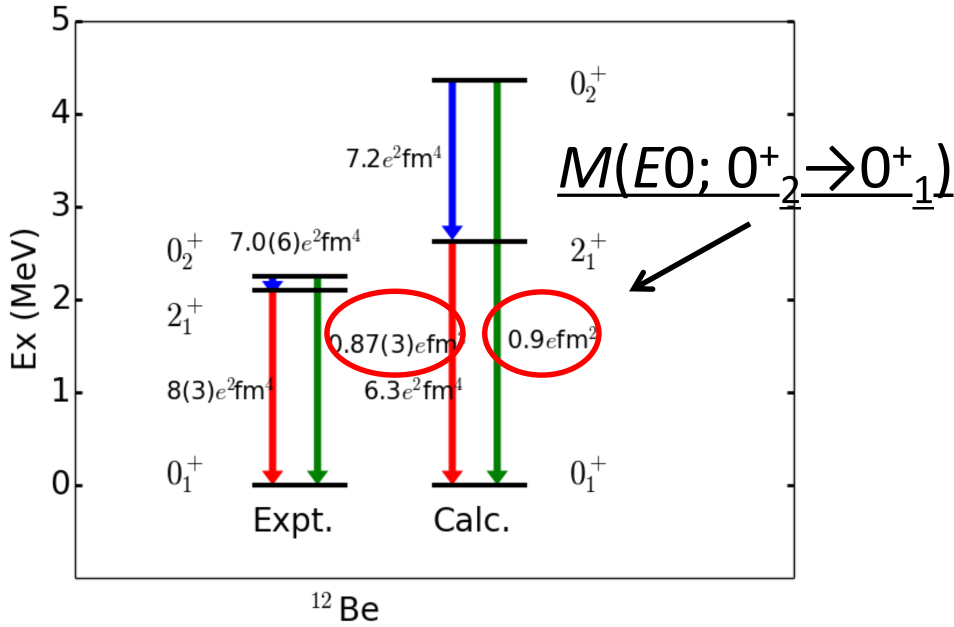
- E2 transition strengths

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



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

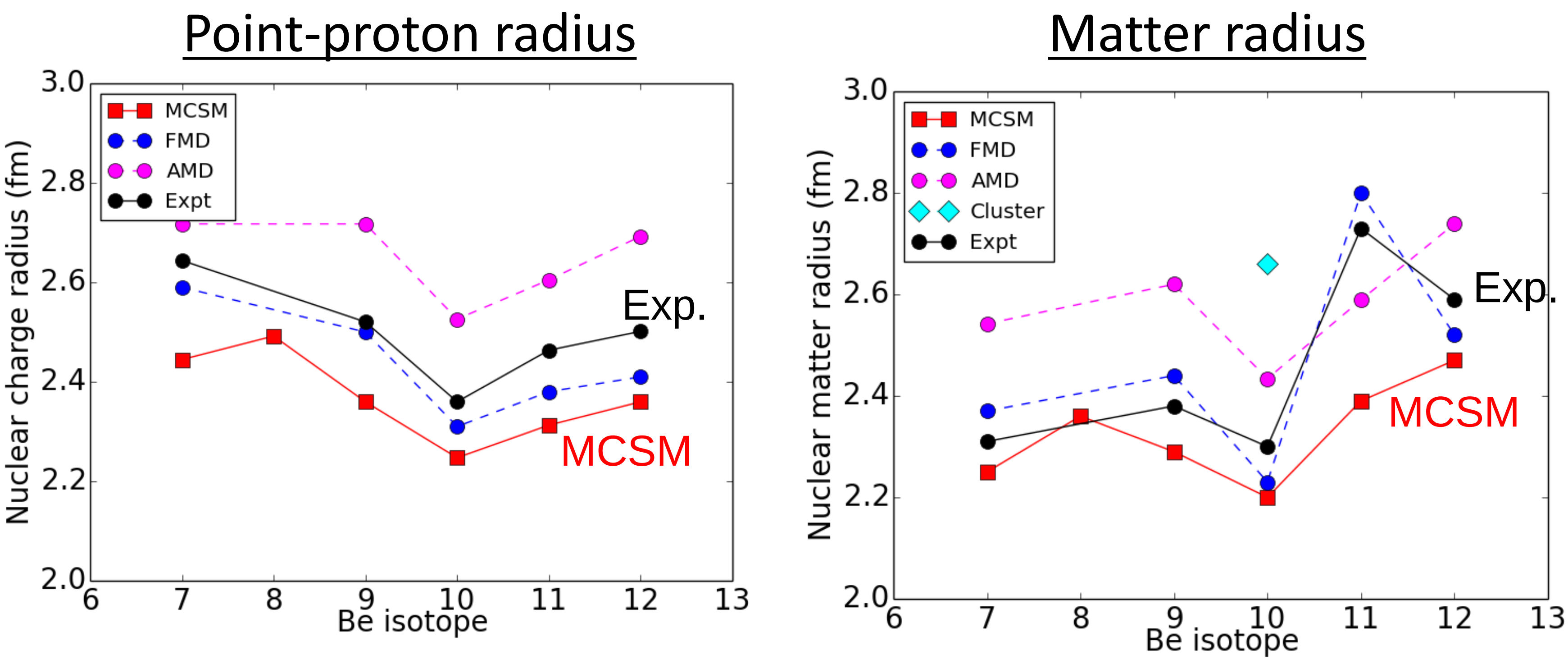
- E2 & E0 transition strengths in 12Be



Expt.:
S. Shimoura, et al., Phys. Lett. B 654 87 (2007)
N. Imai, et al., Phys. Lett. B 673 179 (2009)

MCSM: JISP16 NN, N_{shell} = 6, hw = 15 MeV

Radii of Be isotopes



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)

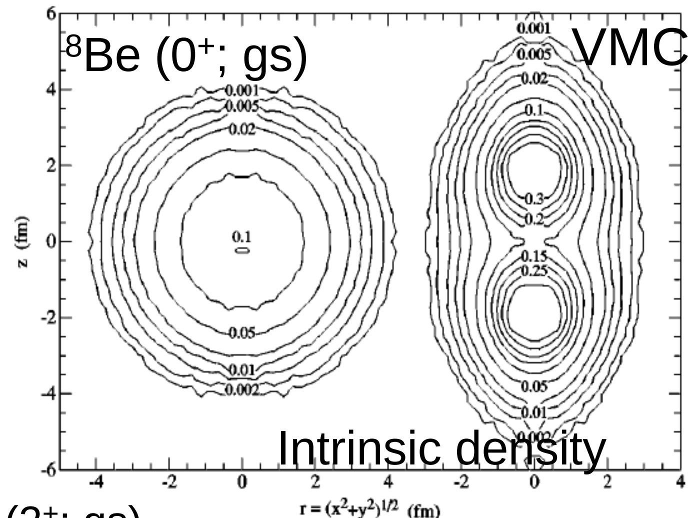
Density distribution from ab initio calc.

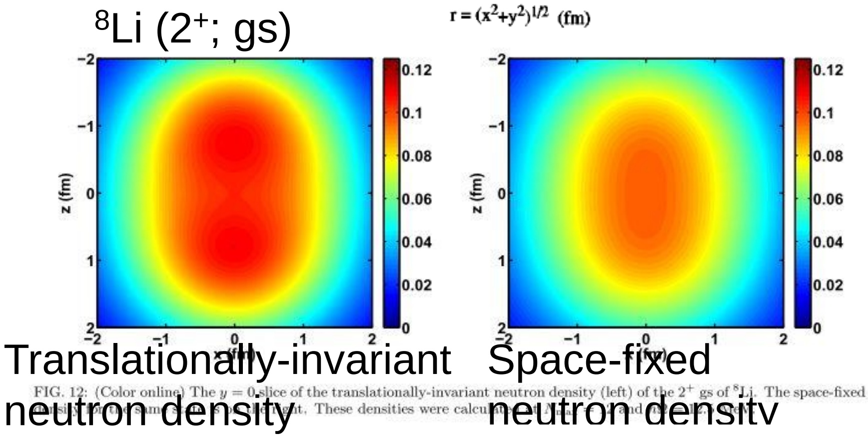
- Green's function Monte Carlo (GFMC)
  - "Intrinsic" density is constructed by aligning the moment of inertia among samples
  - R. B. Wiringa, S. C. Pieper, J. Carlson, & V. R. Pandharipande, Phys. Rev. C62, 014001 (2000)

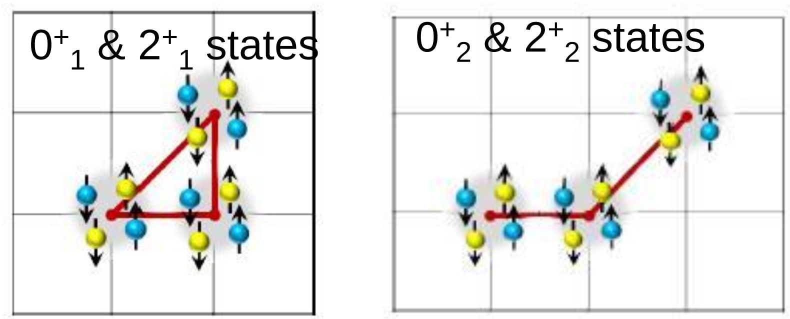
- No-core full configuration (NCFC)
  - Translationally-invariant density is obtained by deconvoluting the intrinsic & CM w.f.
  - C. Cockrell J. P. Vary & P. Maris, Phys. Rev. C86, 034325 (2012)

- 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), …

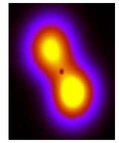
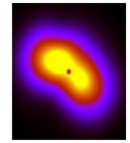
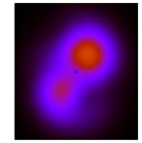
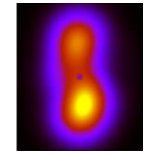
- FMD
  - H. Feldmeier, Nucl. Phys. A515, 147 (1990), …







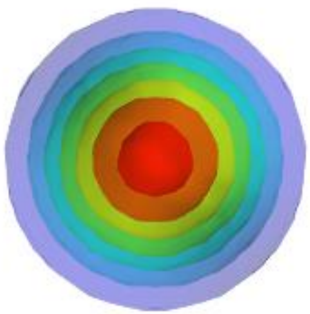
Density distribution in MCSM

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

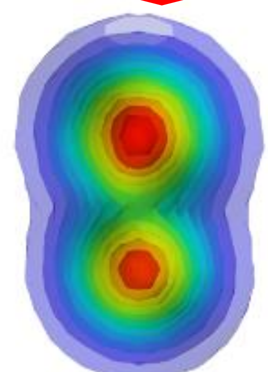
Angular-momentum projection

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

A way to construct an "intrinsic" density



^{8}Be 0^+ ground state



Laboratory frame

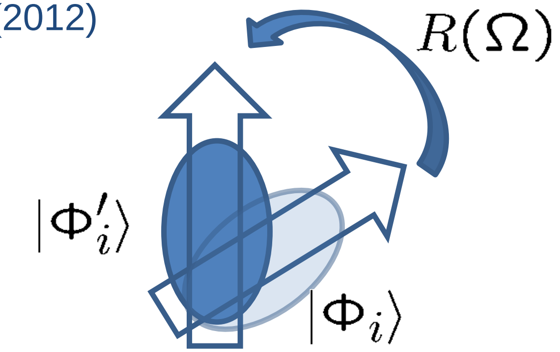
"Intrinsic" (body-fixed) frame

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)



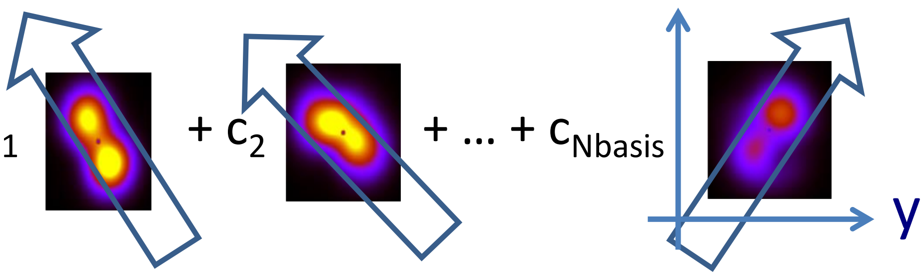
Rotation by diagonalizing Q-moment
($Q_{zz} > Q_{yy} > Q_{xx}$)

- MCSM wave function

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

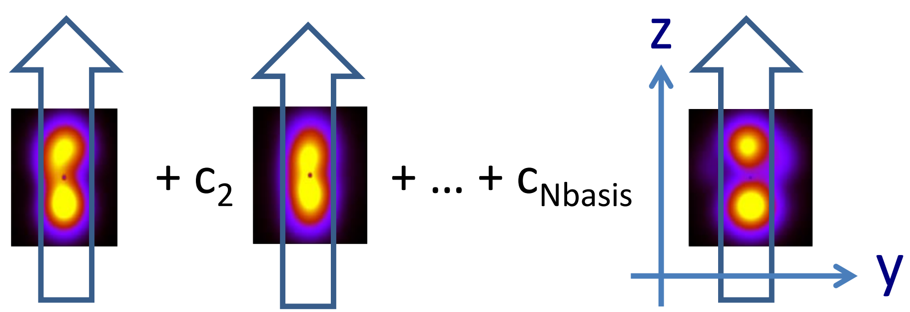
- Wave function w/o the projections

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

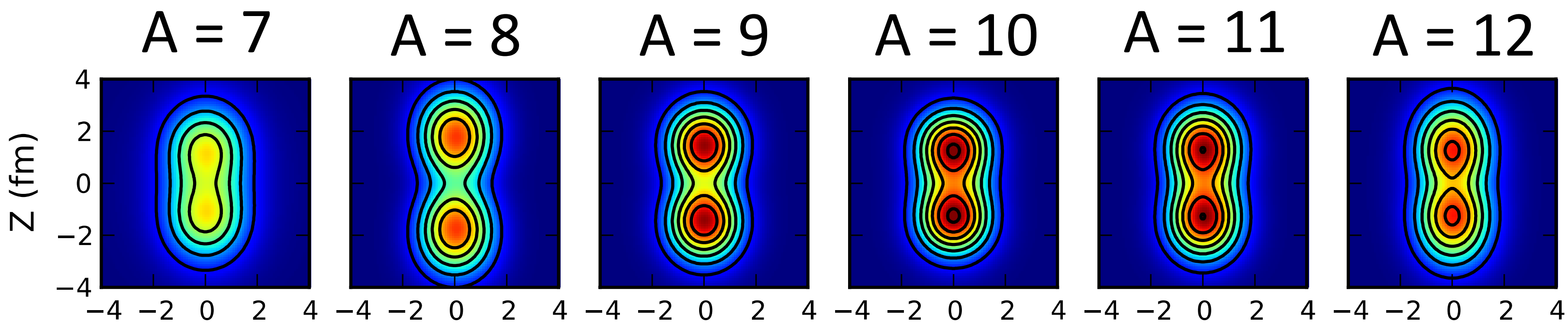


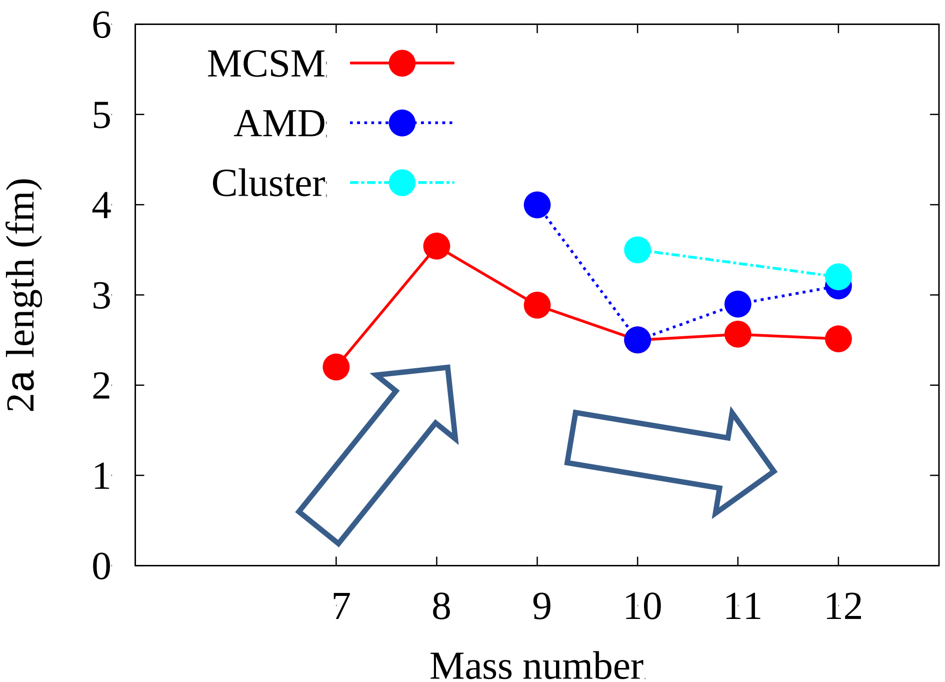
- Wave function w/o the projection w/ the alignment of Q-moment

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

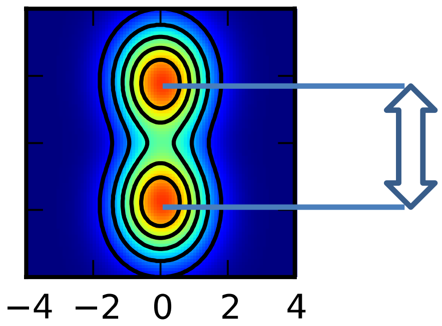


inter α-cluster distance



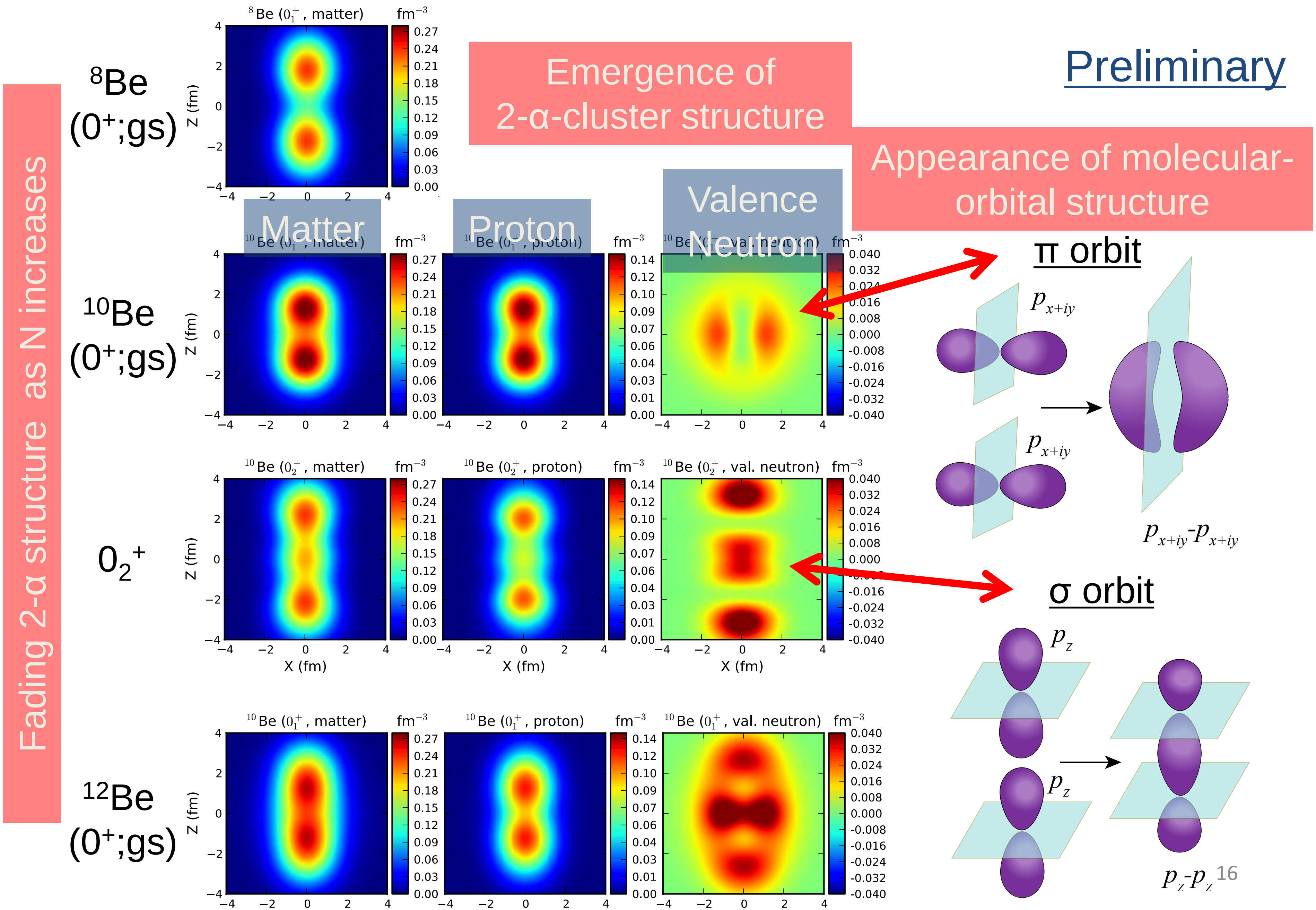


Definition:
Distance btw the positions of each highest proton density



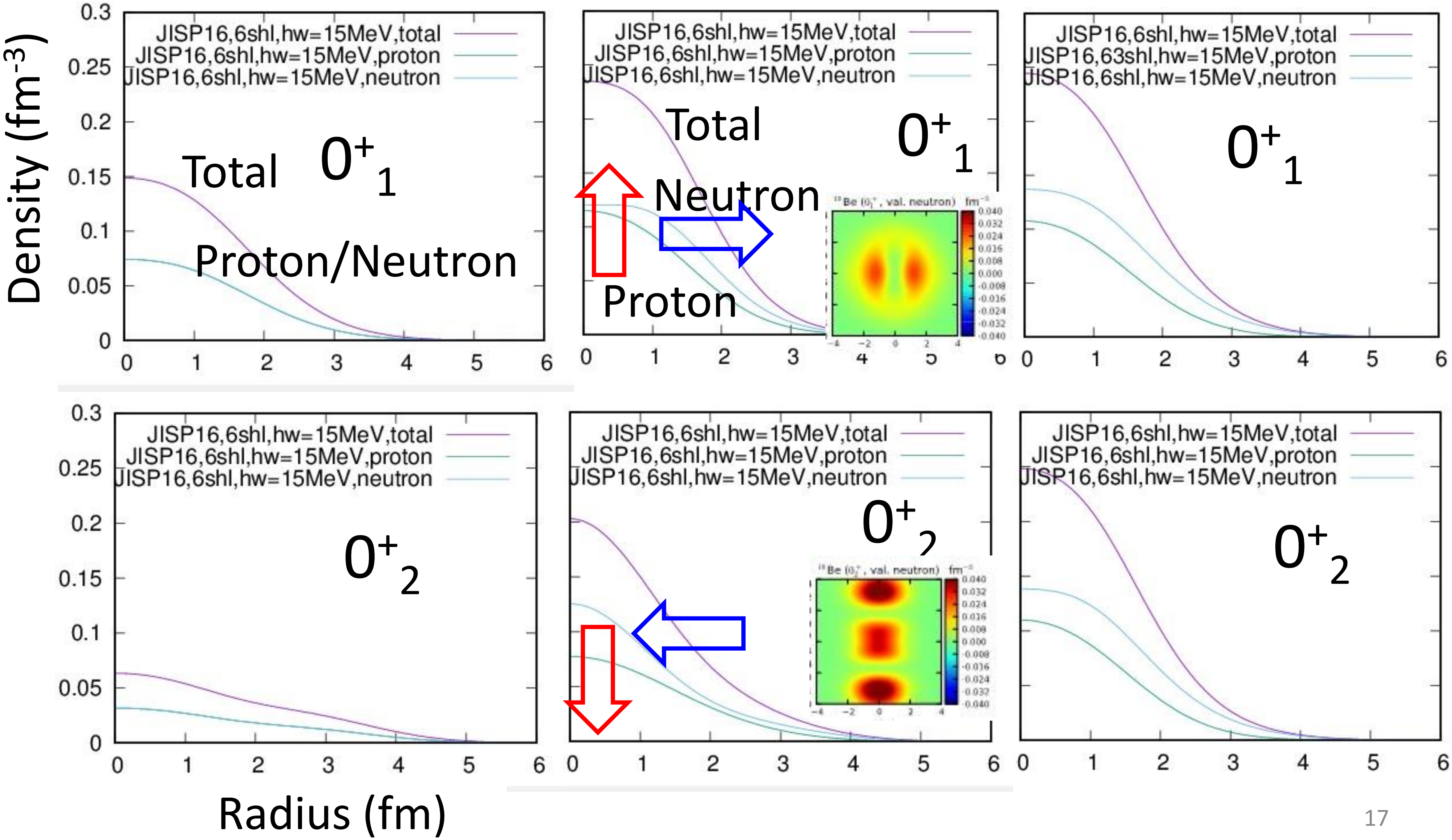
AMD: Y. Kanada-En'yo, Phys. Rev C68, 014319 (2003)
Cluster: M. Ito & K. Ikeda, Rep. Prog. Phys. 77, 096301 (2014)

Density distribution of Be isotopes

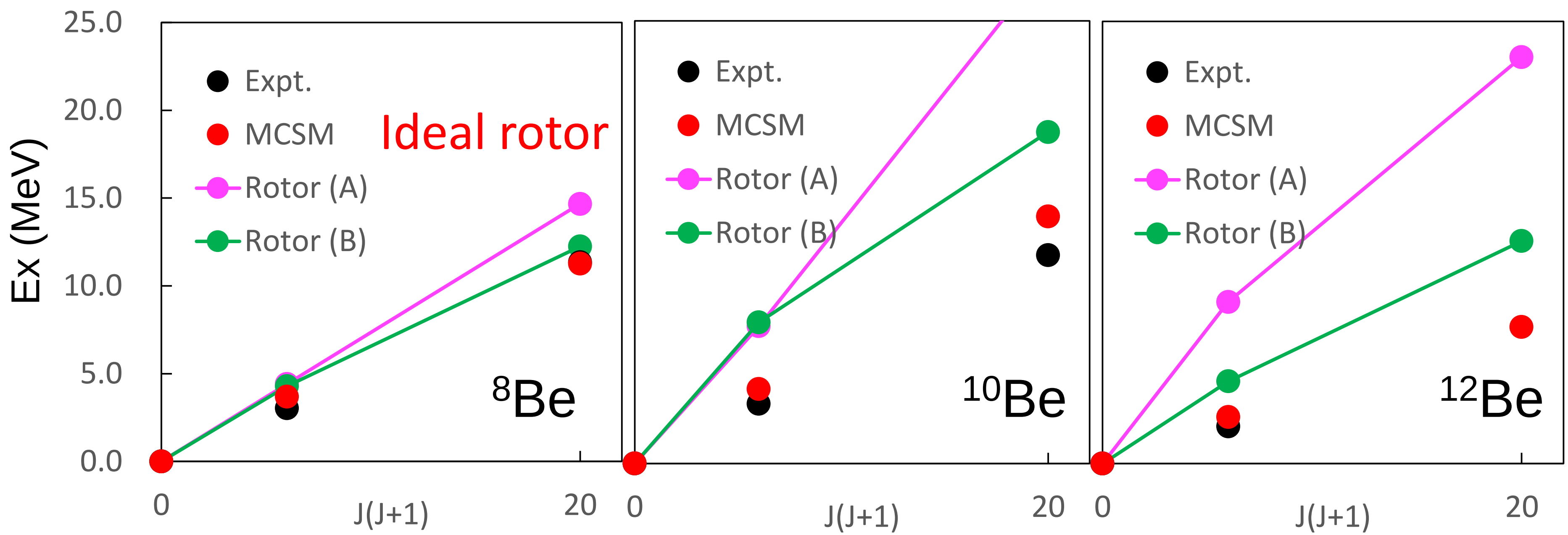


Radial distributions of Be isotopes

^{8}Be ^{10}Be ^{12}Be



Rotational bands of Be isotopes



Projection from MCSM basis vectors for J=0 state

Projection from MCSM basis vectors for J=0 state with amplitudes re-optimized for each J

MCSM basis vector

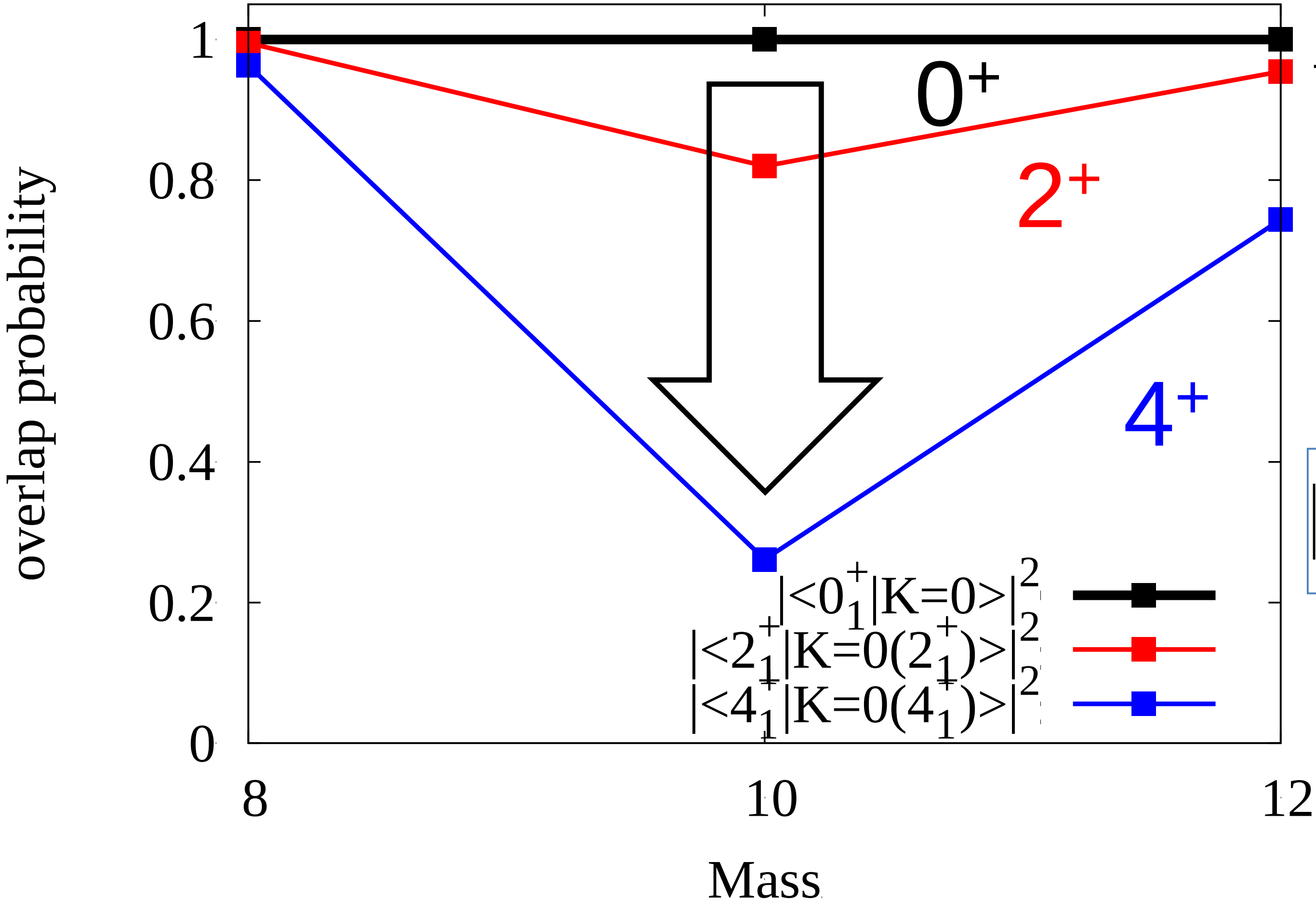
$$|\Psi(J,M,\pi)\rangle = \sum_{i}^{N_{basis}} f_i |\Phi_i(J,M,\pi)\rangle$$

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

K = 0 components

$$\left|P_{K=0}\Psi\right\rangle = \sum_{n=1}^{Nb} P^J_{K=0} c_n \left|\phi_n\right\rangle$$

Large K-mixing in 10Be



Overlap probablitiy

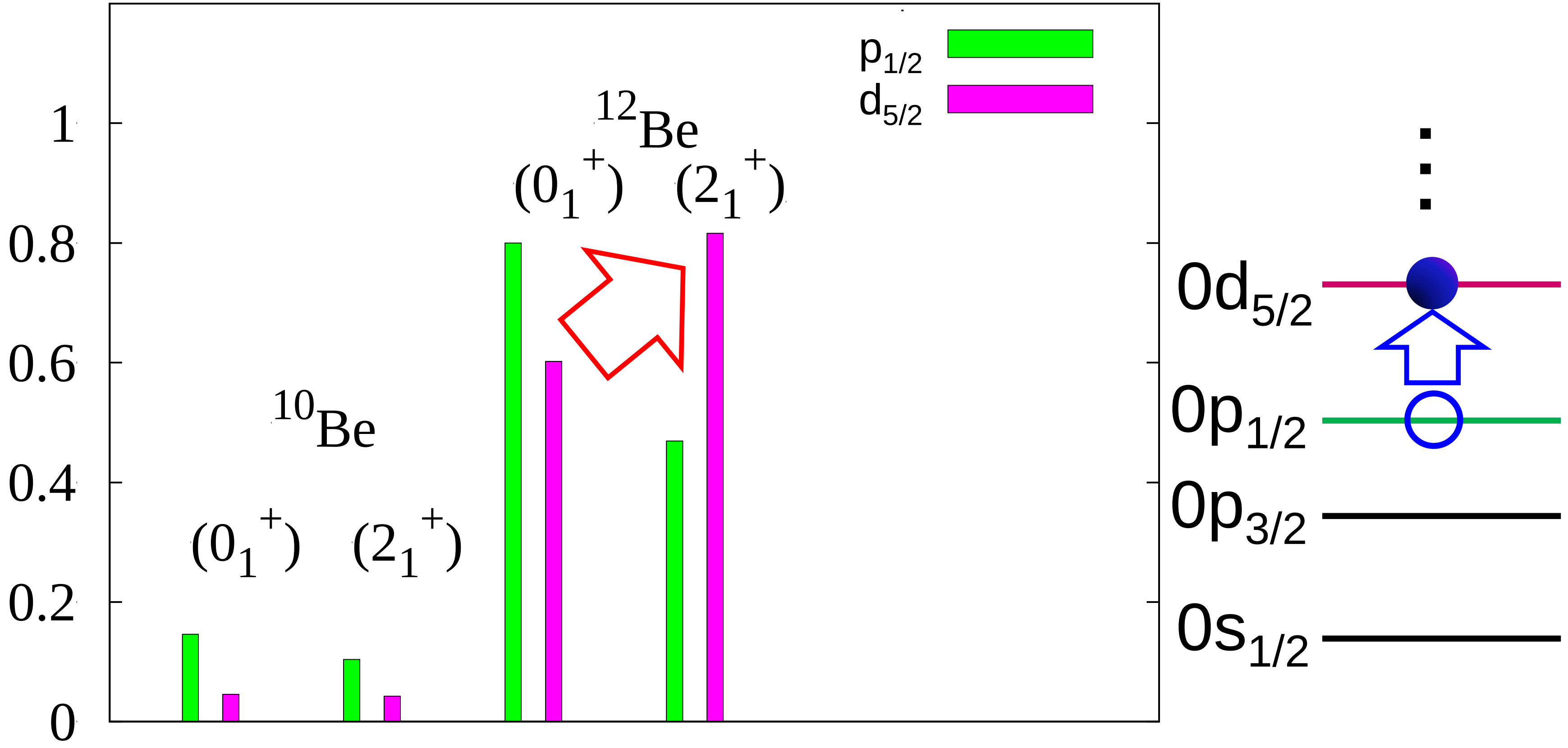
$$\left|\left\langle P^J_{MK}\Psi \middle| P_{K=0}\Psi\right\rangle\right|^2$$

K = 0 components

$$\left|P_{K=0}\Psi\right\rangle = \sum_{n=1}^{Nb} P^J_{K=0} c_n \left|\phi_n\right\rangle$$

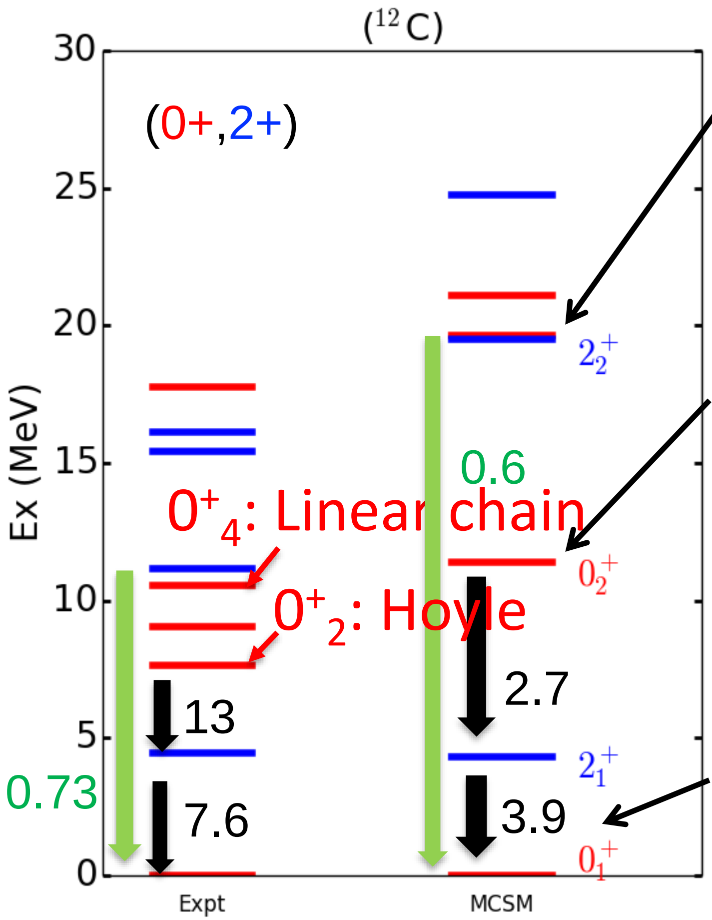
Occupation numbers of valence neutrons

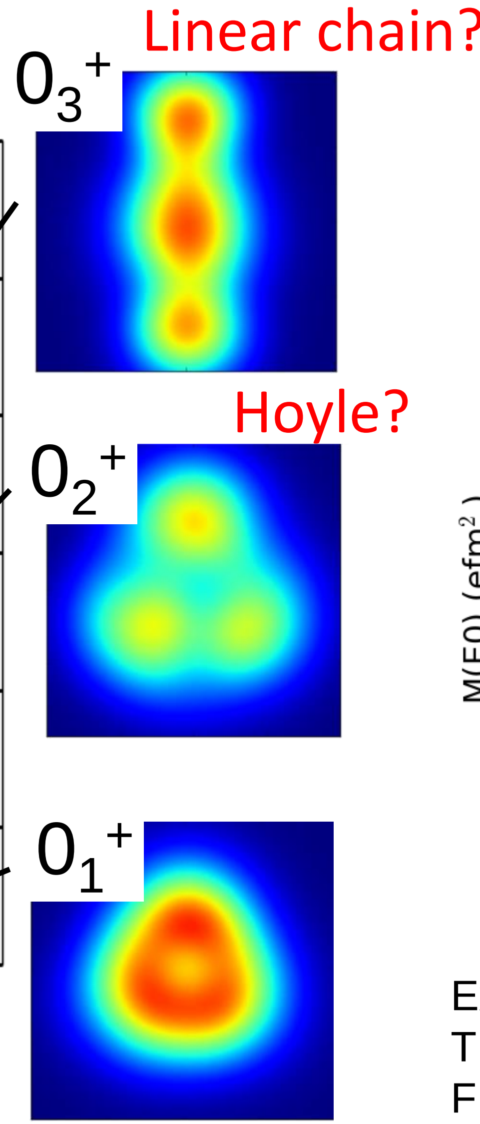
valence neutron $p_{1/2}$ and $d_{5/2}$ occupation number



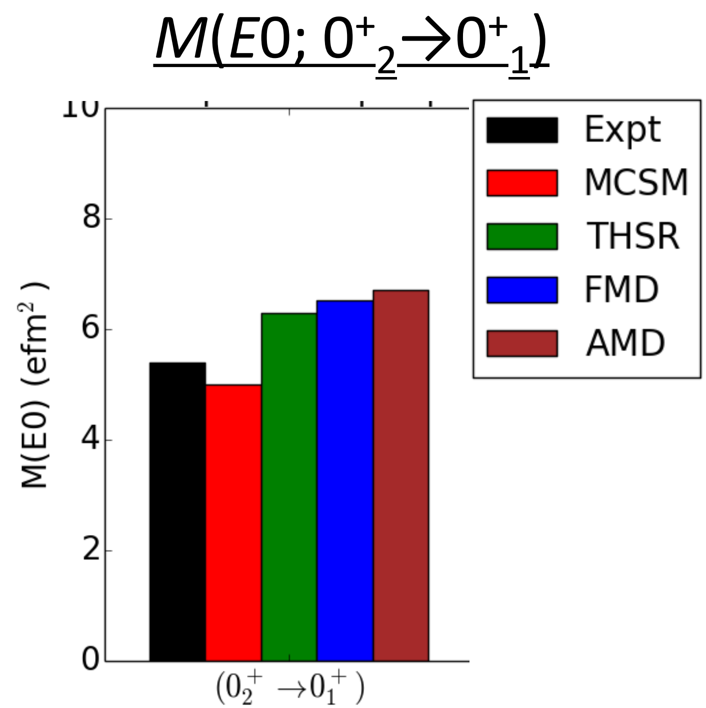
Excitation of valence neutrons from $0p_{1/2}$ to $0d_{5/2}$ orbital in 12Be

Energy level & transition strength of ^{12}C





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

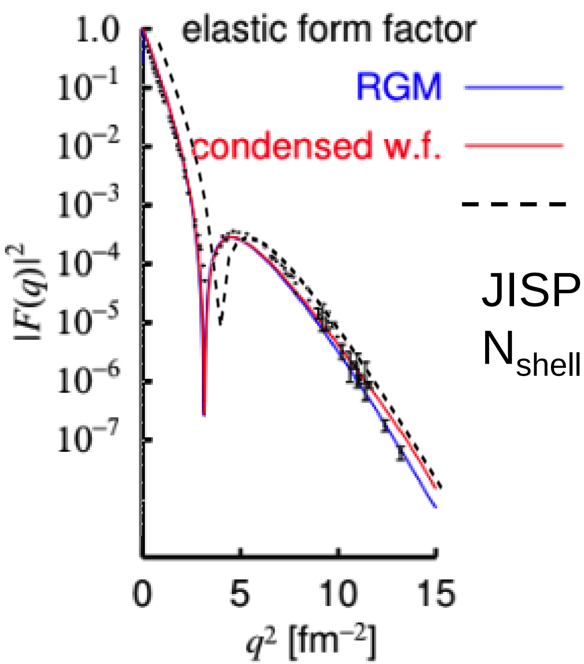


Expt.: P. Strehl 1970
THSR: Y. Funaki 2015
FMD: M. Chernykth 2007
AMD: Y. Kanada-En'yo 2007

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

Elastic and inelastic form factors

Elastic form factor (0^+_1 -> 0^+_1)

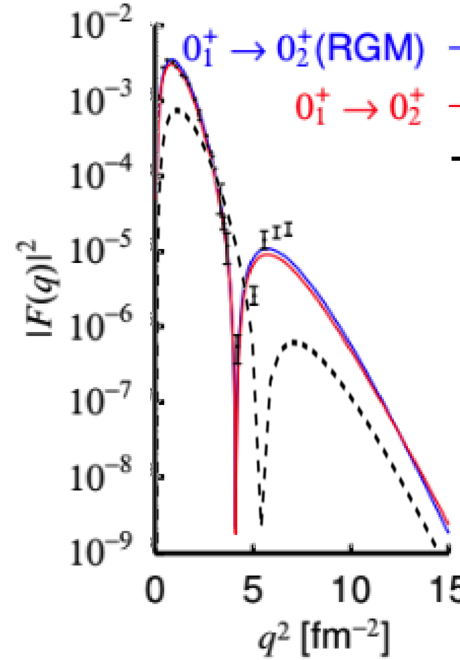


(a)

JISP16 NN

N_{shell} = 4, hw = 15 MeV

Inelastic form factor (0^+_1 -> 0^+_2)



(b)

$$|F(q)|^2 = \frac{4\pi}{12^2}\left|\int_0^\infty \rho^{(J)}_{J,0_1}(r) j_J(qr) r^2 \mathrm{d}r\right|^2 \exp\left(-\frac{1}{2}a_p^2 q^2\right). \quad (1)$$

$$\rho^{(J)}_{J,0_1}(r) = \langle \Psi^{JM}_{\lambda=k} | \sum_{i=1}^{12} \delta(\boldsymbol{r} - \boldsymbol{r}_i) | \Psi^{J=0}_{\lambda=1} \rangle / Y^*_{JM}(\hat{\boldsymbol{r}}), \qquad (2)$$

Figs, & Eqs. taken from Y. Funaki et al., Eur.Phys.J. A28 (2006) 259-263

Preliminary

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.
- Cluster structure of Be & C isotopes can be investigated using MCSM wave functions and we can observe two-alpha cluster of nucleons and molecular-orbital structure of valence neutrons in 10Be.

Future perspective

- Heavier nuclei beyond ^{20}Ne
- Quantitative analysis on cluster structure of Be & C isotopes

Collaborators

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

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"