TRIUMF Theory Workshop (Mar. 3 – 6, 2020)
Progress in Ab Initio Techniques in Nuclear Physics

Intrinsic structure of light nuclei from no-core Monte Carlo shell model

Takashi Abe (CNS, 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 3, 2020

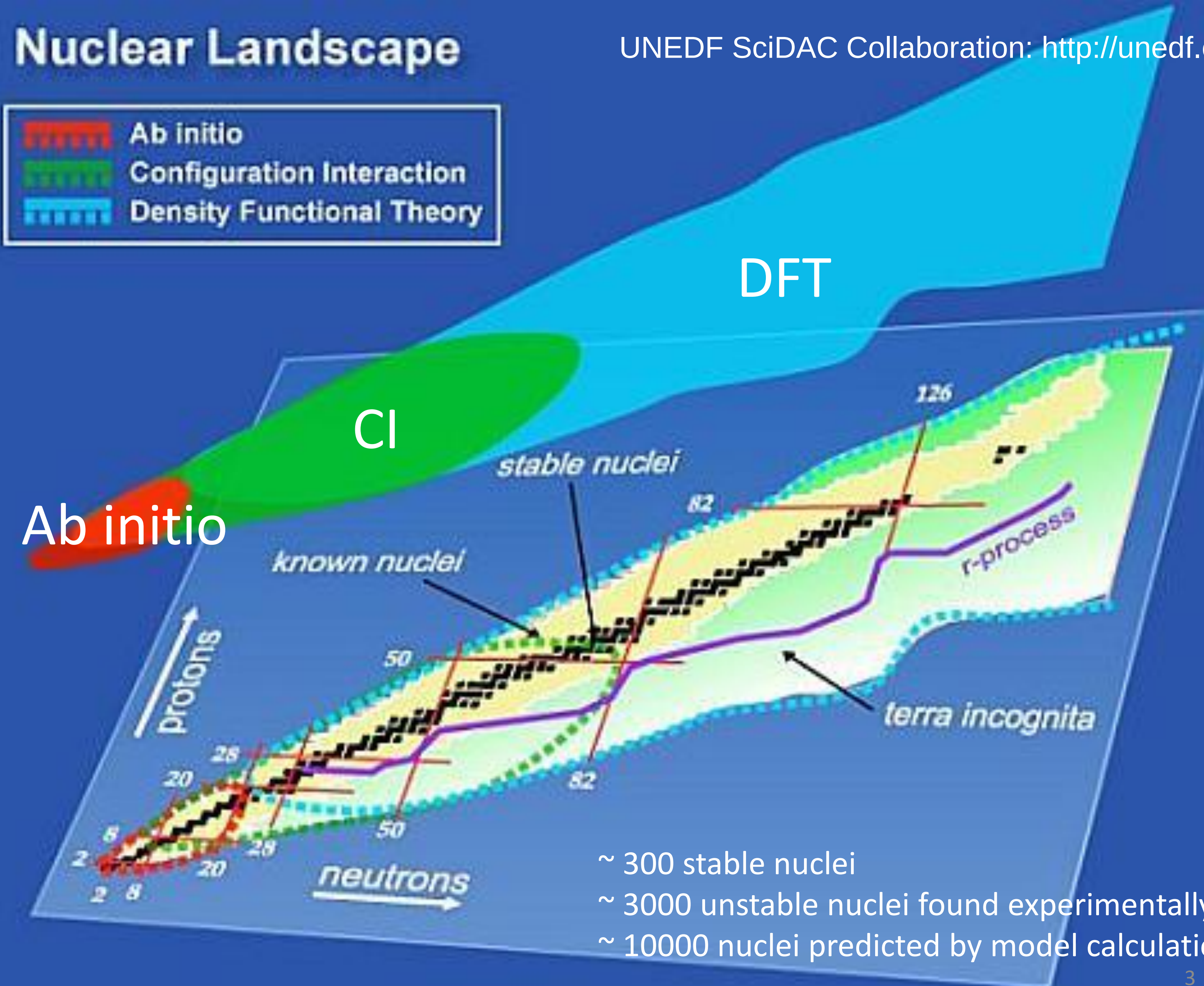
Collaborators

- Takaharu Otsuka (RIKEN, Tokyo)
- Yutaka Utsuno (JAEA)
- Noritaka Shimizu (Tokyo)
- Tooru Yoshida (RIST)
- Yusuke Tsunoda (Tokyo)
- James P Vary (Iowa State U)
- Pieter Maris (Iowa State U)

Supported by MEXT and JICFuS

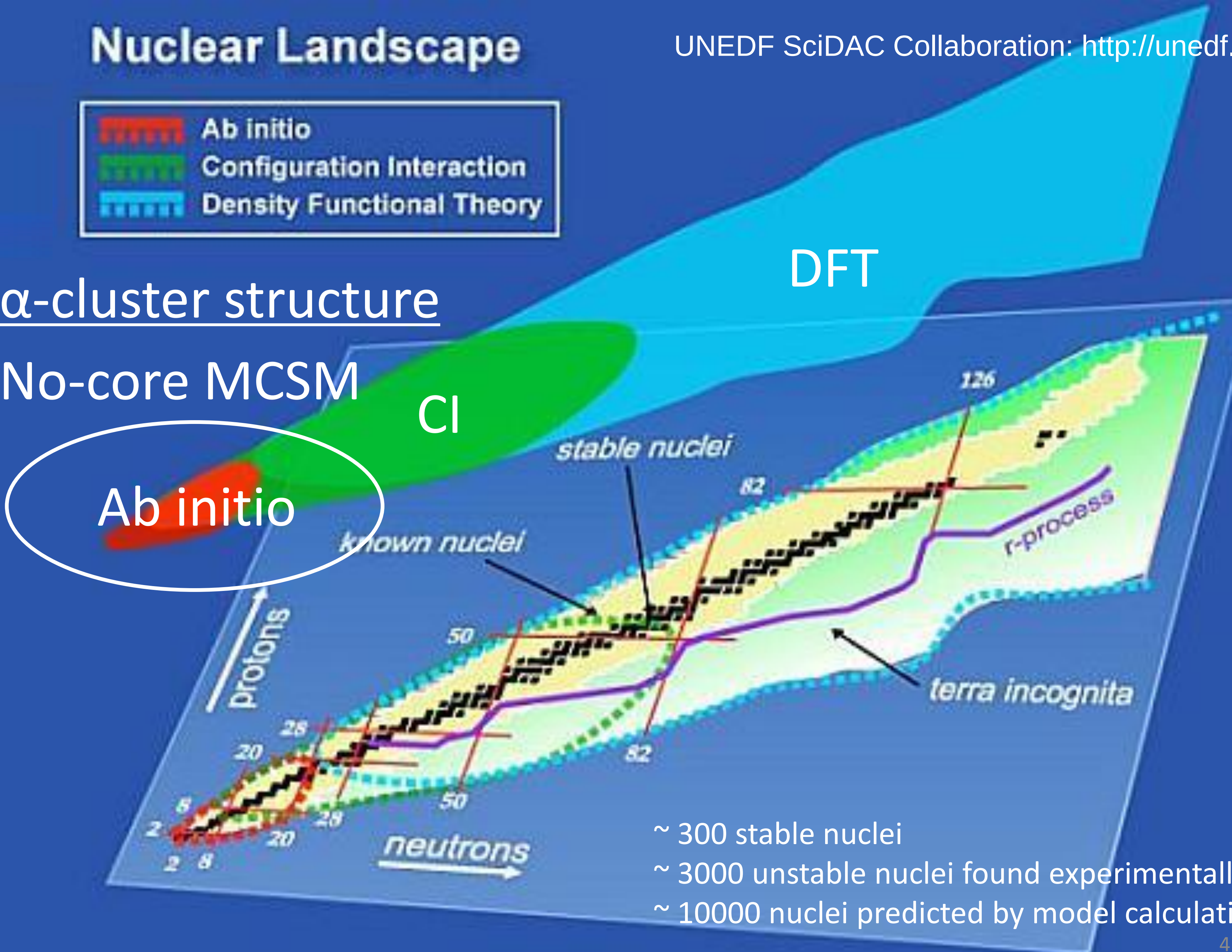
Priority Issue 9 to be Tackled by Using Post K Computer “Elucidation of the Fundamental Laws and Evolution of the Universe”

UNEDF SciDAC Collaboration: http://unedf.org/



~ 300 stable nuclei
~ 3000 unstable nuclei found experimentally
~ 10000 nuclei predicted by model calculations

UNEDF SciDAC Collaboration: http://unedf.org/



<u>α-cluster structure</u>

No-core MCSM

~ 300 stable nuclei
~ 3000 unstable nuclei found experimentally
~ 10000 nuclei predicted by model calculations

"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.

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

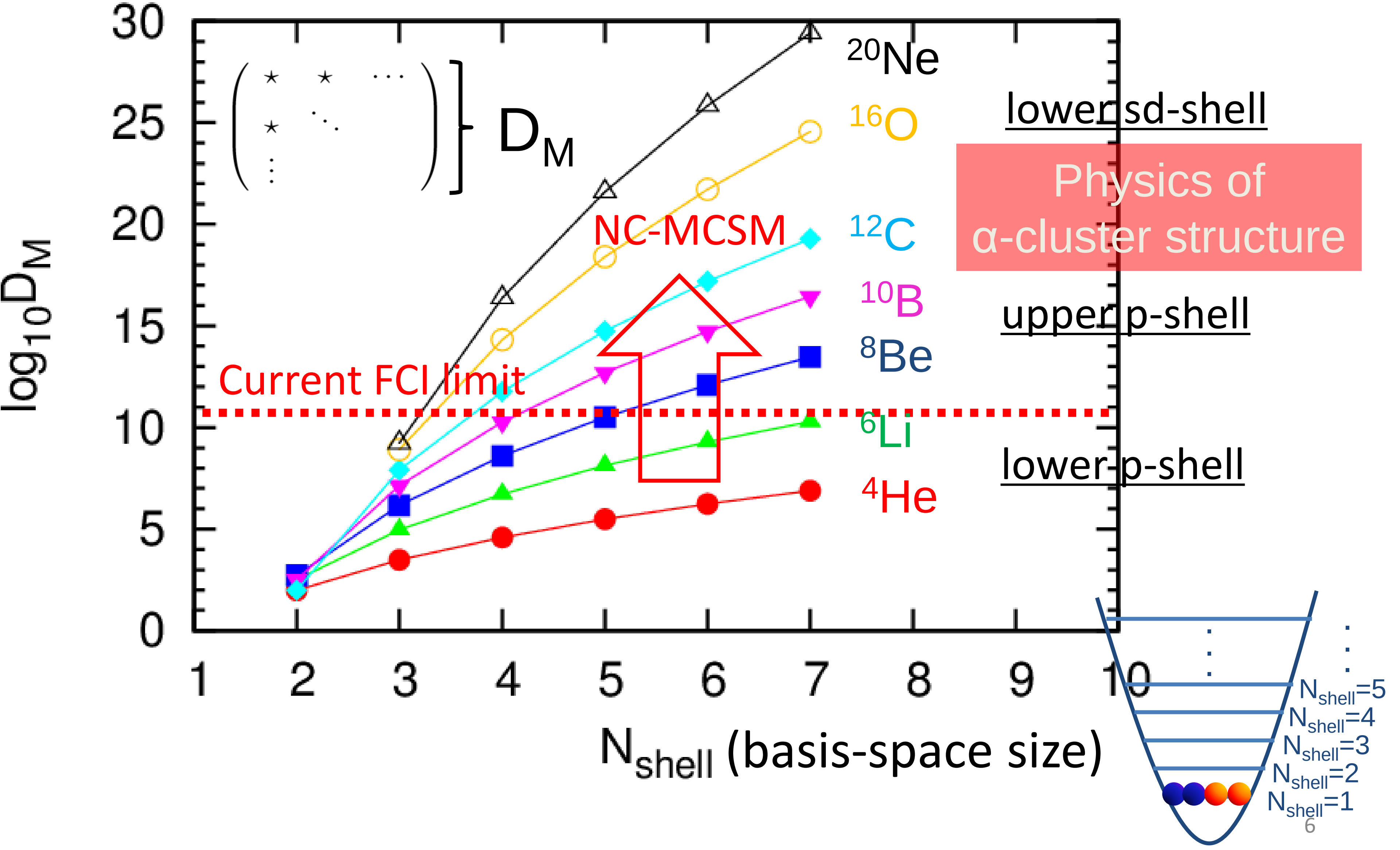
$$H = T + V_{\mathrm{NN}} + V_{\mathrm{3N}} + \cdots + V_{\mathrm{Coulomb}}$$

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

→ Computationally demanding → Monte Carlo shell model (MCSM)

M-scheme dimension

Ab initio calculations w/ NN int only



Monte Carlo shell model (MCSM)

Standard shell model

$$H = \begin{pmatrix} \star & \star & \star & \star & \star & \cdots \\ \star & \star & \star & \star & & \\ \star & \star & \star & & & \\ \star & \star & & \ddots & & \\ \star & & & & & \\ \vdots & & & & & \end{pmatrix}$$

Diagonalization

$$\begin{pmatrix} E_0 & & & 0 \\ & E_1 & & \\ & & E_2 & \\ & & & \ddots \\ 0 & & & \end{pmatrix}$$

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

$$H \sim \begin{pmatrix} \star & \star & \cdots \\ \star & \ddots & \\ \vdots & & \end{pmatrix}$$

Diagonalization

$$\begin{pmatrix} E'_0 & & 0 \\ & E'_1 & \\ 0 & & \ddots \end{pmatrix}$$

Important bases stochastically selected ~ O(100)

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

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

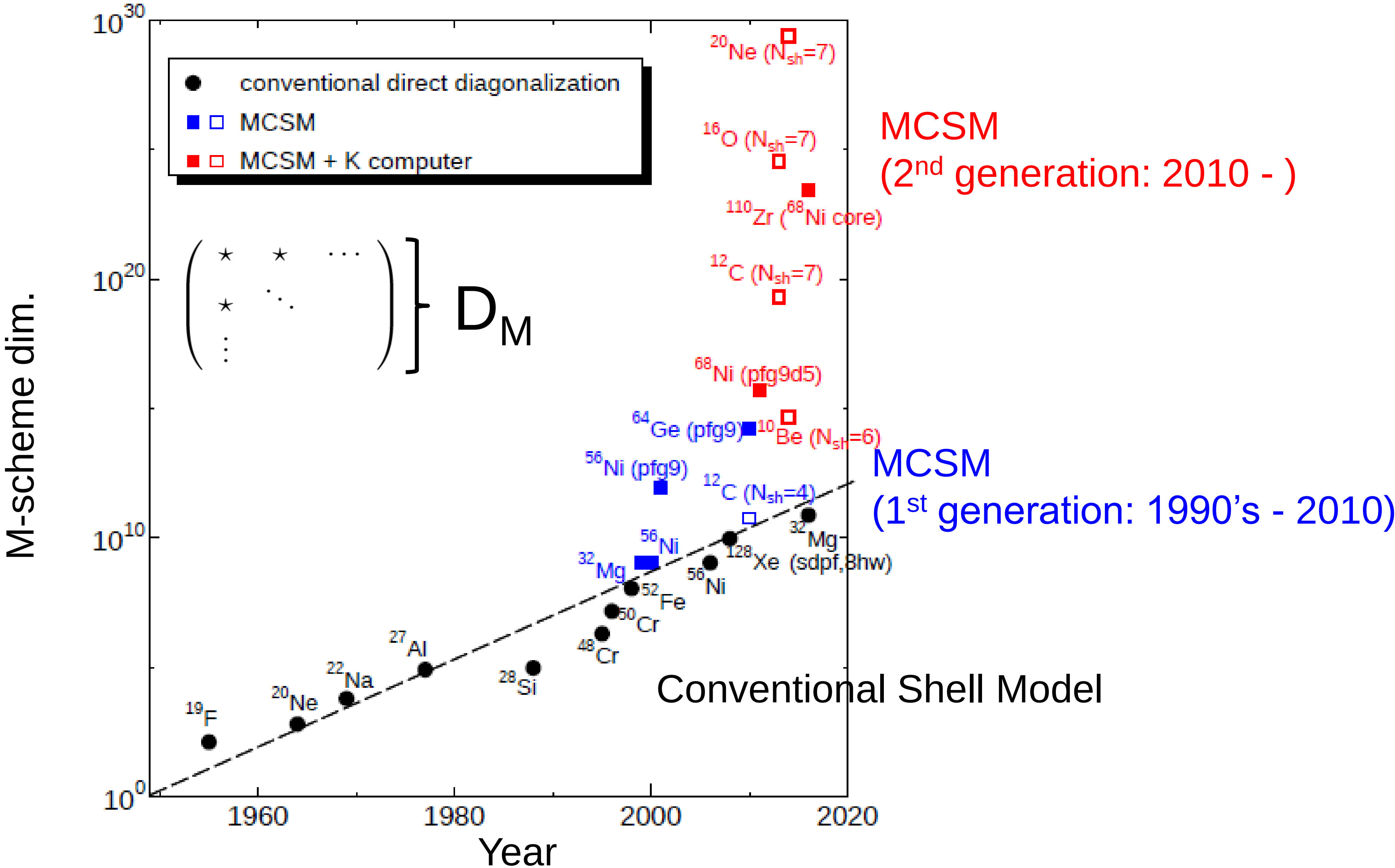
diagonalization

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

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

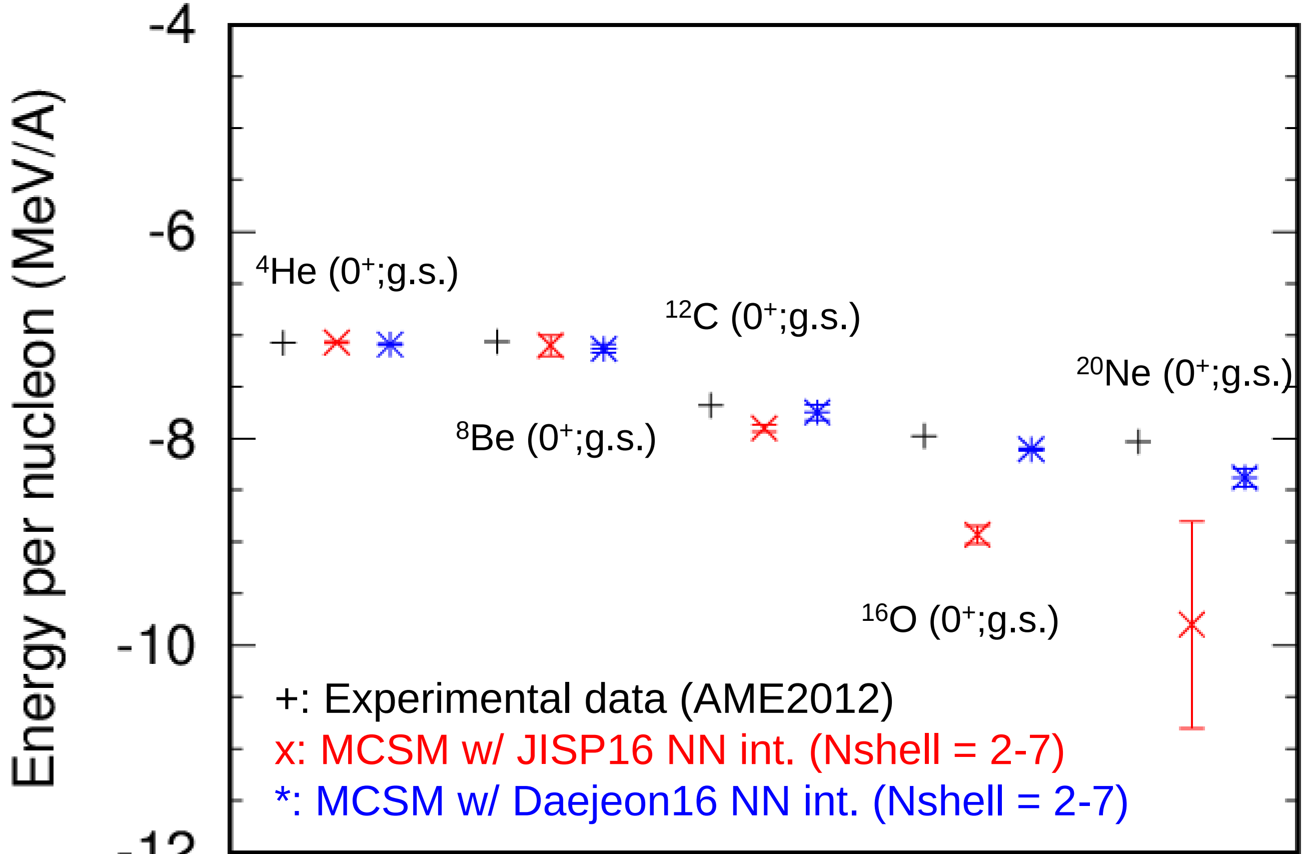
stochastic sampling & CG method

Historical evolution/development of the MCSM



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

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.

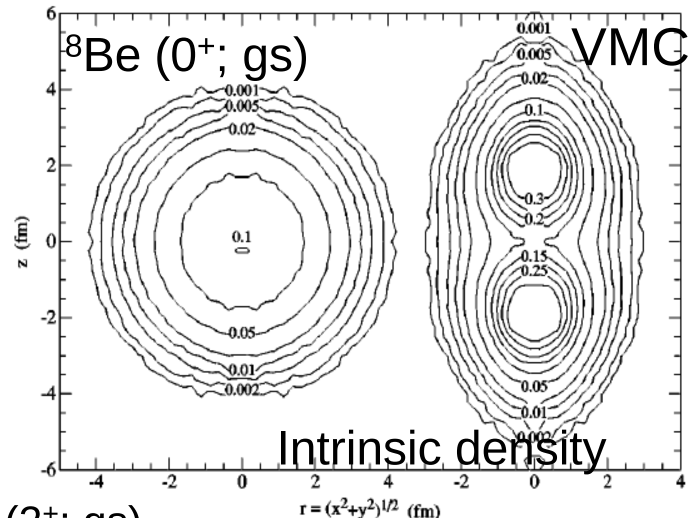
Density distribution from ab initio calc.

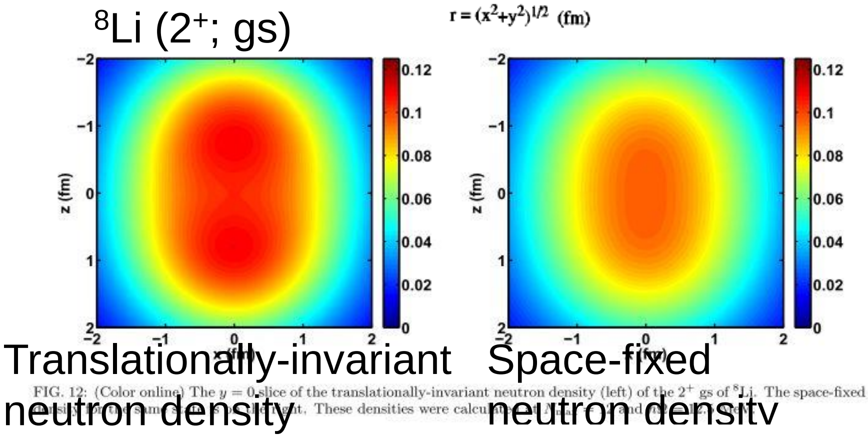
- Green's function Monte Carlo (GFMC)
  - "Intrinsic" density is constructed
    by aligning the moment of inertia among samples
    R. B. Wiringa, S. C. Pieper, J. Carlson, & V. R. Pandharipande,
    Phys. Rev. C62, 014001 (2000)

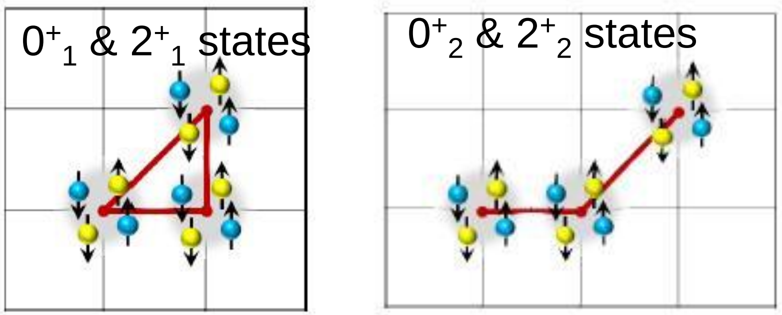
- No-core full configuration (NCFC)
  - Translationally-invariant density is obtained
    by deconvoluting the intrinsic & CM w.f.
    C. Cockrell J. P. Vary & P. Maris, Phys. Rev. C86, 034325 (2012)

- 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), …

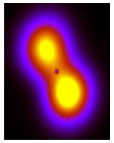
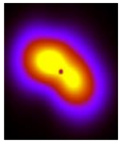
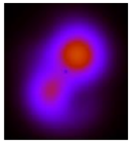
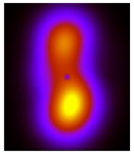
- FMD
    H. Feldmeier, Nucl. Phys. A515, 147 (1990), …







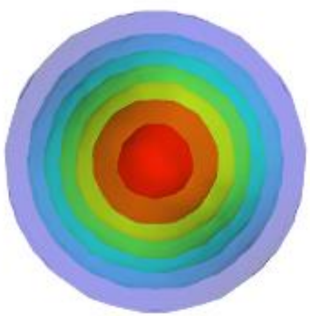
Density distribution in MCSM

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

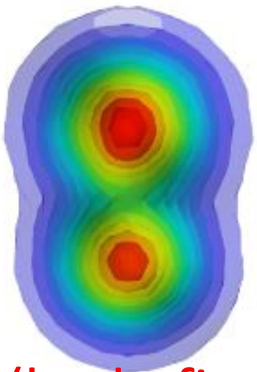
Angular-momentum projection

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

A way to construct an "intrinsic" density



^{8}Be 0^+ ground state



Laboratory frame

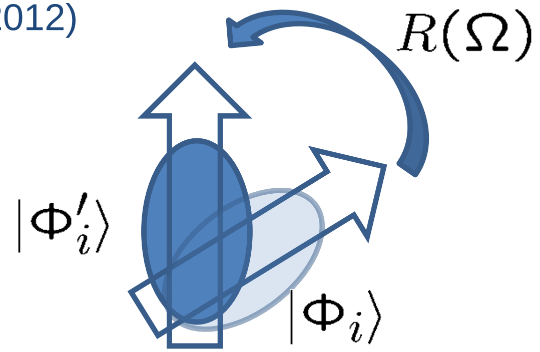
"Intrinsic" (body-fixed) frame

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)

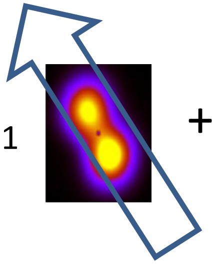
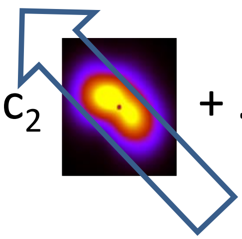
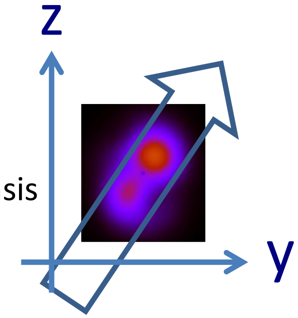


Rotation by diagonalizing Q-moment ($Q_{zz} > Q_{yy} > Q_{xx}$)

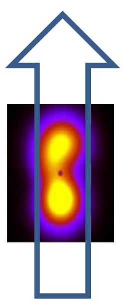
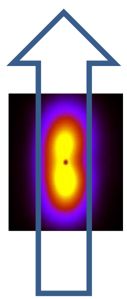
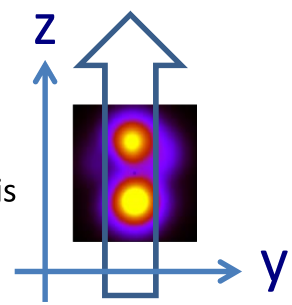
- MCSM wave function

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

- Wave function w/o the projections

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

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

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

Density distribution of Be isotopes

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

Preliminary

Emergence of 2-α-cluster structure

Appearance of molecular-orbital structure

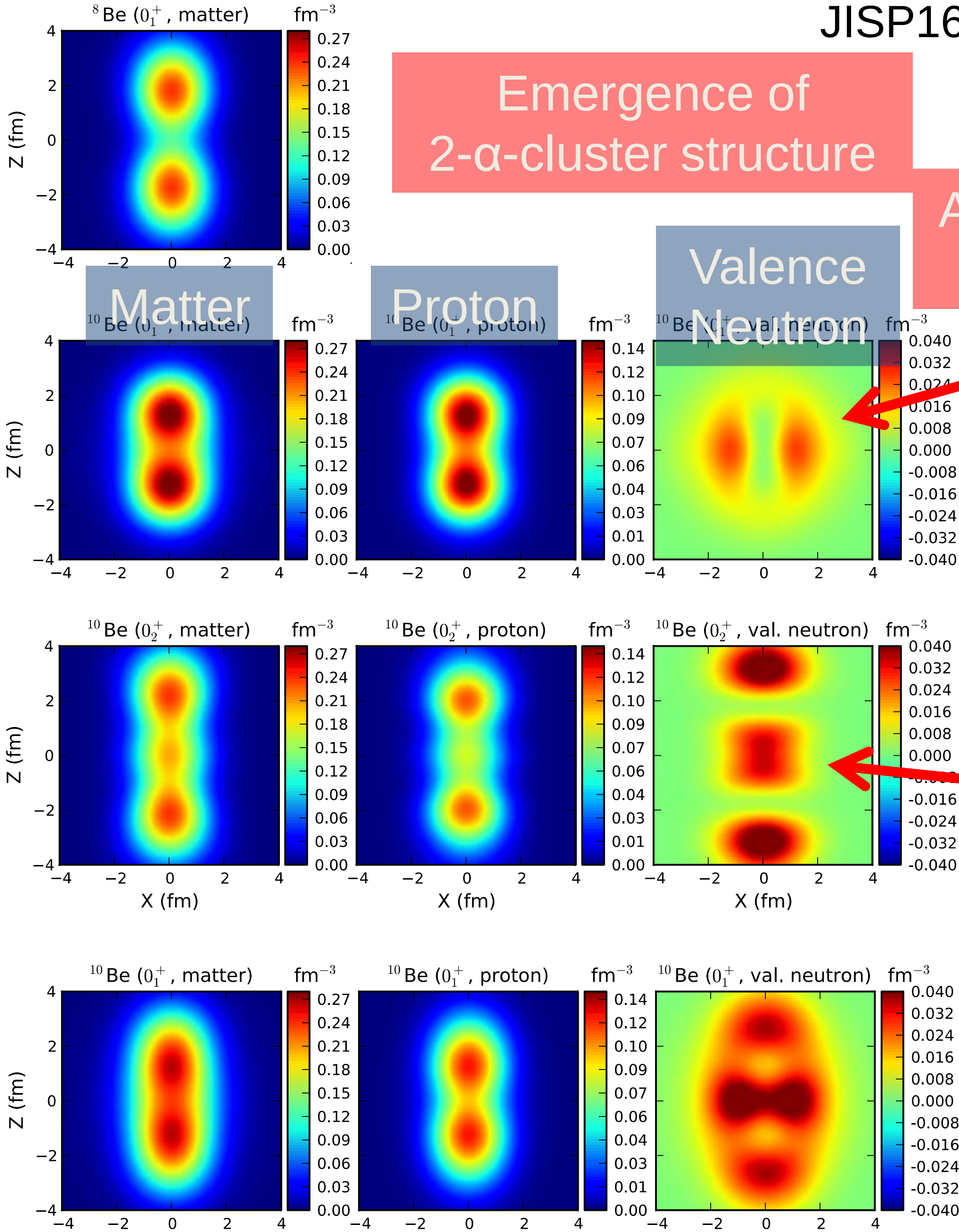
Fading 2-α structure as N increases

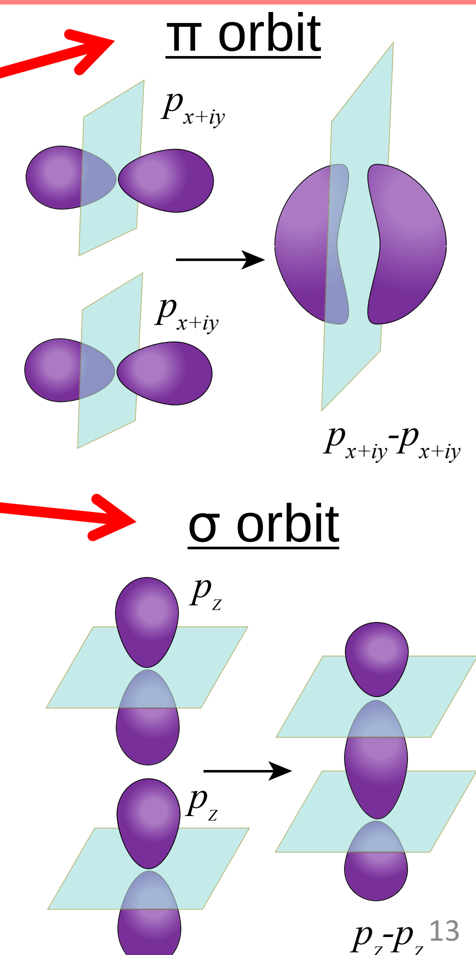
^{8}Be (0^+;gs)

^{10}Be (0^+;gs)

0_2^+

^{12}Be (0^+;gs)





T-plot in MSCM

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

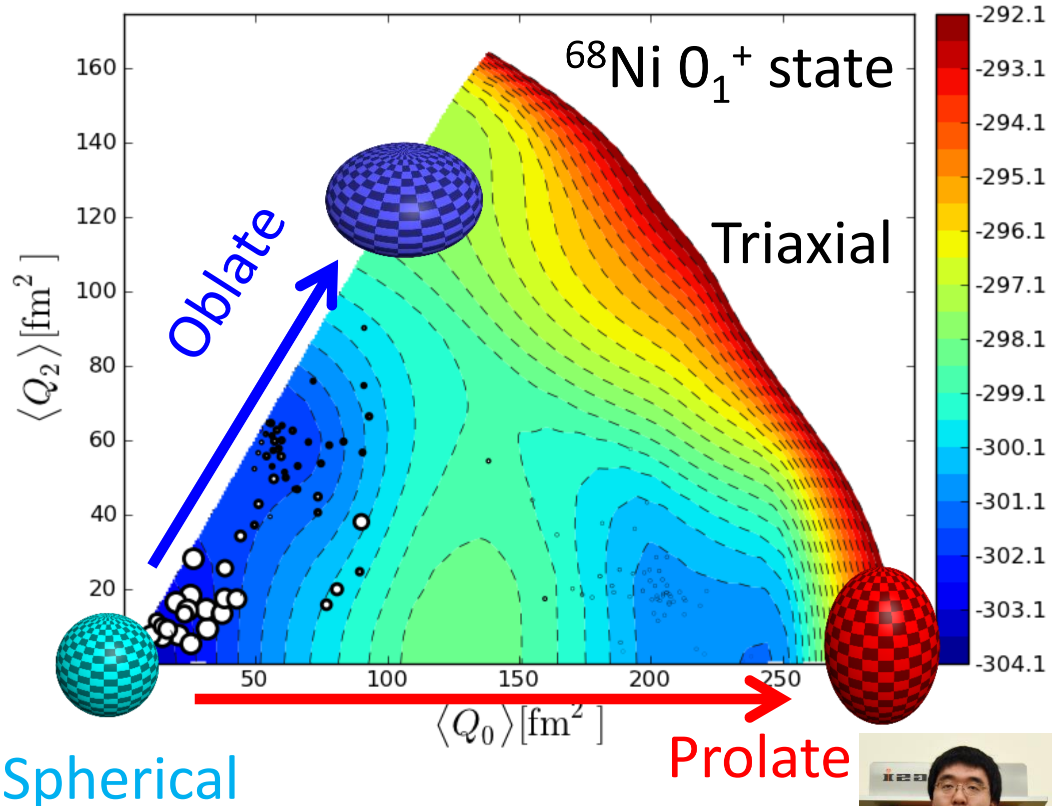
  Deformed SD -> info of intrinsic shape ($|\Phi_i\rangle$)

  Coefficient (c_i)

- Potential Energy Surface (PES):
  Calculated by Q-constrained HF

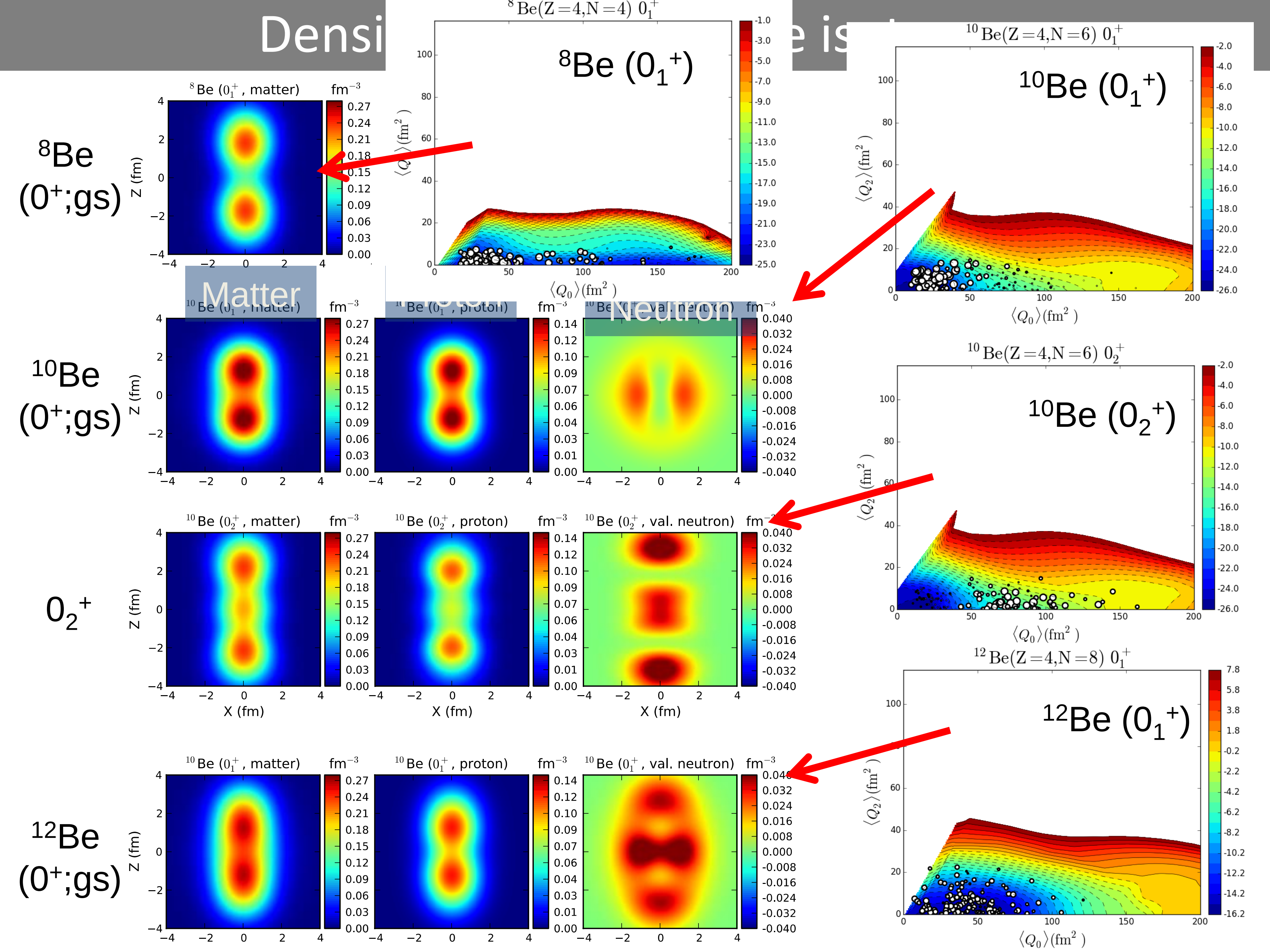
- Location of circles:
  Quadrupole deformation of
  unprojected deformed SDs

- Area of circles:
  Overlap probability
  btw deformed SD & MCSM wf



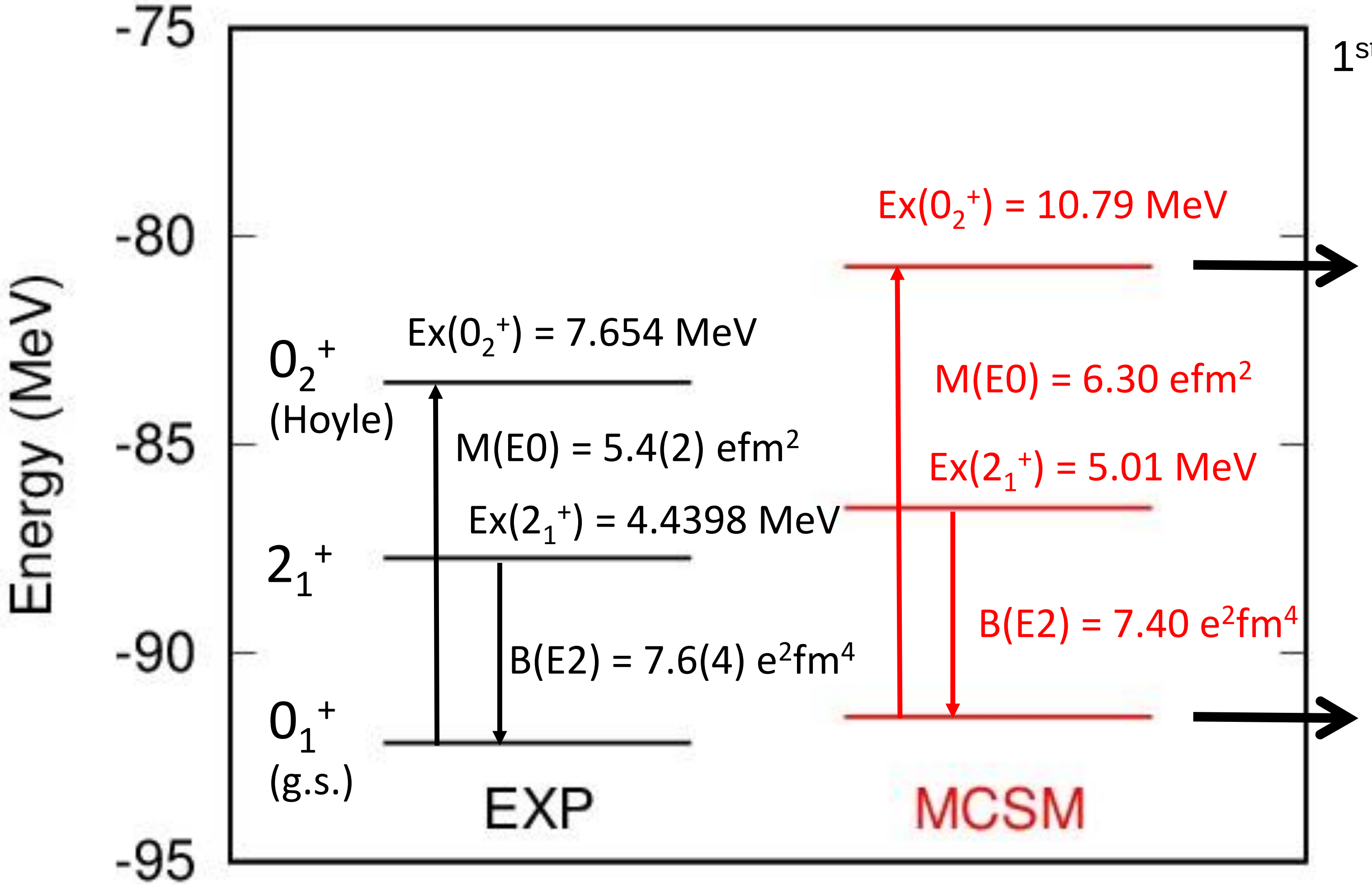
Y. Tsunoda, et al., Phys Rev C89, 031301 (R) (2014).

Densi… e is…



^{8}Be (0$^+$;gs)
^{10}Be (0$^+$;gs)
0$_2$$^+$
^{12}Be (0$^+$;gs)
Matter
Proton
Neutron
^{8}Be (0$_1^+$, matter)
^{10}Be (0$_1^+$, matter)
^{10}Be (0$_1^+$, proton)
^{10}Be (0$_1^+$, val. neutron)
^{10}Be (0$_2^+$, matter)
^{10}Be (0$_2^+$, proton)
^{10}Be (0$_2^+$, val. neutron)
fm^{-3}
Z (fm)
X (fm)
^{8}Be(Z=4,N=4) 0$_1^+$
^{8}Be (0$_1^+$)
^{10}Be(Z=4,N=6) 0$_1^+$
^{10}Be (0$_1^+$)
^{10}Be(Z=4,N=6) 0$_2^+$
^{10}Be (0$_2^+$)
^{12}Be(Z=4,N=8) 0$_1^+$
^{12}Be (0$_1^+$)
$\langle Q_0 \rangle$(fm^2)
$\langle Q_2 \rangle$(fm^2)

Excitation spectrum of ^{12}C

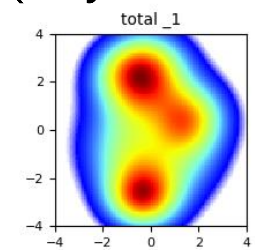


Daejeon16 NN, N_{shell} = 7, hw = 20 MeV
w/o energy-variance extrapolation

Preliminary

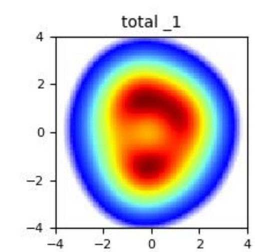
Intrinsic density

1st excited 0^+ state
(Hoyle state?)



r_{pp} = 2.60 fm

Ground state



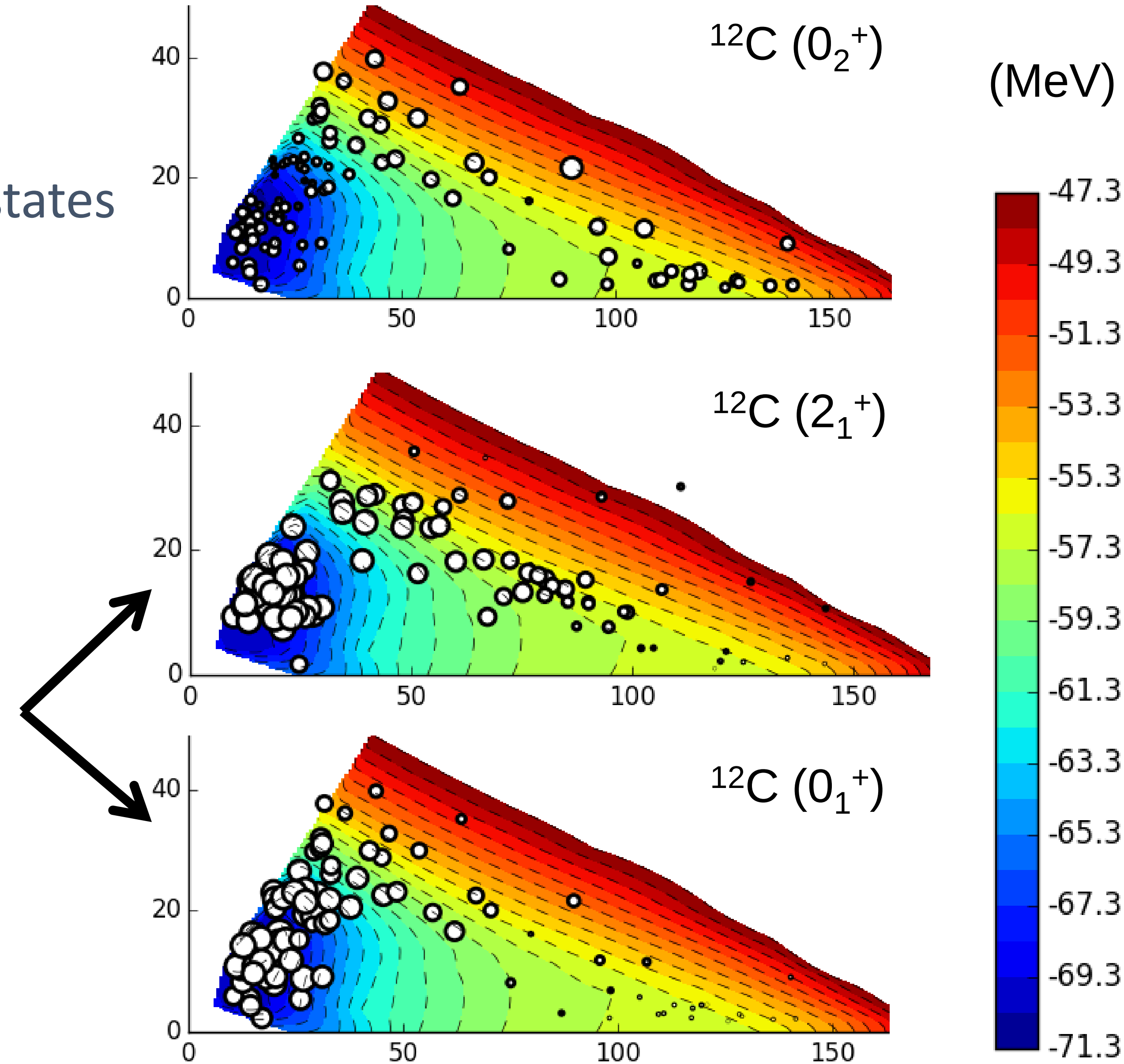
r_{pp} = 2.28 fm

r_{pp} = 2.32(2) fm (exp)

T-plot of ^{12}C low-lying states

Scattered more than those of ground & 2^+ states

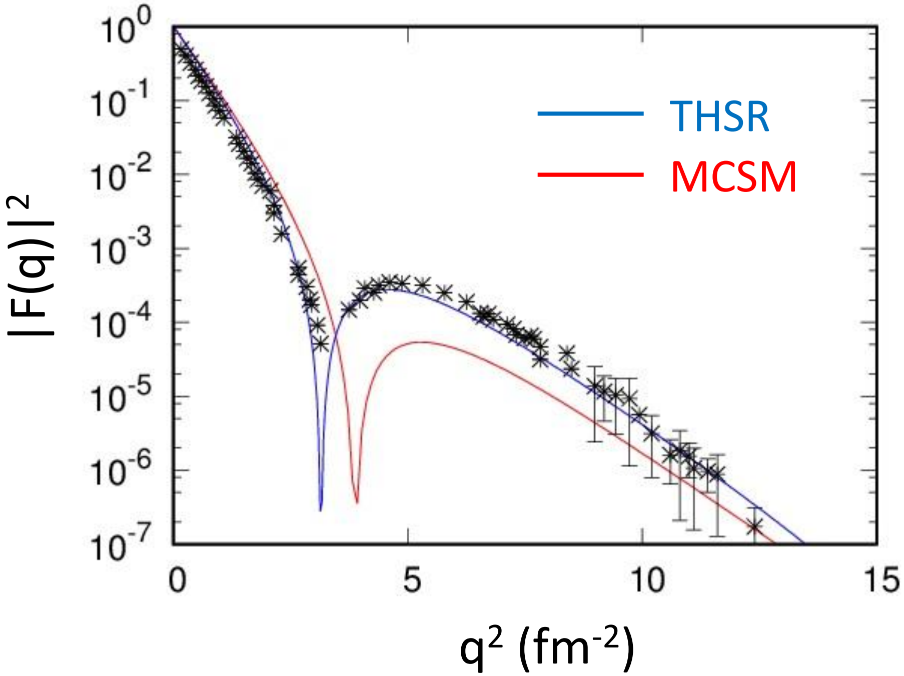
Similar distributions



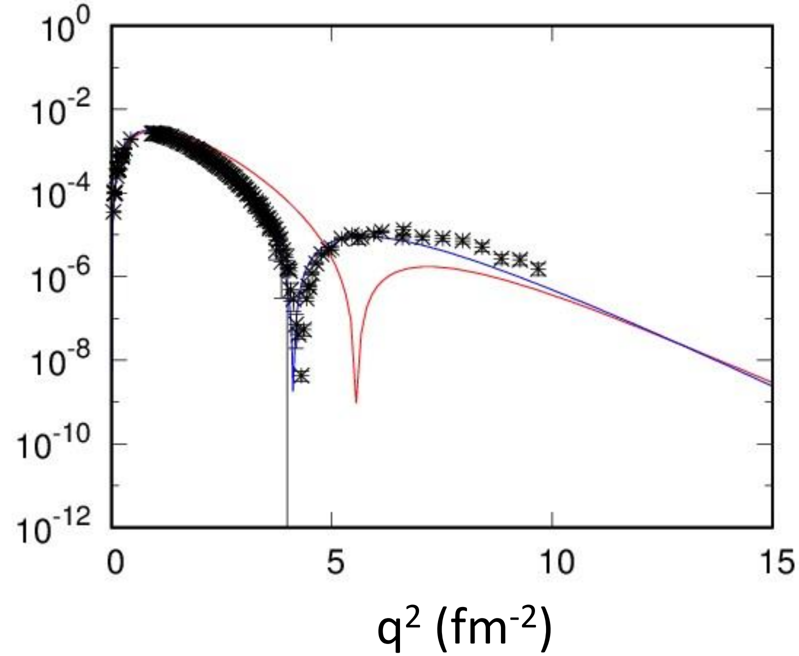
Elastic/Inelastic form factors of ^{12}C

Preliminary

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



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



Daejeon16 NN, N_{shell} = 7, hw = 20 MeV

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

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

THSR & experimental data:
Provided by Y. Funaki et al.,
Eur. Phys. J. A28 (2006) 259-263.

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.
- Intrinsic structure of Be & C isotopes can be investigated using MCSM wave functions. In the Be isotopes, we can observe two-alpha cluster structure of nucleons and molecular-orbital structure of valence neutrons. T-plot analysis of low-lying states of Be & C isotopes was also shown.

Future perspective

- Heavier (sd-shell) nuclei beyond ^{20}Ne enable to provide a comparison with recent experiments
- Quantitative analysis on alpha-cluster structure of Be & C isotopes