TRIUMF Theory Workshop (Feb. 23 – 26, 2016)
Progress in Ab Initio Techniques in Nuclear Physics

No-core MCSM calculations in light nuclei

Takashi Abe (U of Tokyo)

TRIUMF
Feb. 23 – 26, 2016

Collaborators

- U of Tokyo
  - Takaharu Otsuka (Department of Physics & CNS)
  - Noritaka Shimizu (CNS)
  - Tooru Yoshida (CNS)
- JAEA
  - Yutaka Utsuno
- Iowa State U
  - James P. Vary
  - Pieter Maris

Outline

- Motivation
- Monte Carlo shell model (MCSM)
- Extrapolations of the basis space
- Cluster structure of Be isotopes
- Summary & outlook

Ab inito approaches

- Major challenge in nuclear physics

  - Understand the nuclear structure & reactions from *ab-initio* calculations w/ realistic nuclear forces (potentials)

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

    GFMC, NCSM (A ~ 12-16), CC (sub-shell closure +/- 1,2),

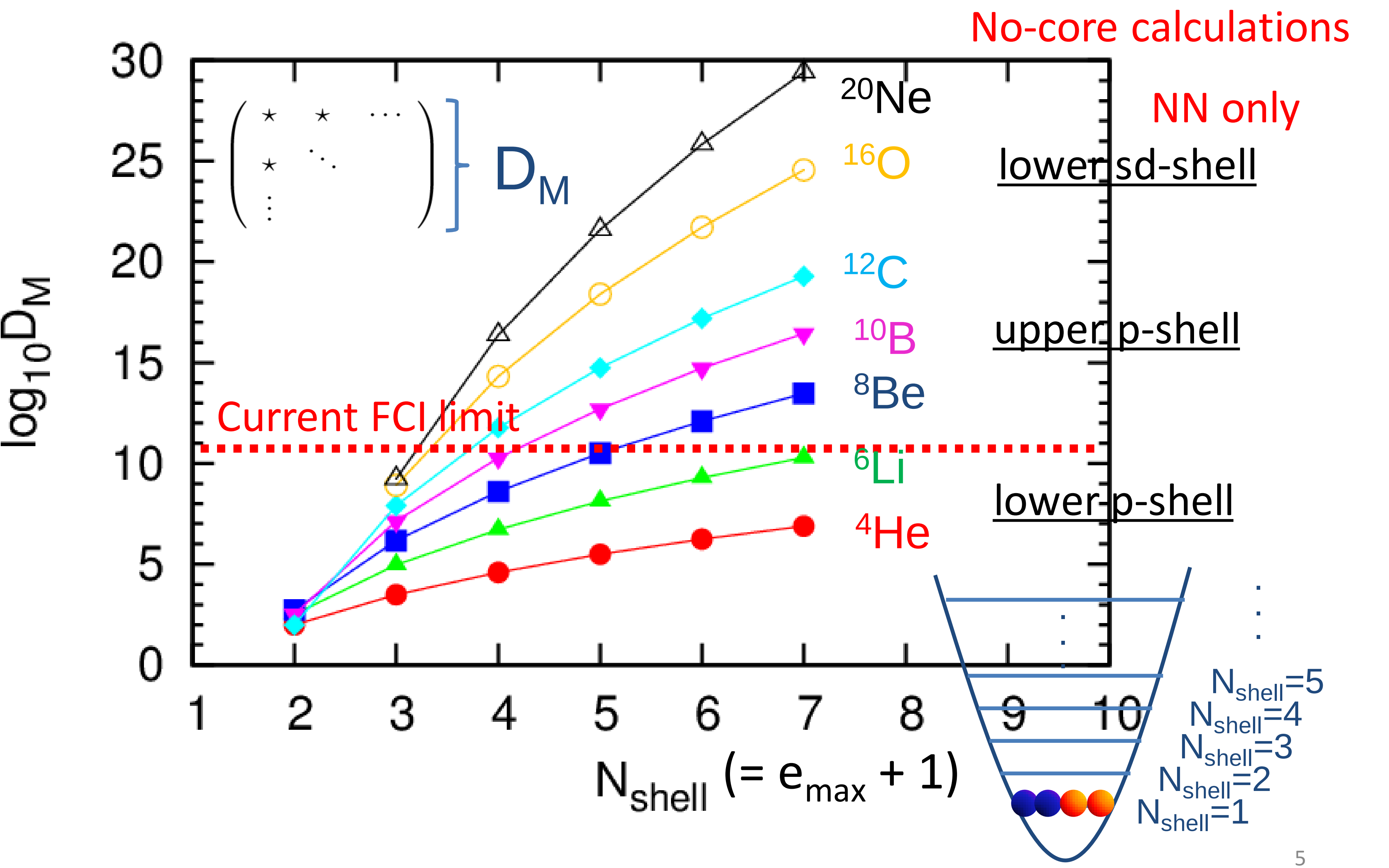
    Self-consistent Green's Function theory, IM-SRG, Lattice EFT, …

→ demand for extensive computational resources

✓ *ab-initio*(-like) SM approaches (which attempt to go) beyond standard methods

- IT-NCSM, IT-CI: R. Roth (TU Darmstadt), P. Navratil (TRIUMF), …
- SA-NCSM: T. Dytrych, J. P. Draayer, K. D. Launey (Louisiana State U), …
- No-Core Monte Carlo Shell Model (MCSM)

M-scheme dimension in N_{shell} truncation



Monte Carlo shell model (MCSM)

- Importance truncation

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

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

All Slater determinants

$d > O(10^{10})$

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

$d_{MCSM} \sim O(100)$

Review: T. Otsuka , M. Honma, T. Mizusaki, N. Shimizu, Y. Utsuno, Prog. Part. Nucl. Phys. 47, 319 (2001)

SM Hamiltonian & MCSM many-body w.f.

- 2nd-quantized non-rel. Hamiltonian (up to 2-body term, so far)

$$H = \sum_{\alpha\beta}^{N_{sps}} t_{\alpha\beta} c_\alpha^\dagger c_\beta + \frac{1}{4} \sum_{\alpha\beta\gamma\delta}^{N_{sps}} \bar{v}_{\alpha\beta\gamma\delta} c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma \quad \bar{v}_{ijkl} = v_{ijkl} - v_{ijlk}$$

- Eigenvalue problem

$$H|\Psi(J,M,\pi)\rangle = E|\Psi(J,M,\pi)\rangle$$

- MCSM many-body wave function & basis function

$$|\Psi(J,M,\pi)\rangle = \sum_i^{N_{basis}} f_i |\Phi_i(J,M,\pi)\rangle \qquad |\Phi(J,M,\pi)\rangle = \sum_K g_K P^J_{MK} P^\pi |\phi\rangle$$

These coeff. are obtained by the diagonalization.

- Deformed SDs

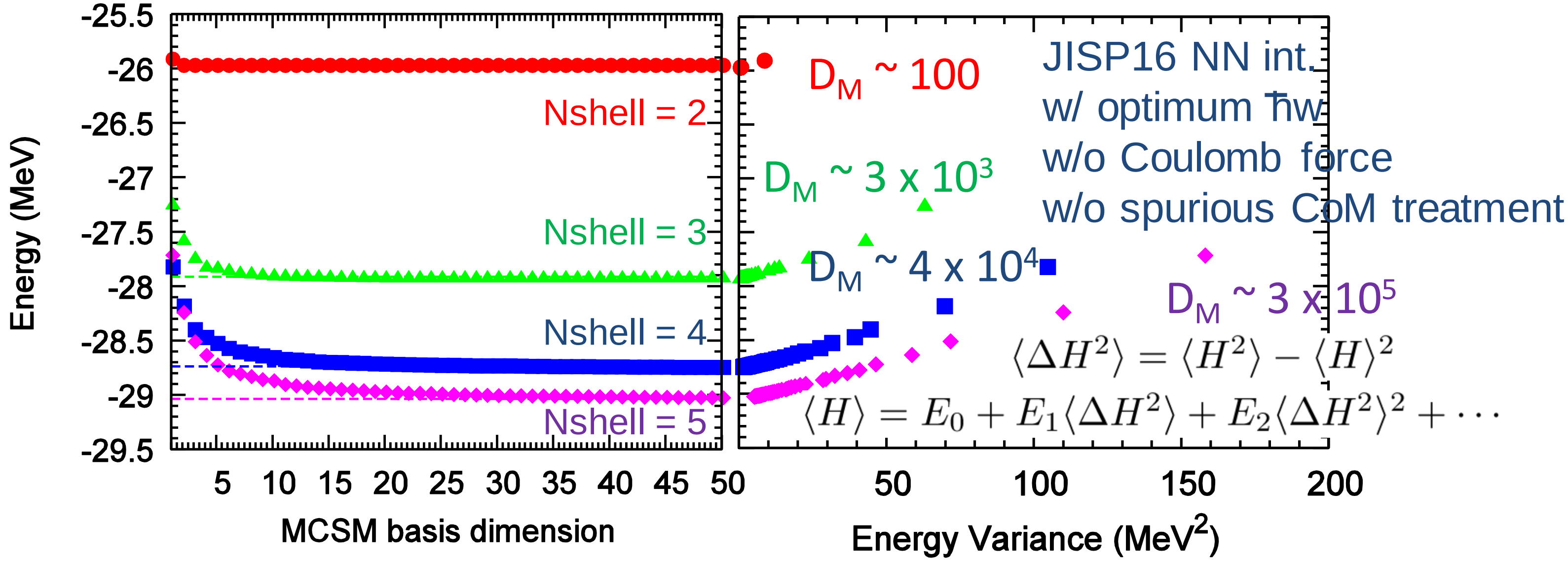
This coeff. is obtained by a stochastic sampling & CG.

$$|\phi\rangle = \prod_i^A a_i^\dagger |-\rangle \qquad a_i^\dagger = \sum_\alpha^{N_{sps}} c_\alpha^\dagger D_{\alpha i}$$

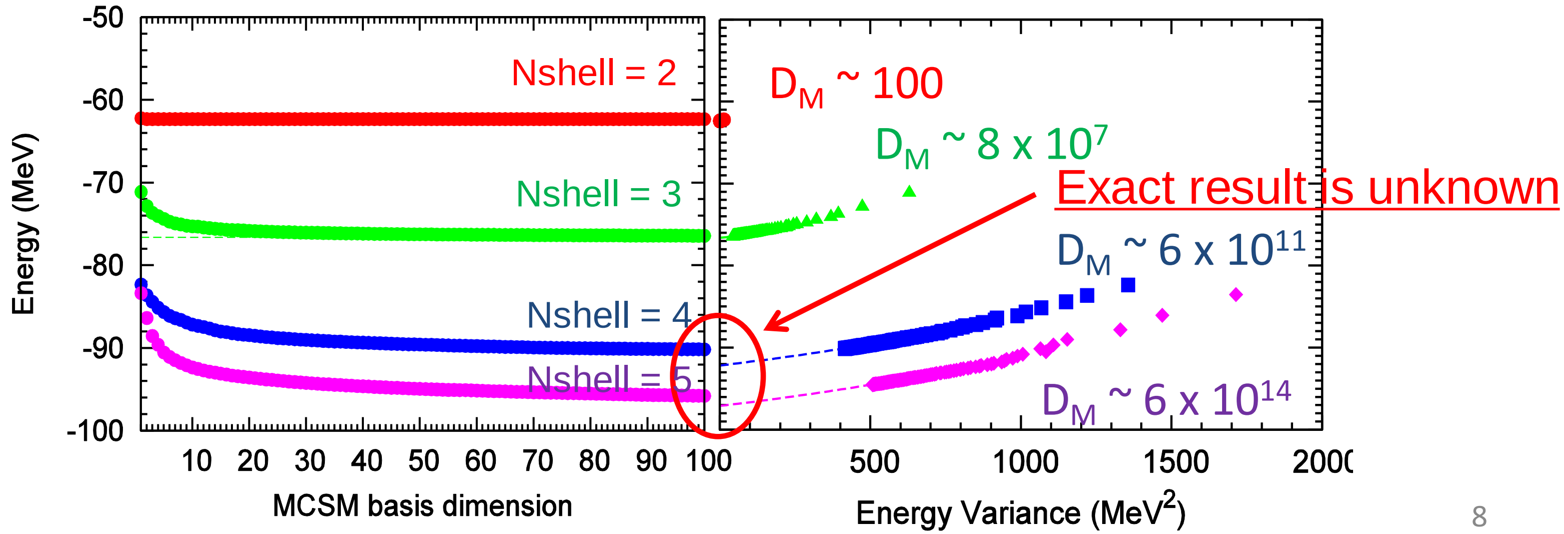
($c_\alpha{}^\dagger$ ... spherical HO basis)

Energies wrt # of basis & energy variance

^{4}He(0^+;gs)



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



Extrapolations in the no-core MCSM

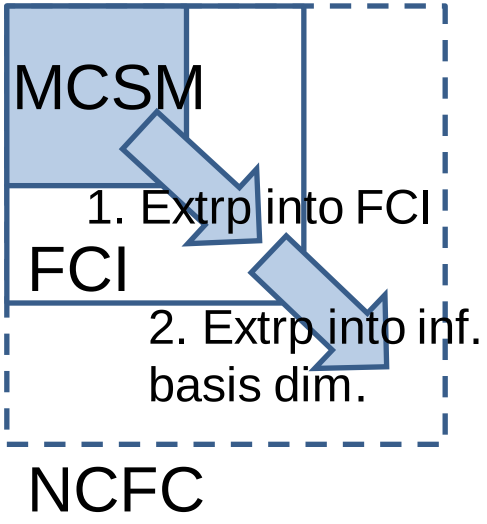
- Two steps of the extrapolation

1. Extrapolation of our MCSM (approx.) results to the FCI (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)

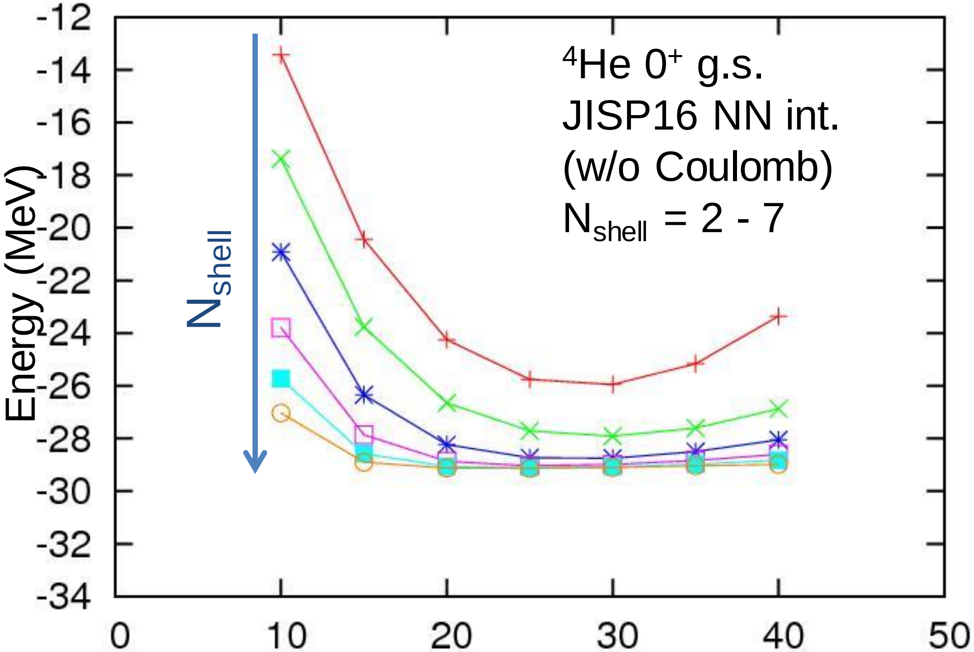
2. Extrapolation into the infinite model space
   - Exponential fit w.r.t. N w/ fixed hw
   - IR- & UV-cutoff extrapolations

Largely developed by Arizona, Oak Ridge, Ohio, Iowa, Chalmers, …



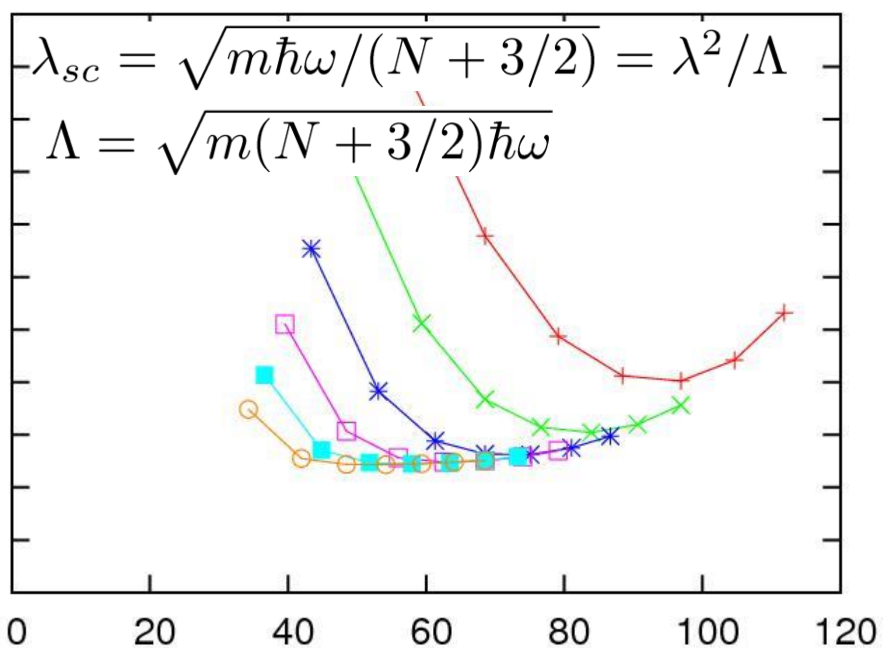
Traditional extrapolation

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



IR-cutoff extrapolation

$$E(\lambda) = E(\lambda=0) + a\exp(-b/\lambda)$$

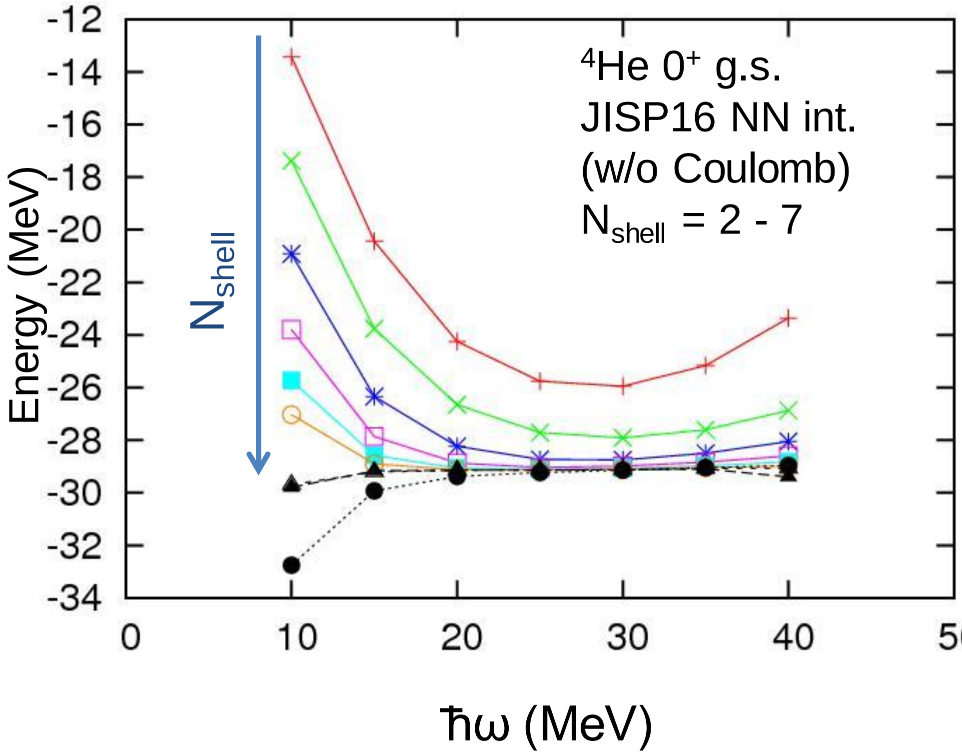


(N_{shell}, ħω) ⟷ (Λ, λsc)

Λ: UV cutoff   λsc: IR cutoff

Traditional extrapolation

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

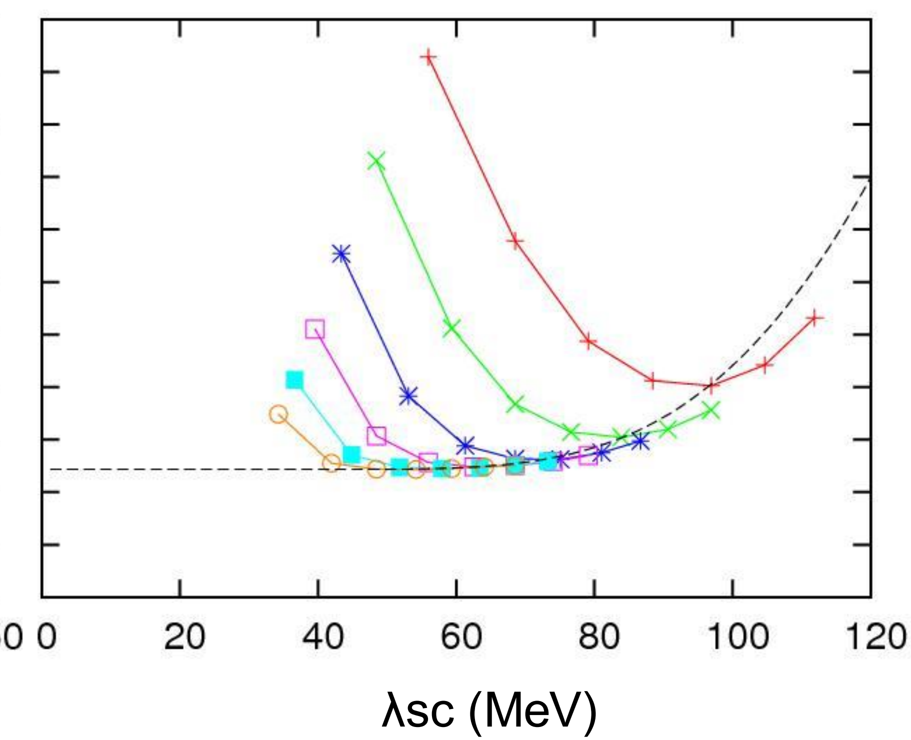


MCSM(empirical): -29.4 ~ -29.1 MeV
(N_{shell} = 3 - 7, hw = 15 - 35 MeV)

O(100) keV error

IR-cutoff extrapolation

$$E(\lambda) = E(\lambda=0) + a\exp(-b/\lambda)$$



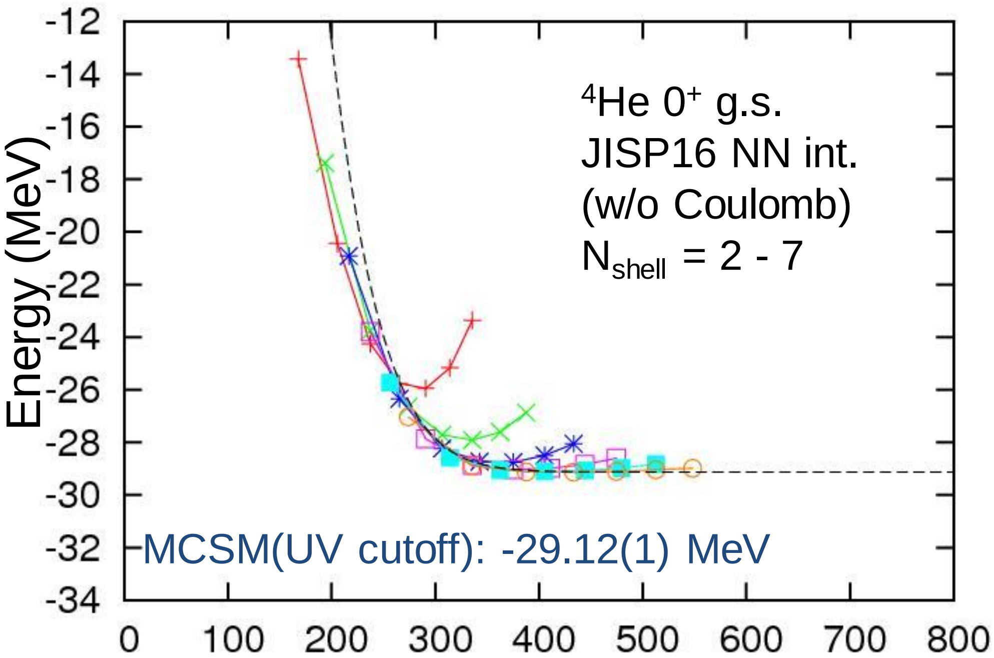
MCSM(IR cutoff): ~ -29.14(1) MeV

O(10) keV error

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

UV-cutoff extrapolation

$$E(\Lambda) = E(\Lambda = \infty) + c\exp(-\Lambda^2/d^2)$$

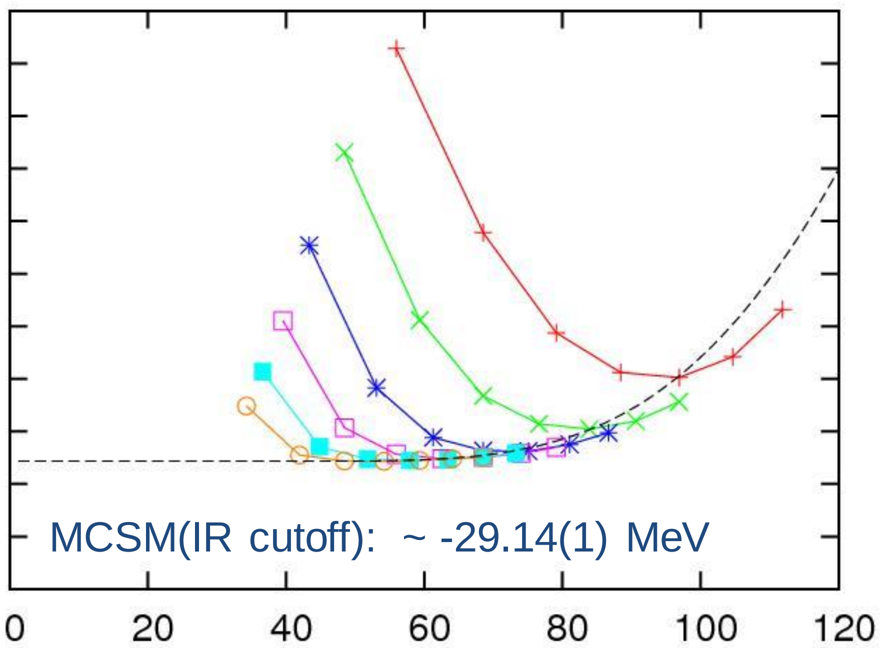


Λ_{UV} (MeV)

O(10) keV error

IR-cutoff extrapolation

$$E(\lambda) = E(\lambda = 0) + a\exp(-b/\lambda)$$



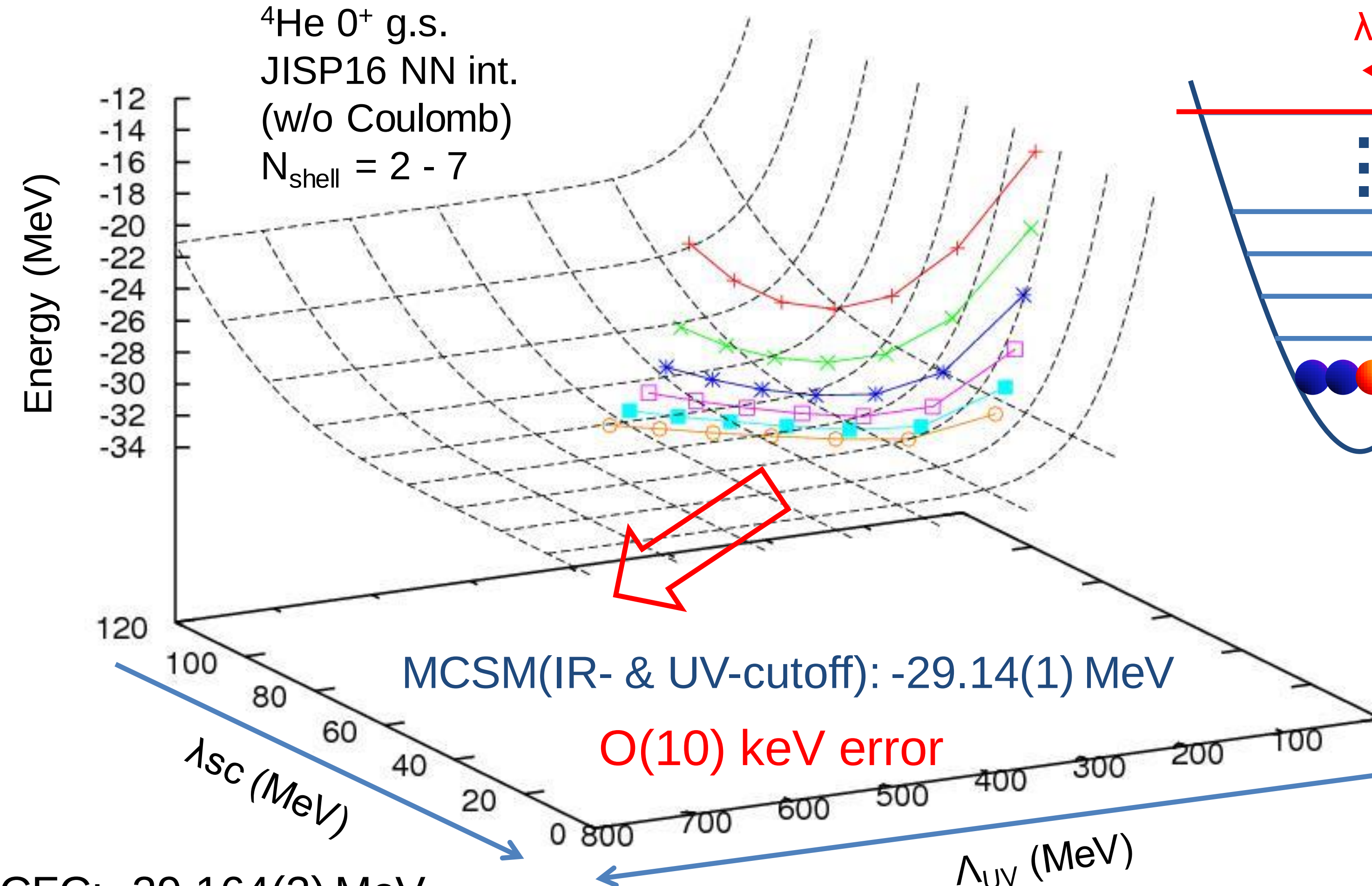
λsc (MeV)

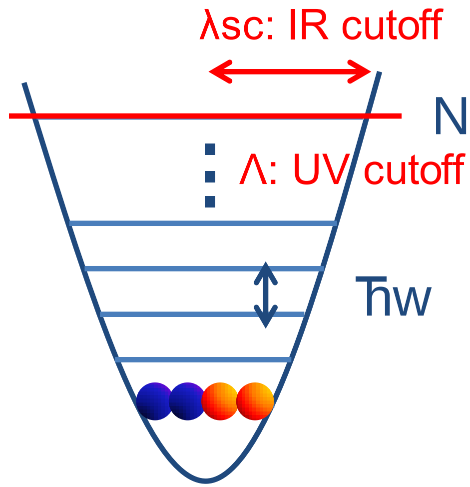
c.f.) NCFC: -29.164(2) MeV

Extrapolated results to infinite N_{max} space

IR- & UV-cutoff extrapolation

$$E(\lambda, \Lambda) = E(\lambda = 0, \Lambda = \infty) + a\exp(-b/\lambda) + c\exp(-\Lambda^2/d^2)$$

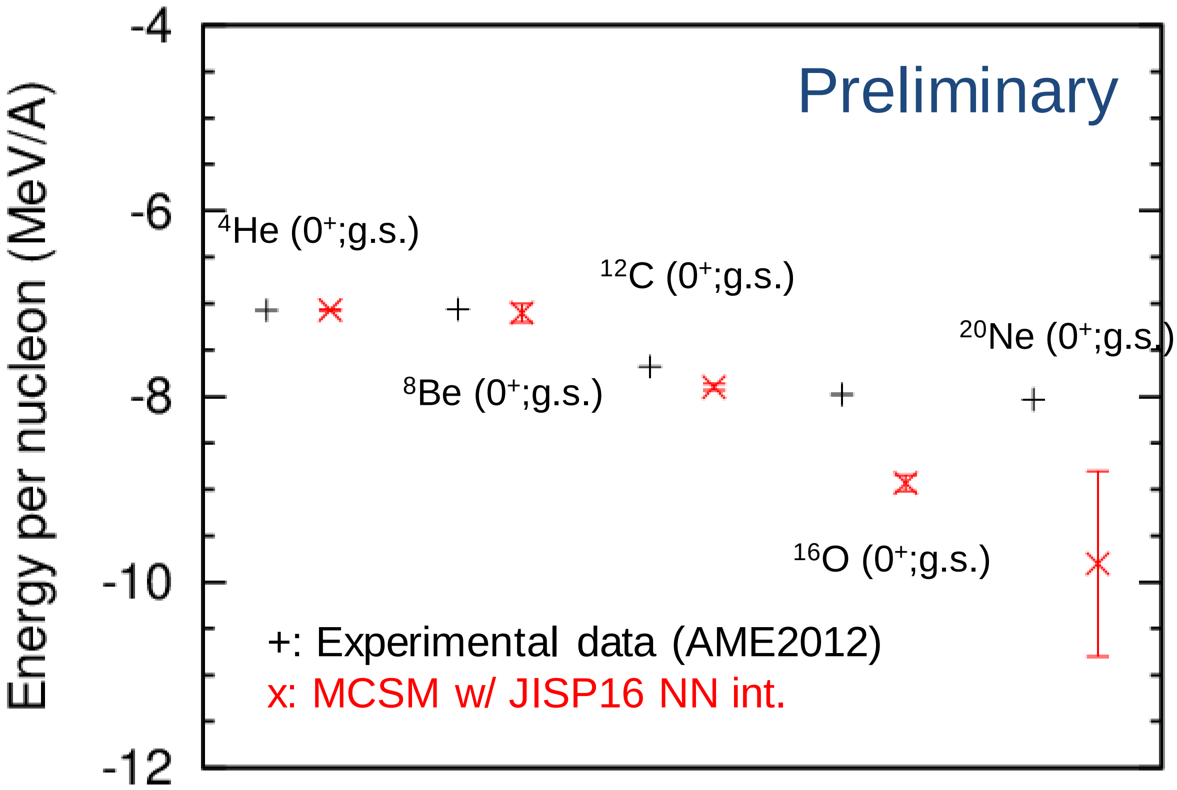




c.f.) NCFC: -29.164(2) MeV

Extrapolated results to infinite N_{max} space

Comparison of MCSM results w/ experiments



JISP16 NN int.
(w/ perturbative Coulomb)

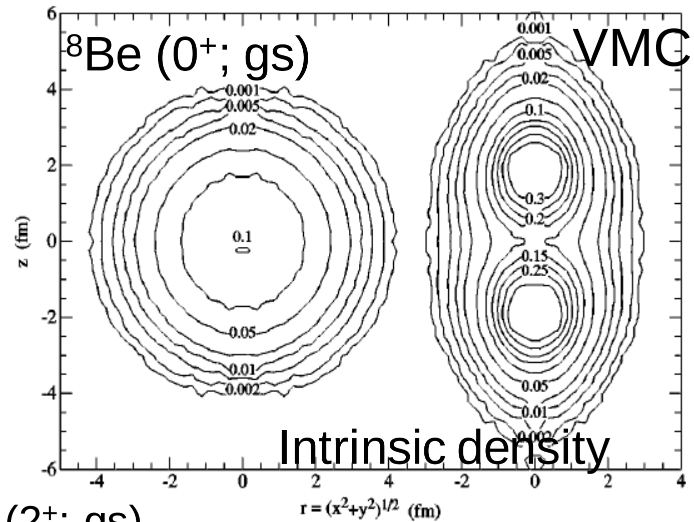
MCSM results are obtained by traditional extrapolation w/ optimum harmonic oscillator energies.
Coulomb interaction is included perturbatively.

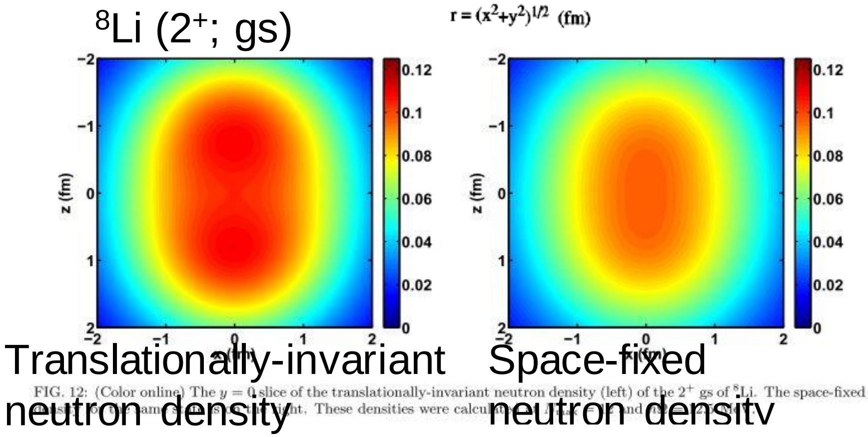
MCSM results show good agreements w/ experimental data up to ^{12}C, slightly overbound for ^{16}O, and clearly overbound for ^{20}Ne.

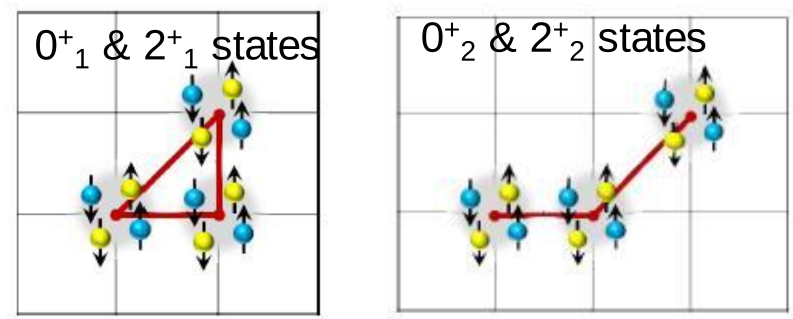
Density distribution from ab initio calc.

- 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 in carbon-12
  E. Epelbaum, H. Krebs, T. A. Lahde,
  D. Lee, & U.-G. Meissner,
  Phys. Rev. Lett. 109, 252501 (2012)
- Fermionic Molecular Dynamics (FMD)

  M. Chernykh, H. Feldmeier, T. Neff, P. von Neumann-Cosel, A Richiter, Phys. Rev. Lett. 98, 032501 (2007)

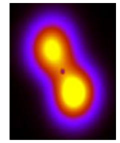
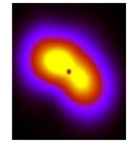
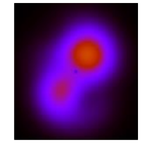
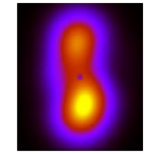






Density distribution in MCSM

T. Yoshida (CNS)

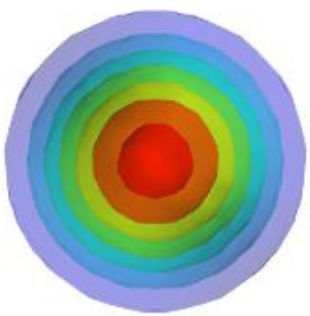
$$|\Phi\rangle = \sum_{i=1}^{N_{basis}} c_i|\Phi_i\rangle = $$ c_1  $+ c_2$  $+ c_3$  $+ c_4$  + …

Angular-momentum projection

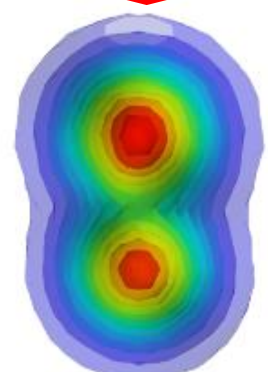
$$|\Psi\rangle = \sum_{i=1}^{N_{basis}} c_i P^J P^\pi |\Phi_i\rangle$$

Rotation of each basis by diagonalizing Q-moment

$$|\Phi'\rangle = \sum_{i=1}^{N_{basis}} c_i R(\Omega_i)|\Phi_i\rangle$$



^{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)

Density distribution of Be isotopes

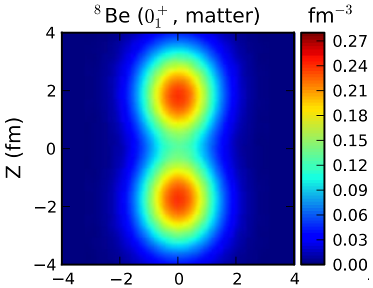
Preliminary

T. Yoshida (CNS)

2-α structure is vanishing as A increases

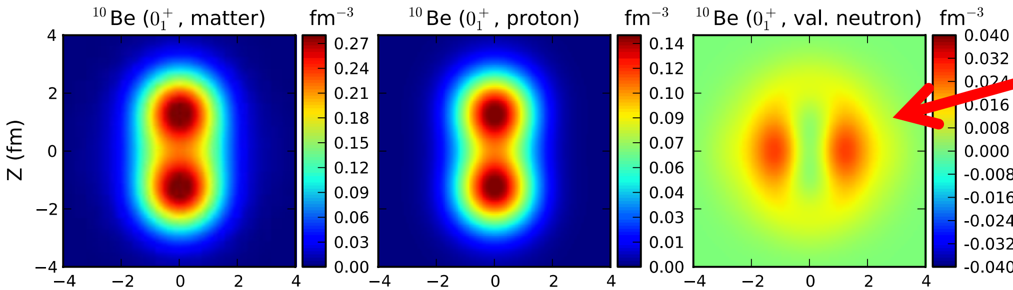
2-α-cluster structure

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

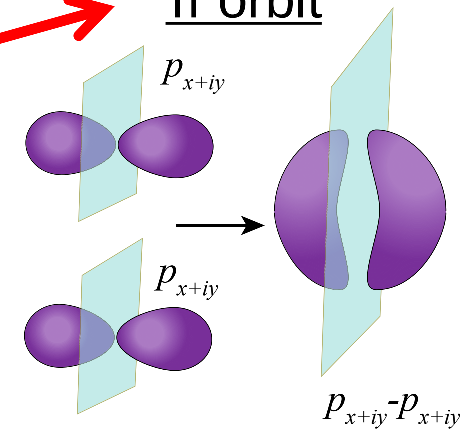


Molecular-orbital states

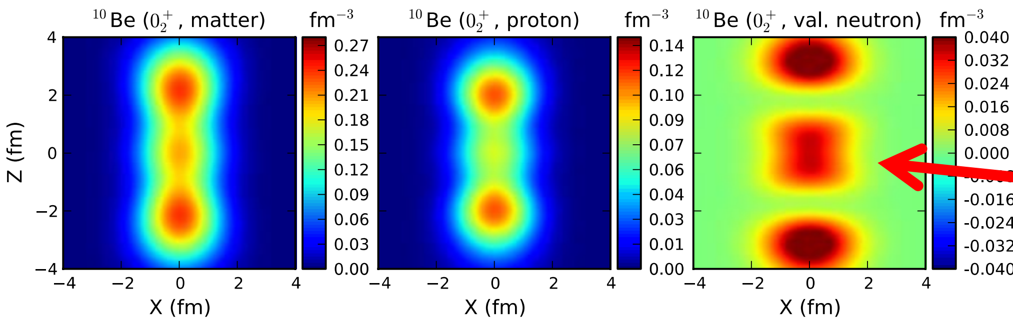
^{10}Be (0$^+$;gs)



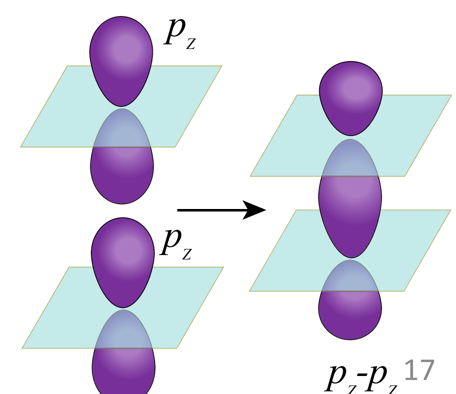
π orbit



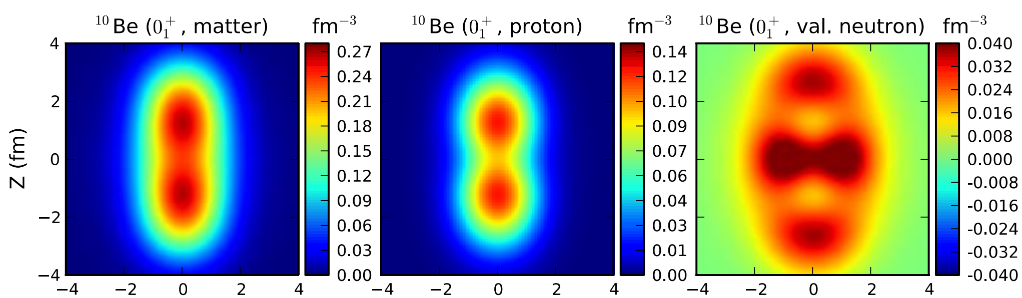
0_2^+



σ orbit



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



Summary

- MCSM results of g.s. energies for light nuclei can be extrapolated to the infinite basis space.
- JISP16 NN interaction gives good agreement w/ experimental data up to ^{12}C, slightly overbound for ^{16}O, and clearly overbound for ^{20}Ne.
- Intrinsic cluster structure of Be isotopes can be visualized using MCSM wave functions.

Perspective

- Extrapolation to the infinite basis space
  - Need better error estimate for the extrapolations
  - Extrapolate other observables (rms radius, …)
  - Test another IR- & UV-cutoff extrapolation scheme
- Physics
  - Study cluster structure of C isotopes (including excited states)