HPCI戦略プログラム分野5「物質と宇宙の起源と構造」全体シンポジウム
素粒子・原子核・宇宙「京からポスト京に向けて」シンポジウム

軽い核におけるモンテカルロ殻模型による第一原理計算の現状

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課題2

実施計画

研究開発課題説明資料より抜粋（一部加工）

	H23	H24	H25	H26	H27
チューニング、アルゴリズム改良	「京」でのチューニング アルゴリズムの改良		アルゴリズムの改良		
軽い核の第一原理計算（質量数 < 30）	4主殻 p殻核		5主殻 核力から媒質補正なしに（軽い）原子核をつくる Beクラスター構造 クラスター構造	sd殻核	6主殻 ^{12}C ホイル状態（宇宙：元素合成）
閉殻芯を仮定した中重核計算（質量数 60 – 150）	1バレンス殻計算 有効相互作用の確立		2バレンス殻 有効相互作用の確立 ⇒ 核力から作る原子核へ向けて rプロセス核（宇宙：元素合成） ^{90}Sr, ^{93}Zr, ^{135}Cs ,..^{130}Te, ^{150}Nd,...（社会：原子力ニーズ）（素粒子：2重ベータ崩壊）		
有効相互作用の構築	広い模型空間での有効相互作用理論		3体力の効果 有効核力による3体力寄与の議論		3体力フル計算

“Ab initio” in low-energy nuclear structure physics

- 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.

- Two main sources of uncertainties:
  - Nuclear forces (interactions btw/among nucleons)
    In principle, they should be obtained (directly) by QCD.
  - Many-body methods
    CI: Finite basis space (choice of basis function and truncation), we have to extrapolate to infinite basis dimensions

Shell model (Configuration Interaction, CI)

- Eigenvalue problem of large sparse Hamiltonian matirx

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

$$\begin{pmatrix} H_{11} & H_{12} & H_{13} & H_{14} & H_{15} & \cdots \\ H_{21} & H_{22} & H_{23} & H_{24} & & \\ H_{31} & H_{32} & H_{33} & & & \\ H_{41} & H_{33} & & \ddots & & \\ H_{51} & & & & & \\ \vdots & & & & & \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \\ \Psi_5 \\ \vdots \end{pmatrix} = \begin{pmatrix} E_1 & & & 0 \\ & E_2 & & \\ & & E_3 & \\ & & & \ddots \\ 0 & & & \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \\ \Psi_5 \\ \vdots \end{pmatrix}$$

Large sparse matrix (in M-scheme)

$\sim \mathcal{O}(10^{10})$

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

$$\begin{cases} |\Psi_1\rangle = a^\dagger_\alpha a^\dagger_\beta a^\dagger_\gamma \cdots |-\rangle \\ |\Psi_2\rangle = a^\dagger_{\alpha'} a^\dagger_{\beta'} a^\dagger_{\gamma'} \cdots |-\rangle \\ |\Psi_3\rangle = \cdots \\ \vdots \end{cases}$$

Monte Carlo shell model (MCSM)

- Importance truncation

Standard shell model

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

All Slater determinants

d > O(10^{10})

Monte Carlo shell model

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

Important bases stochastically selected

d_{MCSM} ~ 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)

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

- Eigenvalue problem

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

- MCSM many-body wave function & basis function

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

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)

Recent developments in the MCSM

- Energy minimization by the CG method
  - N. Shimizu, Y. Utsuno, T. Mizusaki, M. Honma, Y. Tsunoda & T. Otsuka, Phys. Rev. C85, 054301 (2012)

~ 30% reduction of # basis

- Efficient computation of TBMEs
  - Y. Utsuno, N. Shimizu, T. Otsuka & T. Abe, Compt. Phys. Comm. 184, 102 (2013)

~ 80% of the peack performance

(~ 10-20% in the old MCSM)

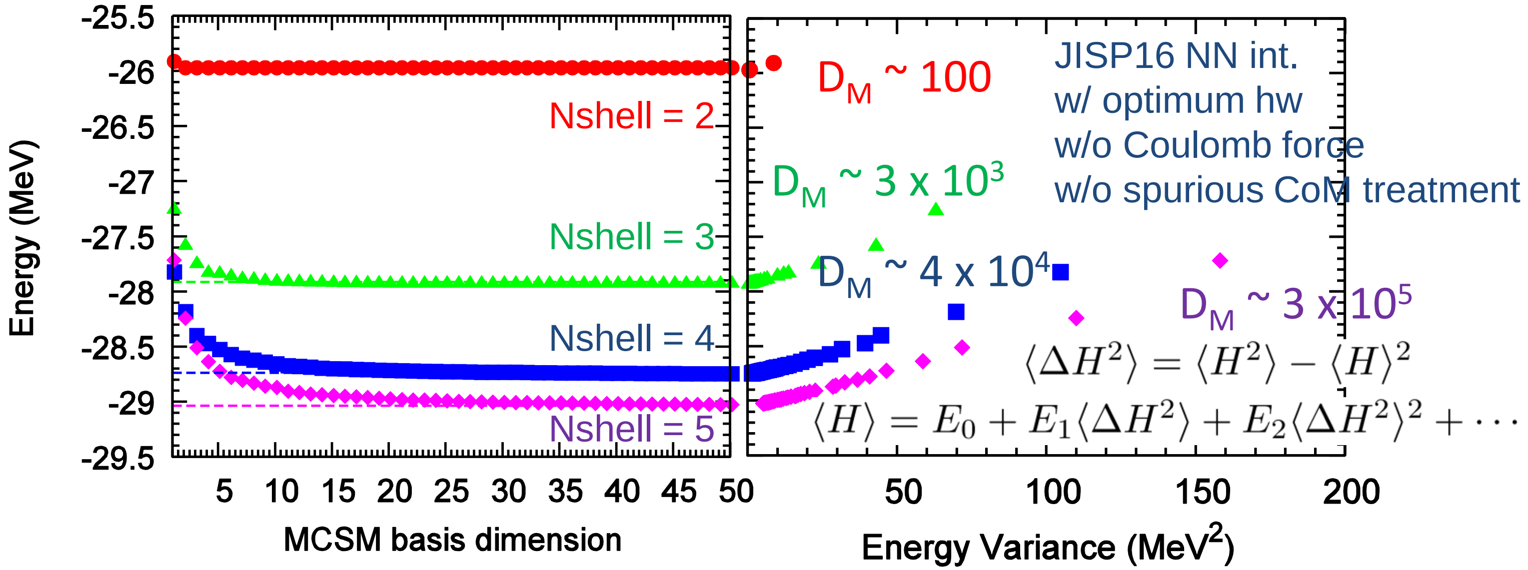
- Energy variance extrapolation
  - N. Shimizu, Y. Utsuno, T. Mizusaki, T. Otsuka, T. Abe & M. Honma, Phys. Rev. C82, 061305 (2010)

Evaluation of exact eignvalue w/ error estimate

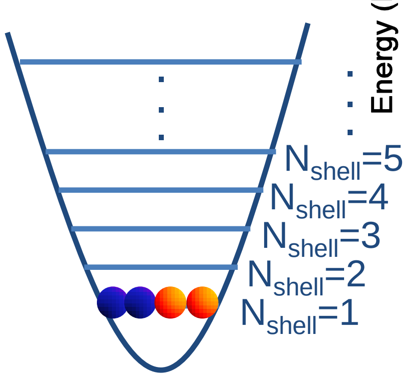
- Summary of recent MCSM developments
  - N. Shimizu, T. Abe, Y. Tsunoda, Y. Utsuno, T. Yoshida, T. Mizusaki, M. Honma, T. Otsuka, Prog. Theor. Exp. Phys. 01A205 (2012)

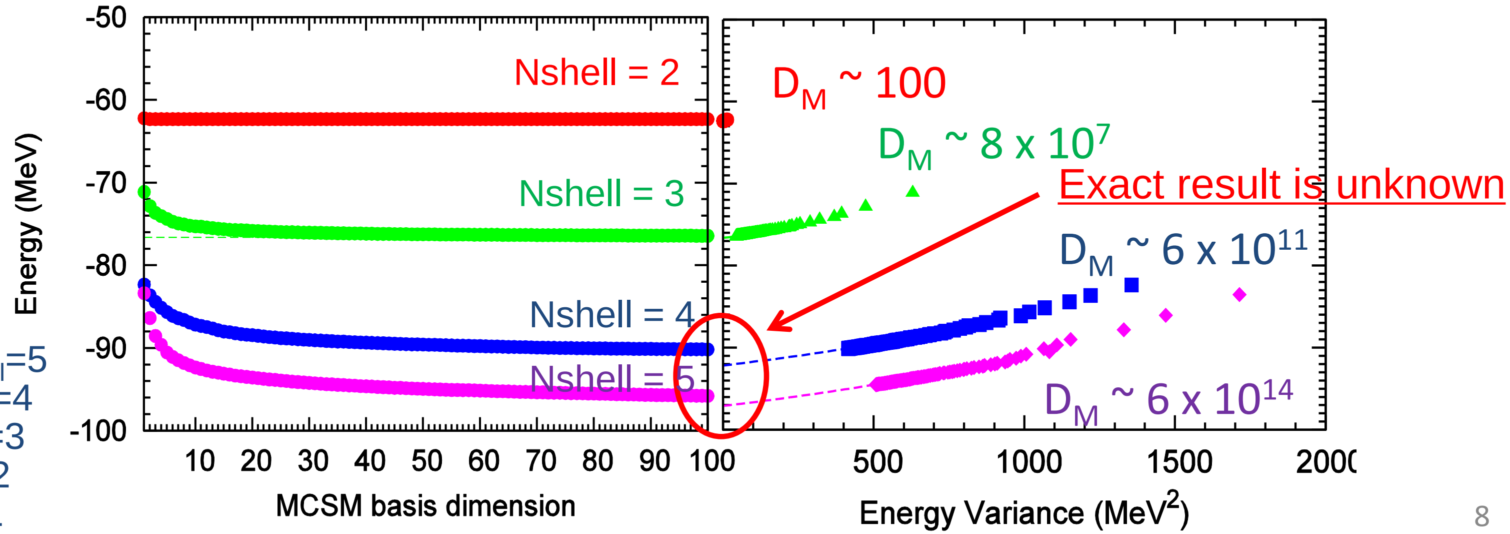
Energies wrt # of basis & energy variance

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

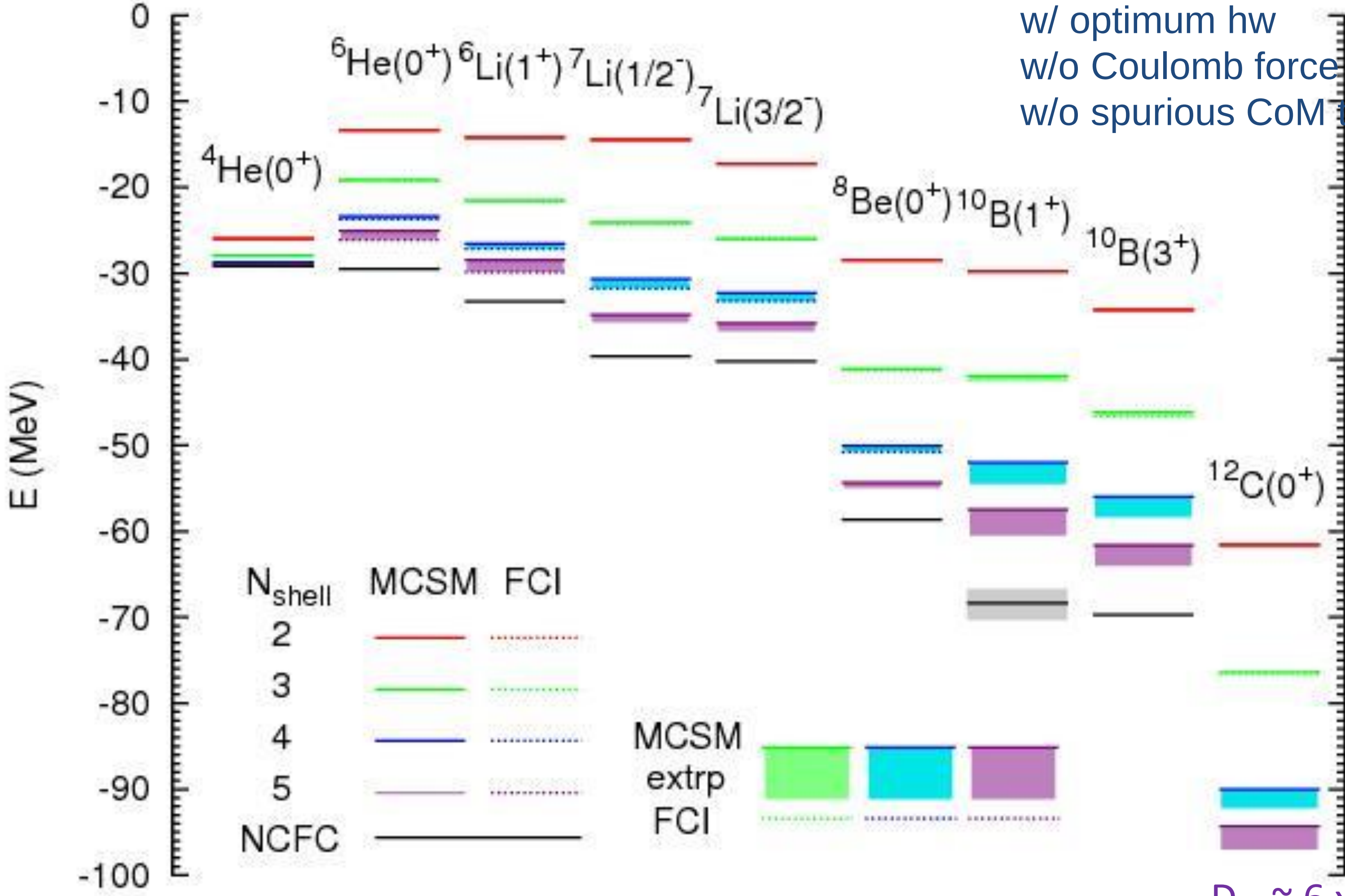


^{12}C(0$^+$;gs)





Energies of the Light Nuclei



JISP16 NN int.
w/ optimum hw
w/o Coulomb force
w/o spurious CoM treatment

$D_M \sim 6 \times 10^{14}$

Some MCSM results are not reachable in the current FCI

Extrapolations in the no-core MCSM

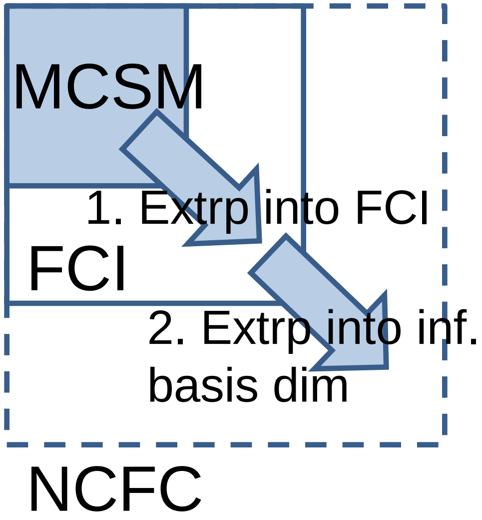
- Two steps of the extrapolation

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

   Energy-variance extrapolation

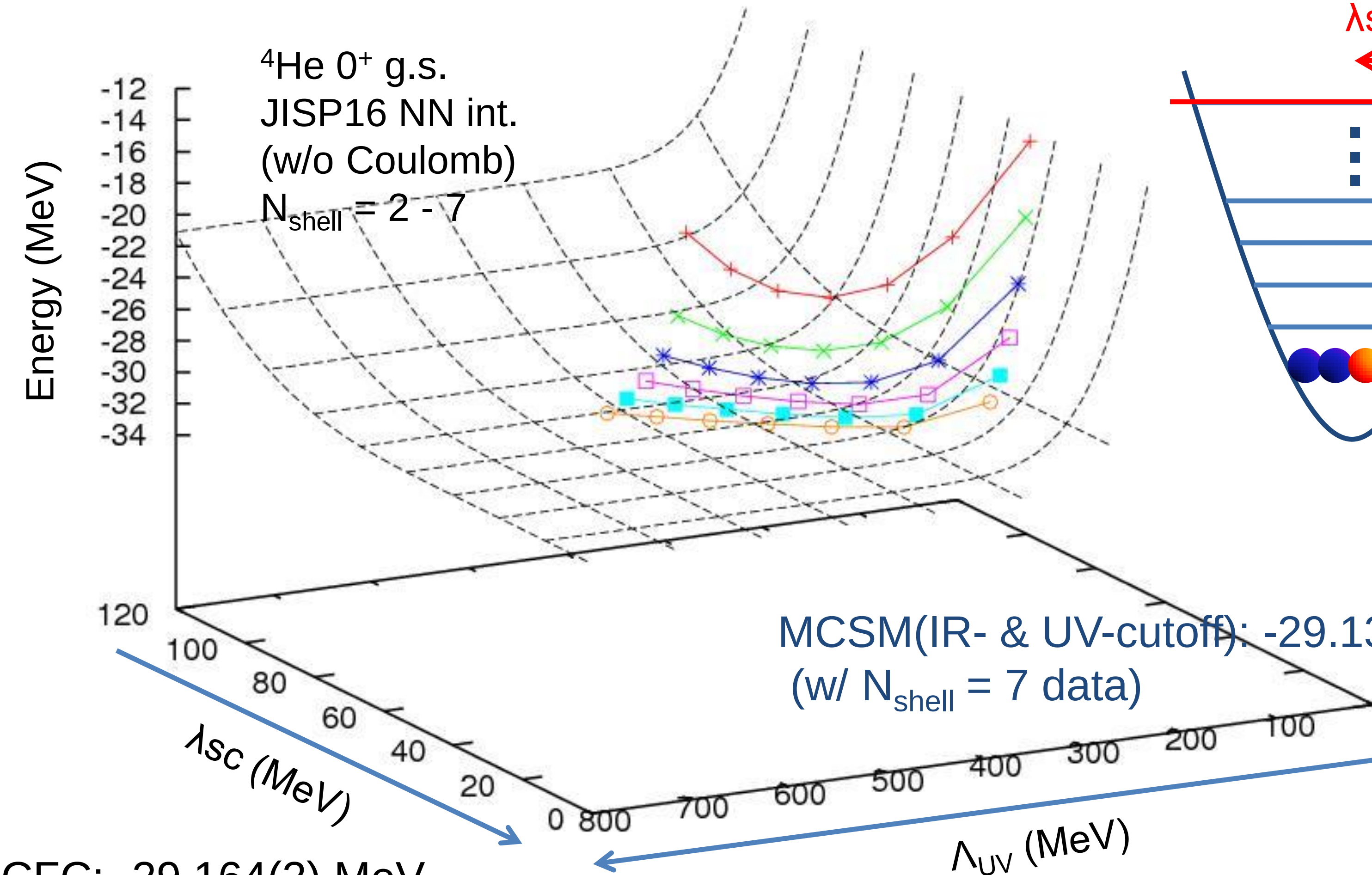
N. Shimizu, Y. Utsuno, T. Mizusaki, T. Otsuka, T. Abe, & M. Honma, Phys. Rev. C82, 061305(R) (2010)

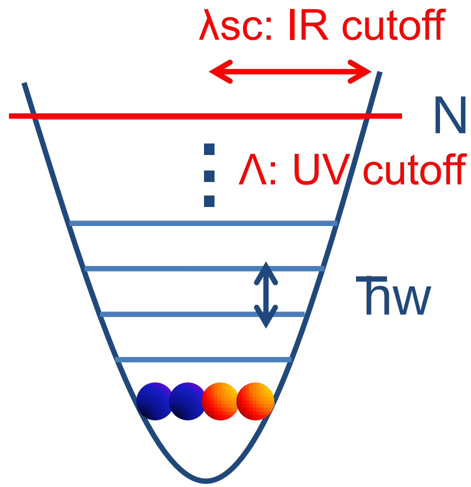
2. Extrapolation into the infinite model space
   - Exponential fit w.r.t. N_{max} in the NCFC
   - IR- & UV-cutoff extrapolations



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}

on going: ^{8}Be, ^{12}C, ^{16}O, …

Effective 2N force from 3N force

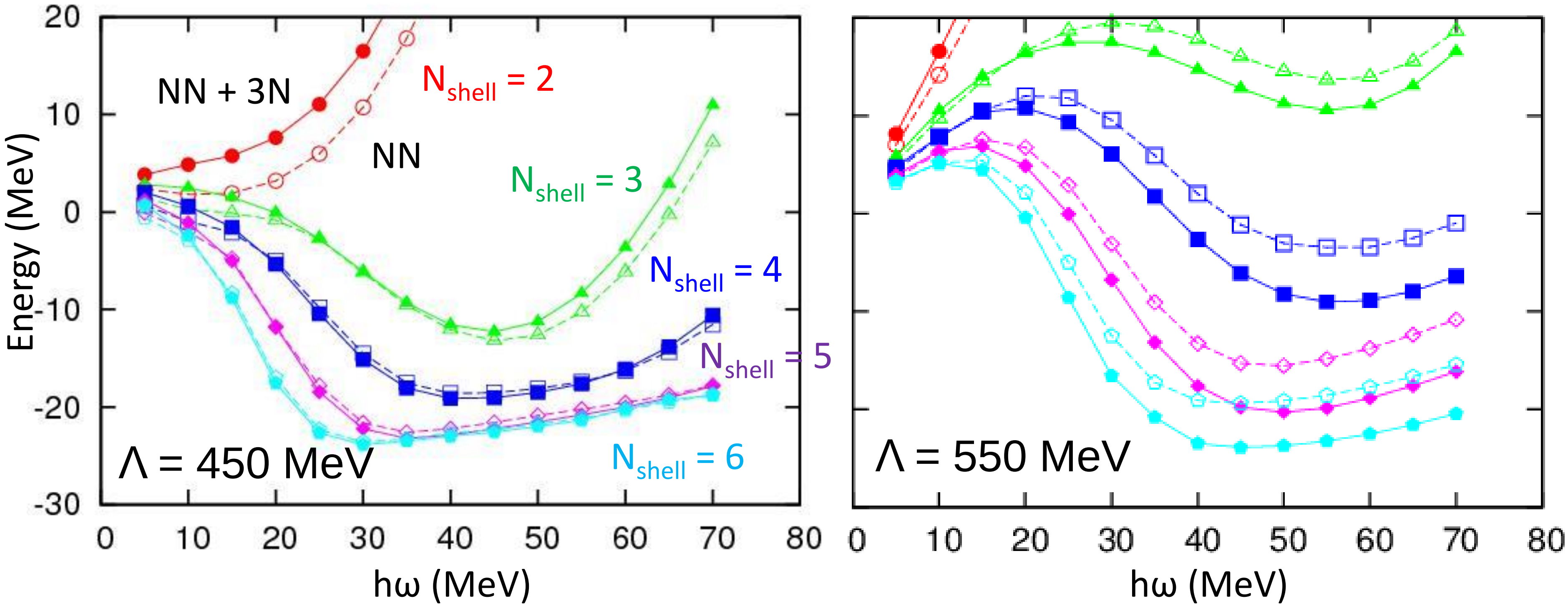
^{4}He 0^+ g.s. energy calculated by FCI & no-core MCSM w/ χEFT N3LO NN (+ "N2LO 3N") potential

Effective 2N potential from initial 3N potential in momentum space

$$\langle k_1', k_2'|V_{12(3)}|k_1, k_2\rangle_A \equiv \sum_{k_3} \langle k_1', k_2', k_3|V_{123}|k_1, k_2, k_3\rangle_A,$$

A: antisymmetrized matrix element

$$\frac{1}{2}\sum_{k_1 k_2}\langle k_1 k_2|V_{12}|k_1 k_2\rangle_A + \frac{1}{3!}\sum_{k_1 k_2 k_3}\langle k_1 k_2 k_3|V_{123}|k_1 k_2 k_3\rangle_A$$
$$= \frac{1}{2}\sum_{k_1 k_2}\langle k_1 k_2|V_{12} + \frac{1}{3}V_{12(3)}|k_1 k_2\rangle_A.$$



Energies with 3NF in the different cutoff scales are consistent in a sufficiently large basis space

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)

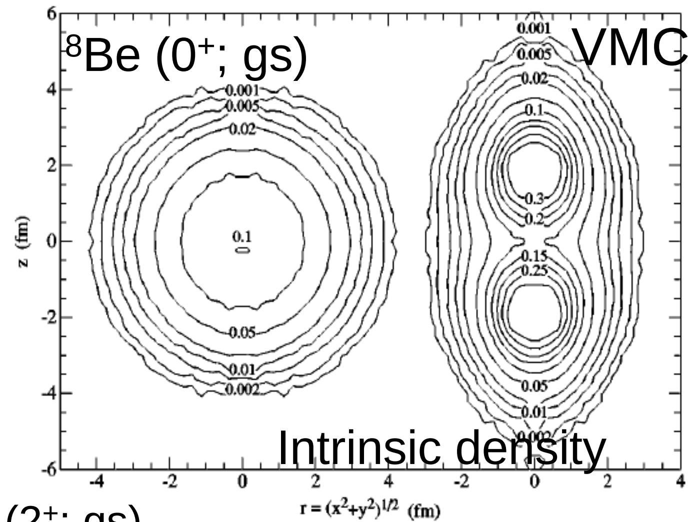
- Lattice EFT

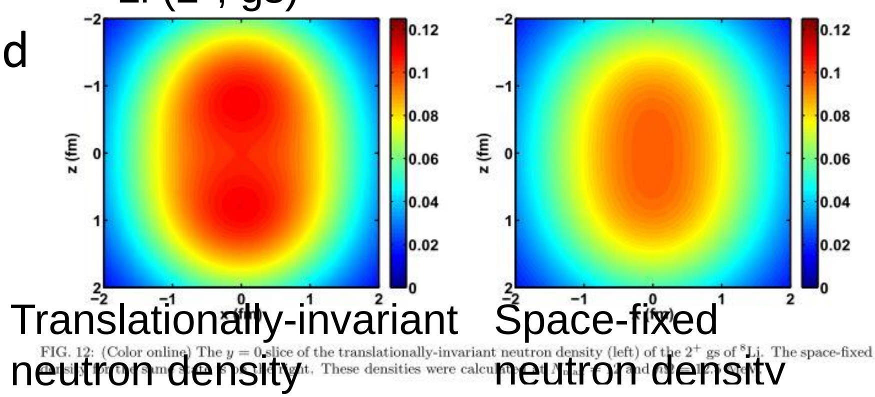
  - Triangle structure in carbon-12

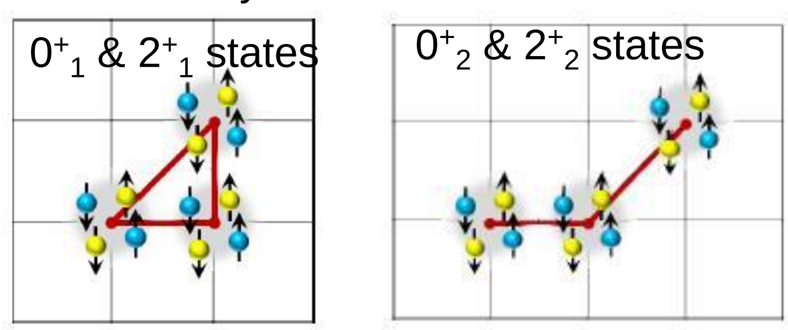
  E. Epelbaum, H. Krebs, T. A. Lahde,

  D. Lee, & U.-G. Meissner,

  Phys. Rev. Lett. 109, 252501 (2012)

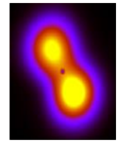
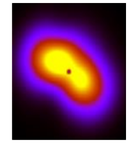
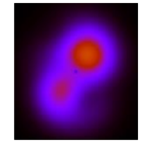
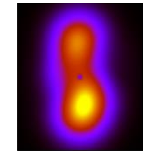






Density distribution in MCSM

T. Yoshida (CNS)

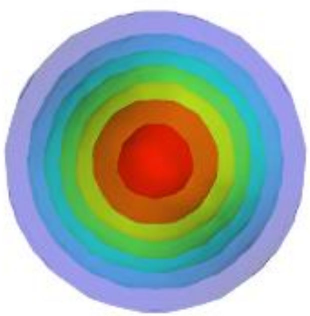
$$|\Phi\rangle = \sum_{i=1}^{N_{basis}} c_i |\Phi_i\rangle = $$ c_1  $+ c_2$  $+ c_3$  $+ c_4$  + …

Angular-momentum projection

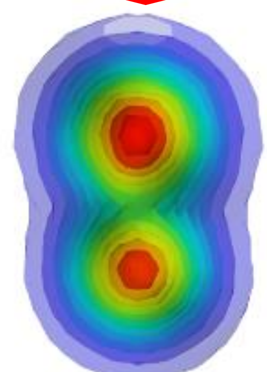
$$|\Psi\rangle = \sum_{i=1}^{N_{basis}} c_i P^J P^\pi |\Phi_i\rangle$$

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

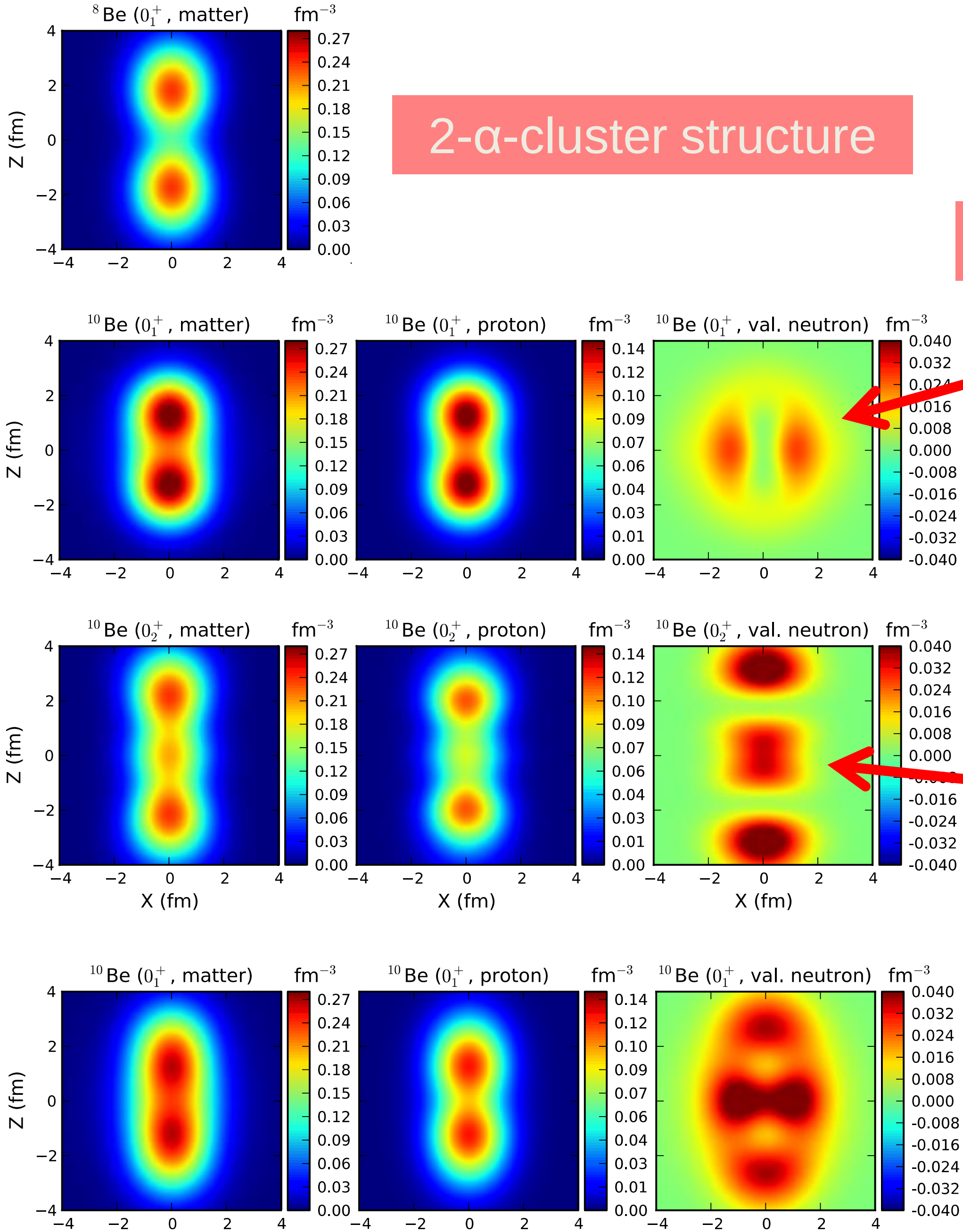
Molecular-orbital states

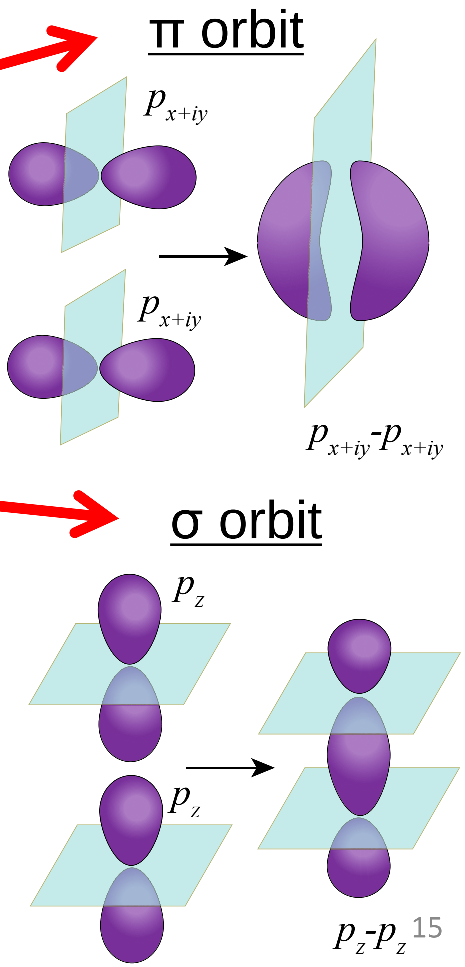
^{8}Be (0^+;gs)

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

0_2^+

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





Summary

- MCSM can be applied to no-core calculations of the p-shell nuclei.

  - Extension to larger basis spaces (N_{shell} = 6, 7, …), extrapolation to infinite basis space, & comparison with another truncation (N_{max})

  - Test calculation of the no-core MCSM with the effective two-body force from the chiral EFT N2LO three-body force

  - Density distributions in the Be isotopes; appearance of alpha clusters & molecular-orbital states

Perspective

- MCSM algorithm/computation

  - Error estimates of the extrapolations

  - Inclusion of the full 3-body force

  Physics

  - sd-shell nuclei

  - alpha-cluster & molecular-orbital states in the p-shell nuclei

Collaborators

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- JAEA
  - Yutaka Utsuno
- Iowa State U
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  - Pieter Maris
- Kyushu Institute of Technology
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- RCNP, Osaka U
  - Michio Kohno