TRIUMF Theory Workshop (Feb. 17 – 20, 2015)
Progress in Ab Initio Techniques in Nuclear Physics

Progress in the no-core Monte Carlo shell model in light nuclei

Takashi Abe (U of Tokyo)

TRIUMF

Feb. 17 – 20, 2015

Ab inito approaches

- Major challenge of nuclear physics

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

  - *ab-initio* approaches in nuclear structure physics (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 (Louisiana State U), …
- No-Core Monte Carlo Shell Model (MCSM)

Shell model (Configuration Interaction, CI)

- Eigenvalue problem of large sparse Hamiltonian matirx

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

$$\underbrace{\begin{pmatrix} H_{11} & H_{12} & H_{13} & H_{14} & H_{15} & \cdots \\ H_{21} & H_{22} & H_{23} & H_{24} & & \\ H_{31} & H_{32} & H_{33} & & & \\ H_{41} & H_{33} & & \ddots & & \\ H_{51} & & & & & \\ \vdots & & & & & \end{pmatrix}}_{\text{Large sparse matrix (in M-scheme)}} \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \\ \Psi_5 \\ \vdots \end{pmatrix} = \begin{pmatrix} E_1 & & & & 0 \\ & E_2 & & & \\ & & E_3 & & \\ & & & \ddots & \\ 0 & & & & \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \\ \Psi_5 \\ \vdots \end{pmatrix}$$

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

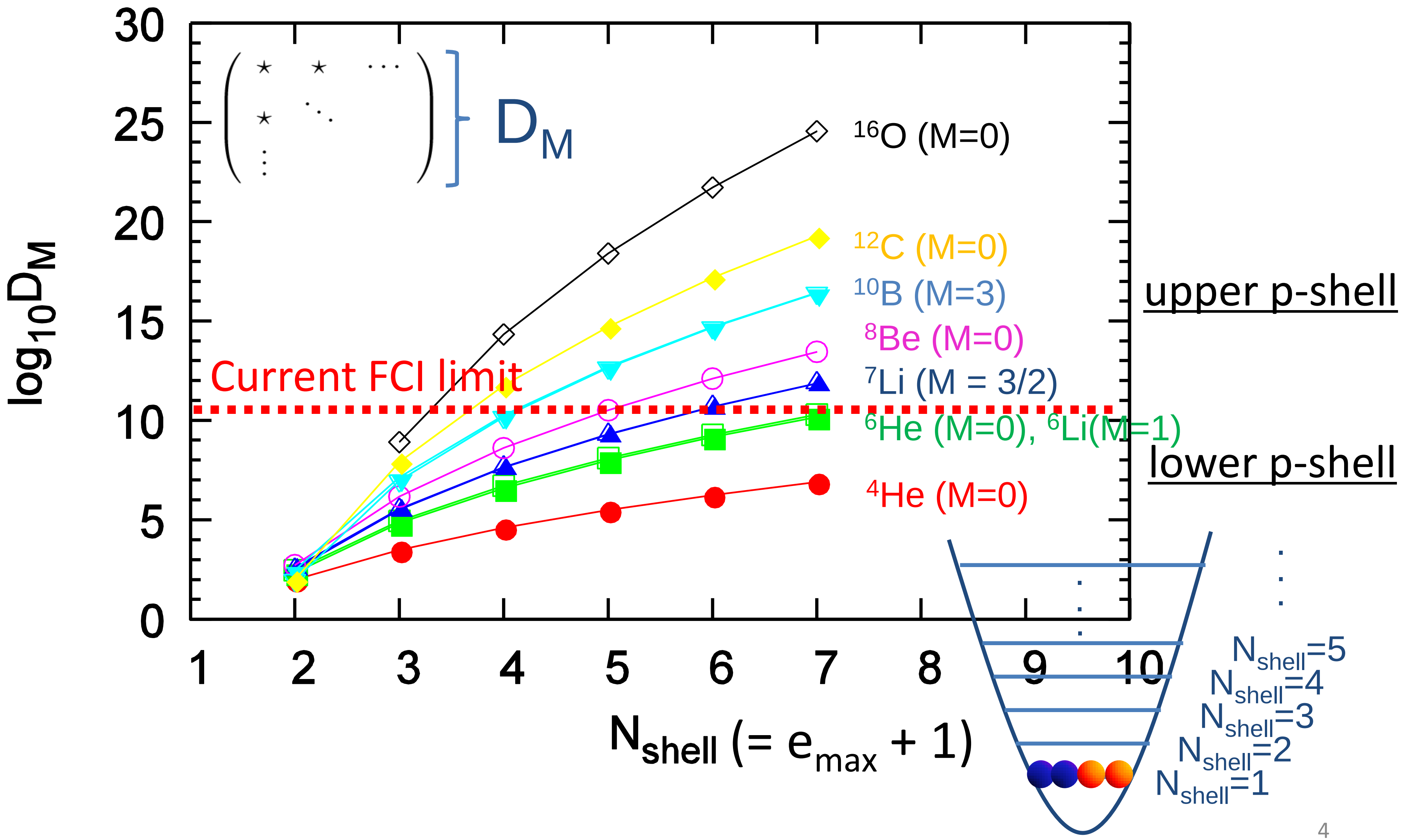
non-zero MEs

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

$$\left\{ \begin{array}{lcl} |\Psi_1\rangle & = & a^\dagger_\alpha a^\dagger_\beta a^\dagger_\gamma \cdots |-\rangle \\ |\Psi_2\rangle & = & a^\dagger_{\alpha'} a^\dagger_{\beta'} a^\dagger_{\gamma'} \cdots |-\rangle \\ |\Psi_3\rangle & = & \cdots \\ & \vdots & \end{array} \right.$$

M-scheme dimension in N_{shell} truncation

No-core calculations



Monte Carlo shell model (MCSM)

- Importance truncation

Standard shell model

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

All Slater determinants

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

Monte Carlo shell model

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

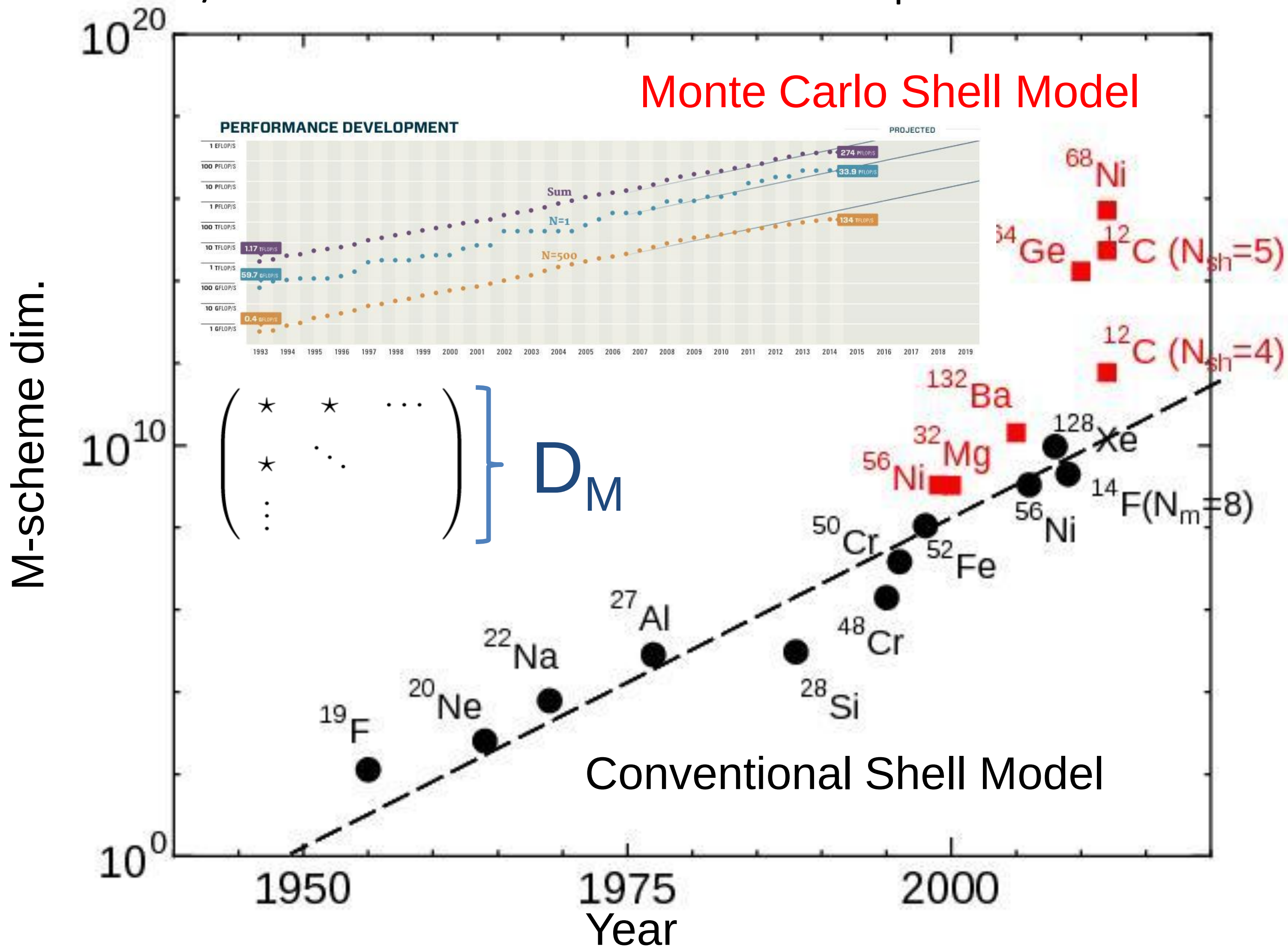
Important bases stochastically selected

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

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

Historical evolution/development of the MCSM

- MCSM w/ an assumed inert core is one of the powerful shell model algorithms.



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.

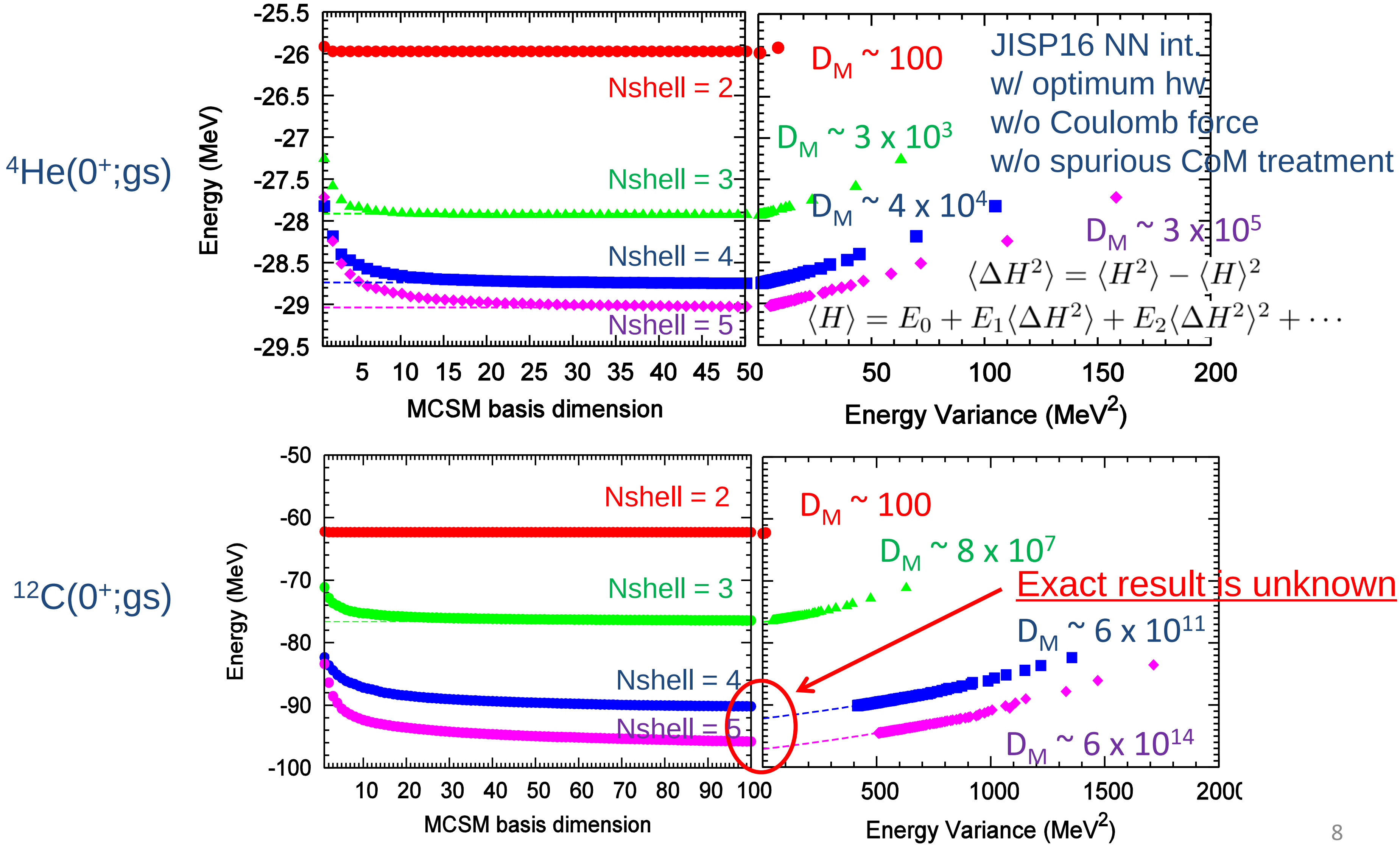
- Deformed SDs

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



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)

TOP500 JUNE 2013

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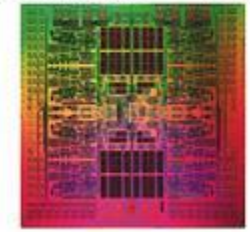
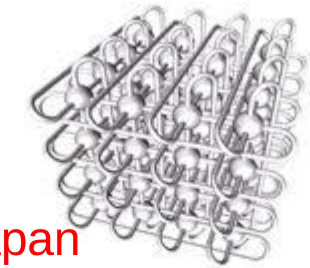
	NAME	SPECS	SITE	COUNTRY	CORES	R_{MAX} PFLOP/S	POWER MW
1	Tianhe-2 (Milkyway-2)	NUDT, Intel Ivy Bridge (12C, 2.2 GHz) & Xeon Phi (57C, 1.1 GHz), Custom interconnect	NUDT	China	3,120,000	33.9	17.8
2	Titan	Cray XK7, Opteron 6274 (16C, 2.2 GHz) + Nvidia Kepler (14C, .732 GHz), Custom interconnect	DOE/SC/ORNL	USA	560,640	17.6	8.3
3	Sequoia	IBM BlueGene/Q, Power BQC (16C, 1.60 GHz), Custom interconnect	DOE/NNSA/LLNL	USA	1,572,864	17.2	7.9
4	K computer	Fujitsu SPARC64 VIIIfx (8C, 2.0GHz), Custom interconnect	RIKEN AICS	Japan	705,024	10.5	12.7
5	Mira	IBM BlueGene/Q, Power BQC (16C, 1.60 GHz), Custom interconnect	DOE/SC/ANL	USA	786,432	8.16	3.95

SPARC64 TM VIIIfx

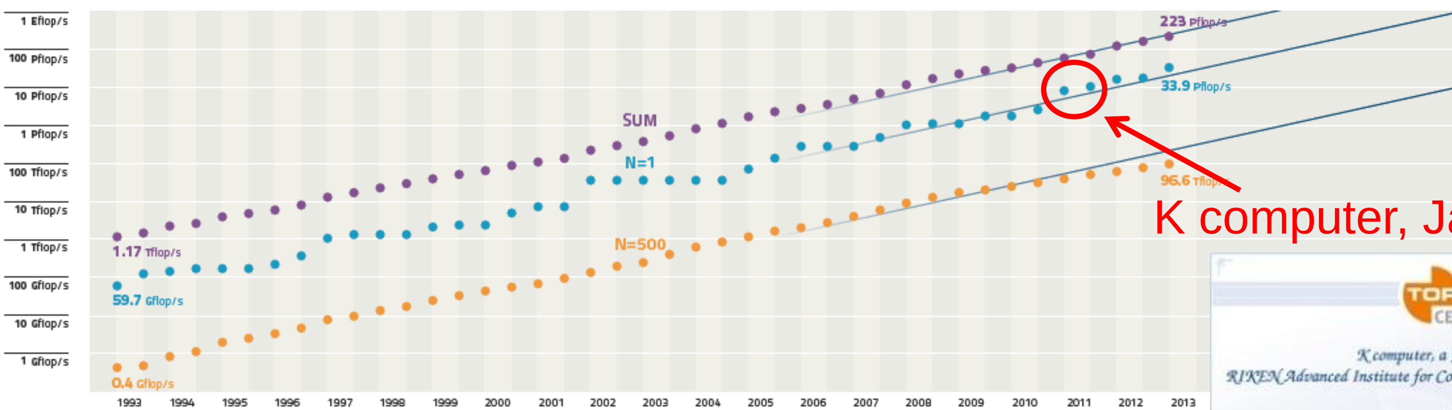


128 GFLOPS/CPU
(8 cores/CPU)

Tofu inter-connection
6D Mesh/Torus



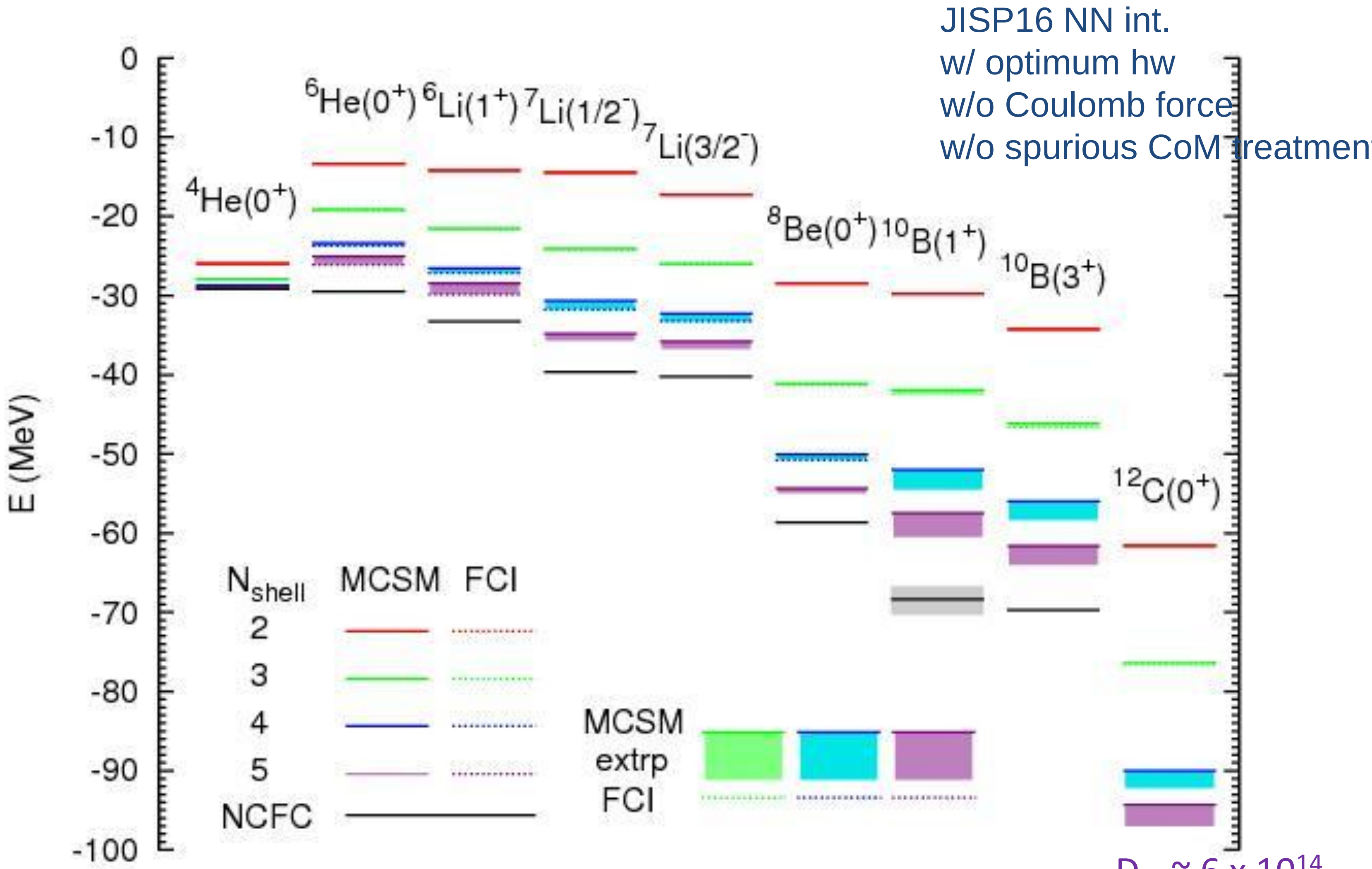
PERFORMANCE DEVELOPMENT



K computer, Japan

HPCI Strategic Program Field 5
"The origin of matter and the universe"

Energies of the Light Nuclei



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

Some MCSM results are not reachable in the current FCI

Extrapolations in the no-core MCSM

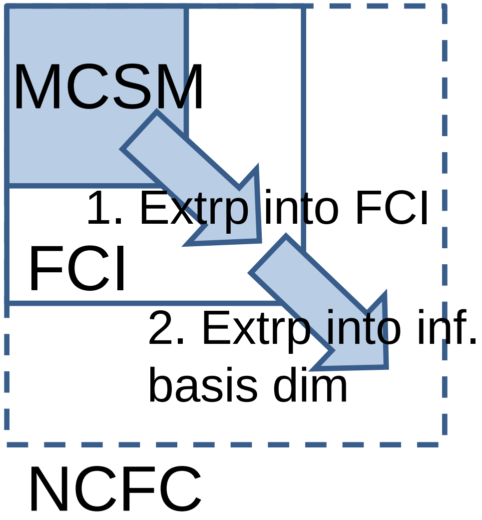
- Two steps of the extrapolation

  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



Extrapolation to the infinite basis space

- Two ways of the extrapolation to the infinite basis space

1. Traditional exponential form (w/ fixed hw)

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

P. Maris, A. M. Shirokov, & J. P. Vary, Phys. Rev. C79, 014308 (2009)

2. Cutoff extrapolations

(N, hw) <-> (λ, Λ)

- IR-cutoff extrapolation (w/ UV-saturated data)

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

- IR- & UV-cutoff extrapolations (w/ any data, ideally)

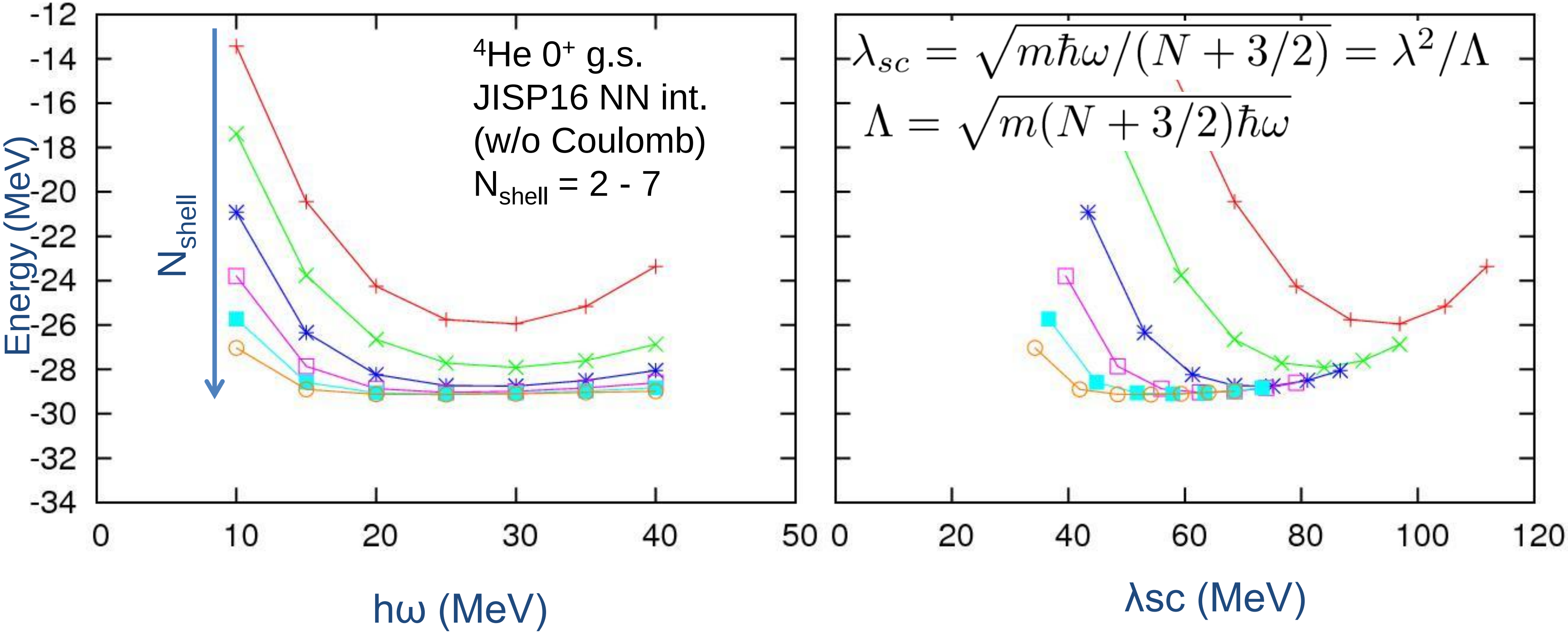
$$E(\lambda, \Lambda) = E(\lambda = 0, \Lambda = \infty) + a\exp(-b/\lambda) + c\exp(-\Lambda^2/d^2)$$

S. A. Coon, M. I. Avetian, M. K. G. Kruse, U. van Kolck, P. Maris, J. P. Vary, Phys. Rev. C86, 054002 (2012)
S. A. Coon, arXiv:1303.6358
S. A. Coon, arXiv:1408.0738

R. J. Furnstahl, G, Hagen, T. Papenbrock, Phys. Rev. C86, 031301(R) (2012)
S. N. More, A. Ekstrom, R. J. Furnstahl, G. Hagen, T. Papenbrock, Phys. Rev. C87, 044326 (2013)
R. J. Furnstahl, S. N. More, T. Papenbrock, arXiv:1312.6876
R. J. Furnstahl, G. Hagen, T. Papenbrock, K. A. Wendt, arXiv:1408.0252

E. D. Jurgenson, P. Maris, R. J. Furnstahl, W. E. Ormand & J. P. Vary, Phys. Rev. C87, 054312 (2013)

Traditional & IR-cutoff extrapolations

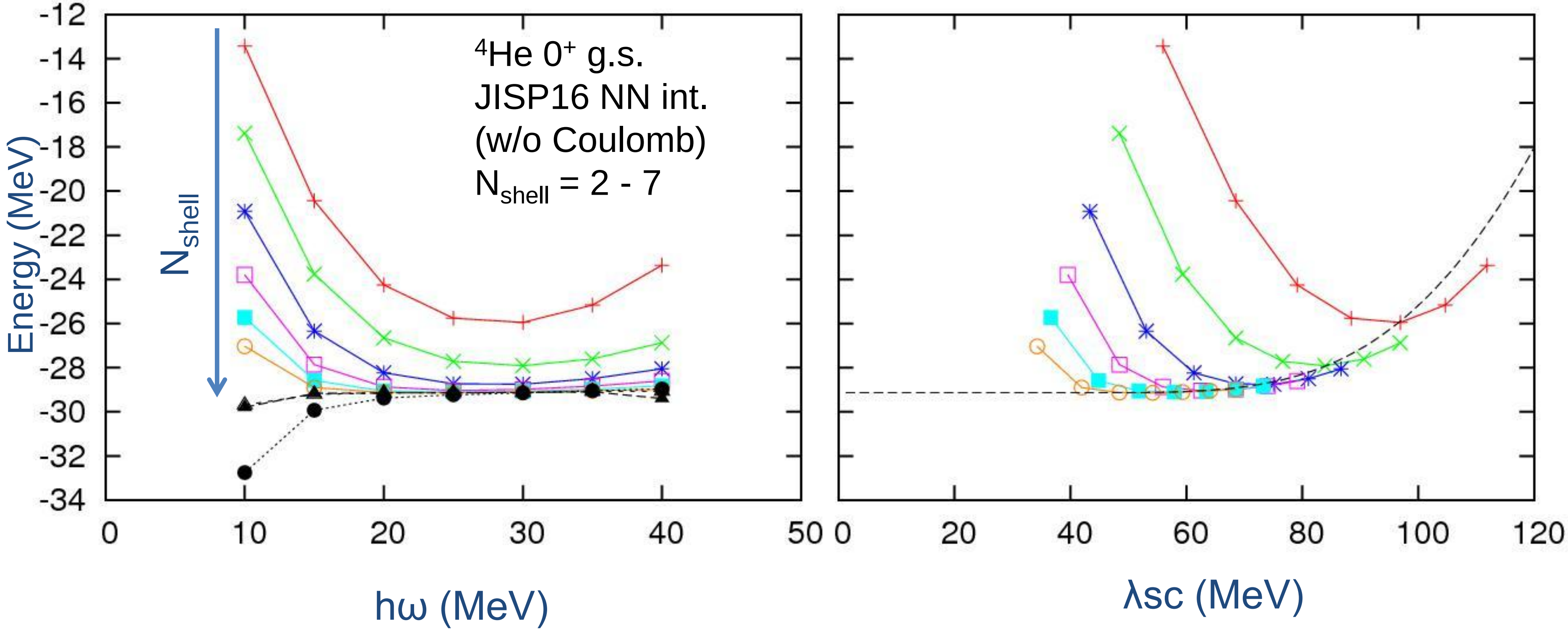


$(N_{shell}, h\omega)$ ⟷ $(\Lambda, \lambda sc)$

Λ: UV cutoff   λsc: IR cutoff

IR cutoff scaling w/ UV saturated data

Traditional & IR-cutoff extrapolations



MCSM(traditional): -29.389 ~ -29.077 MeV
(Nshell = 3 - 7, hw = 15 - 35 MeV)

O(100) keV error?

MCSM(IR cutoff): ~ -29.142 MeV
(w/ UV-saturated data)

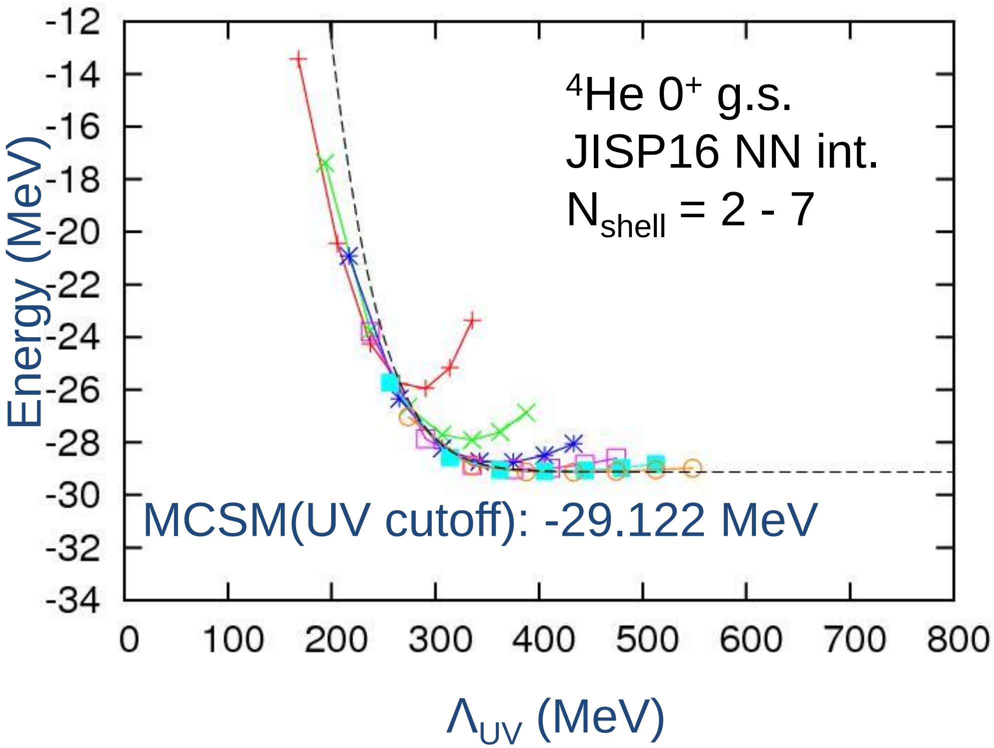
O(10) keV error?

Error estimates are needed.

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

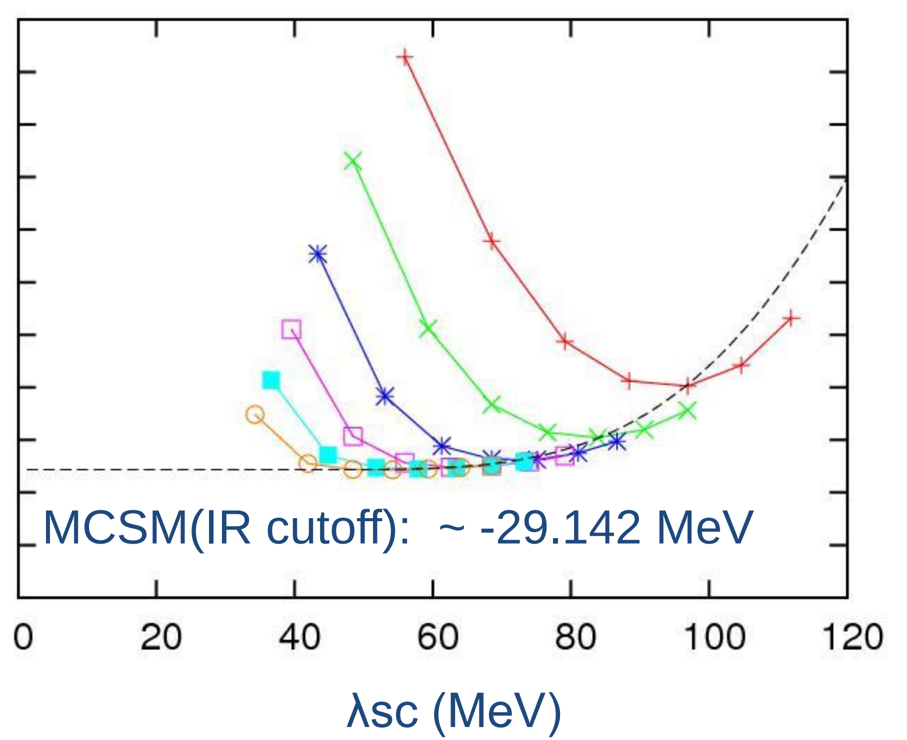
UV-cutoff extrapolation

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



IR-cutoff extrapolation

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



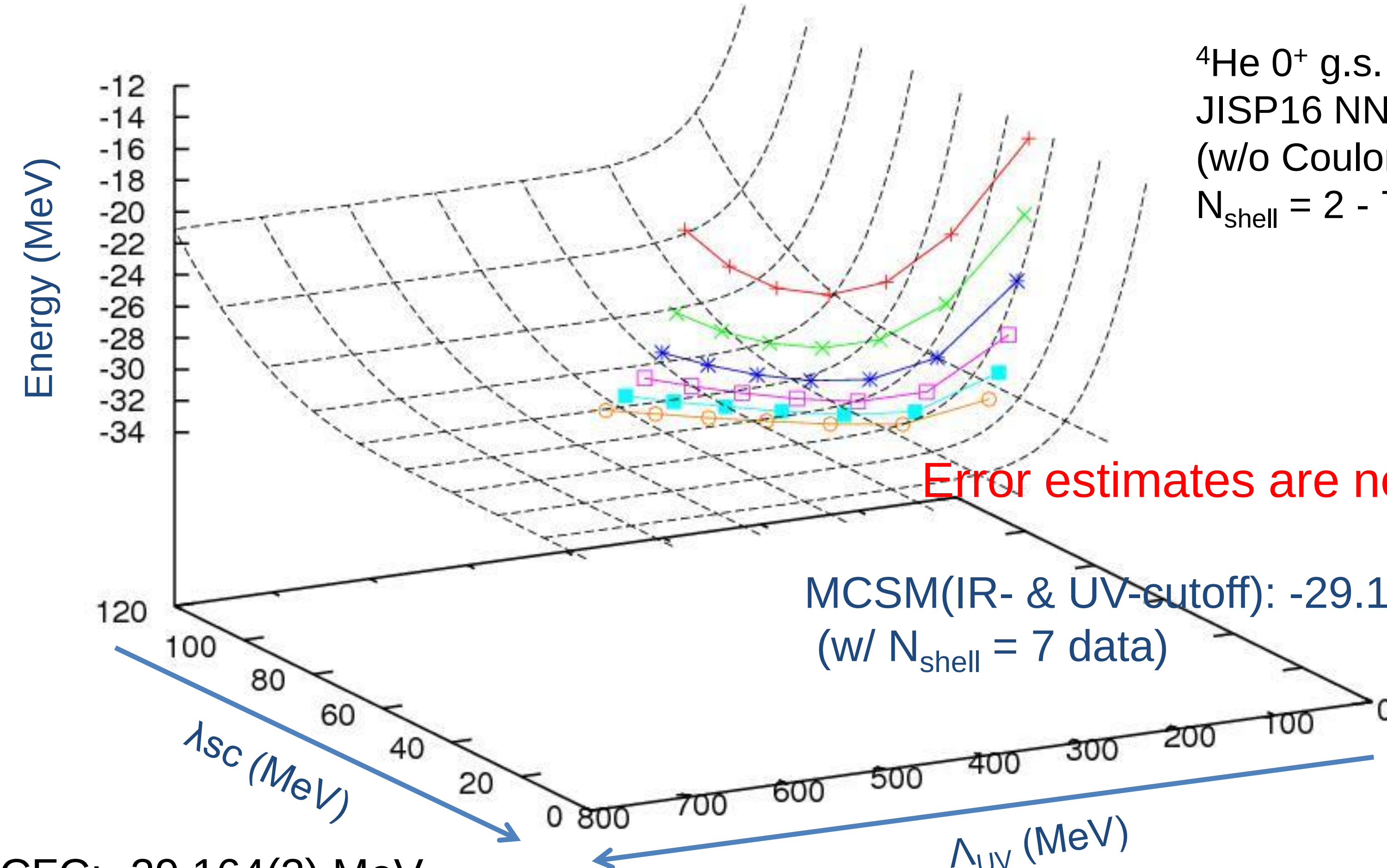
c.f.) NCFC: -29.164(2) MeV

Extrapolated results to infinite N_{max}

on going: ^{8}Be, ^{12}C, ^{16}O, …

IR- & UV-cutoff extrapolation

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



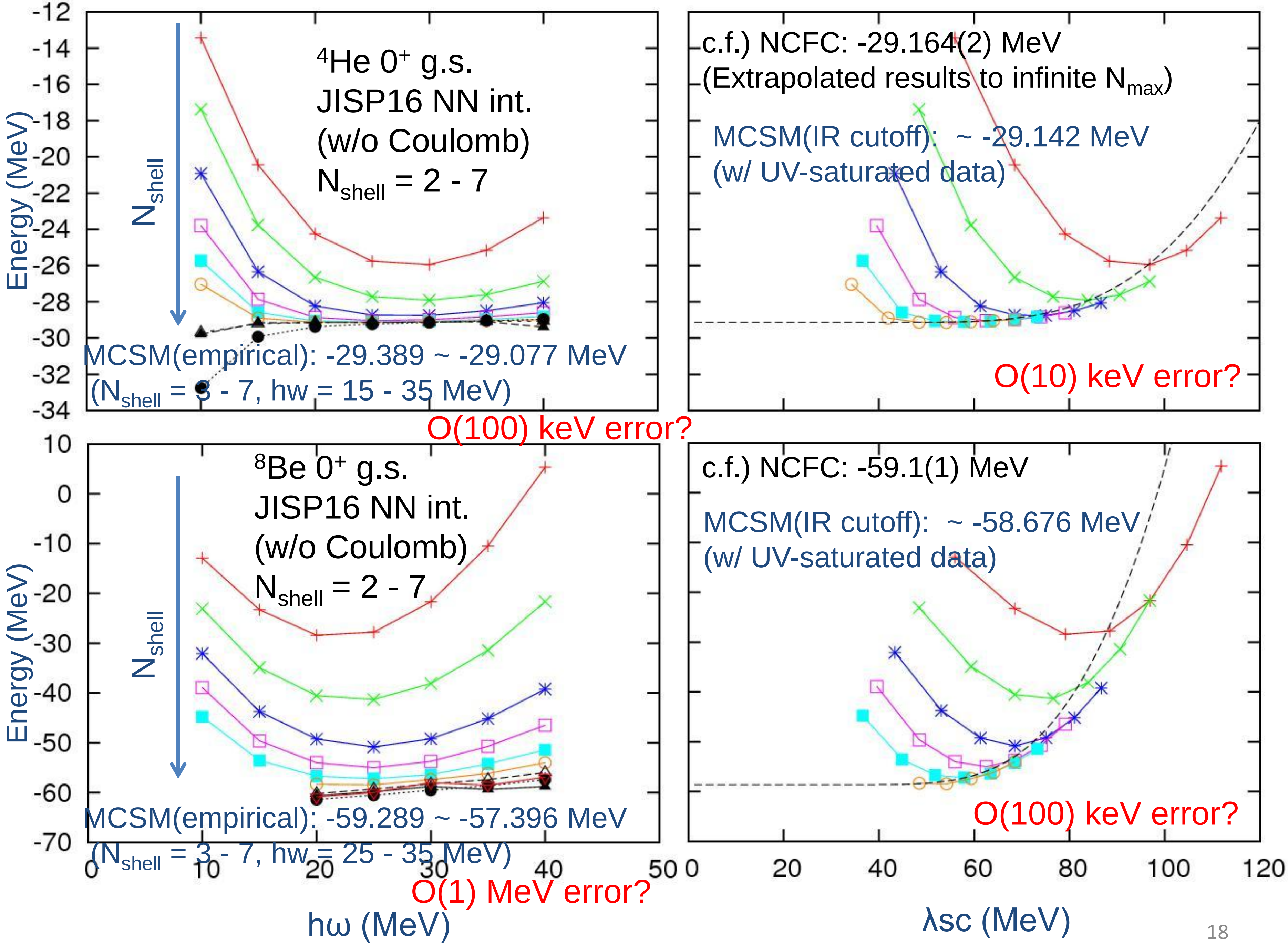
^{4}He 0^+ g.s.
JISP16 NN int.
(w/o Coulomb)
N_{shell} = 2 - 7

Error estimates are needed.

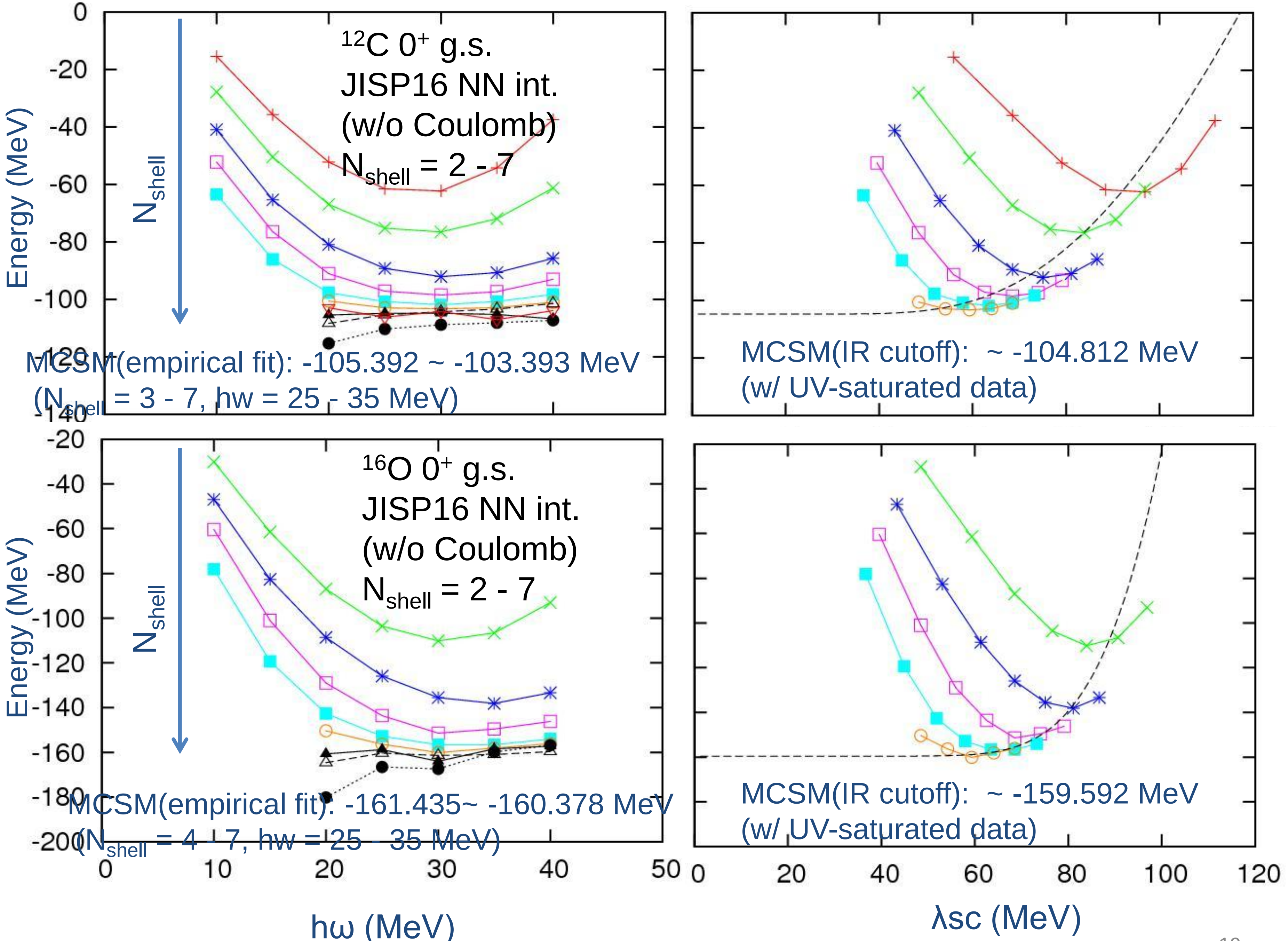
MCSM(IR- & UV-cutoff): -29.139 MeV
(w/ N_{shell} = 7 data)

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

on going: ^{8}Be, ^{12}C, ^{16}O, …



⁴He 0⁺ g.s.
JISP16 NN int.
(w/o Coulomb)
N_shell = 2 - 7
N_shell
MCSM(empirical): -29.389 ~ -29.077 MeV
(N_shell = 3 - 7, hw = 15 - 35 MeV)
O(100) keV error?
c.f.) NCFC: -29.164(2) MeV
(Extrapolated results to infinite N_max)
MCSM(IR cutoff): ~ -29.142 MeV
(w/ UV-saturated data)
O(10) keV error?
⁸Be 0⁺ g.s.
JISP16 NN int.
(w/o Coulomb)
N_shell = 2 - 7
MCSM(empirical): -59.289 ~ -57.396 MeV
(N_shell = 3 - 7, hw = 25 - 35 MeV)
O(1) MeV error?
c.f.) NCFC: -59.1(1) MeV
MCSM(IR cutoff): ~ -58.676 MeV
(w/ UV-saturated data)
O(100) keV error?
Energy (MeV)
hω (MeV)
λsc (MeV)



12C 0+ g.s.
JISP16 NN int.
(w/o Coulomb)
Nshell = 2 - 7
Nshell
Energy (MeV)
MCSM(empirical fit): -105.392 ~ -103.393 MeV
(Nshell = 3 - 7, hw = 25 - 35 MeV)
MCSM(IR cutoff): ~ -104.812 MeV
(w/ UV-saturated data)
16O 0+ g.s.
JISP16 NN int.
(w/o Coulomb)
Nshell = 2 - 7
MCSM(empirical fit): -161.435~ -160.378 MeV
(Nshell = 4 - 7, hw = 25 - 35 MeV)
MCSM(IR cutoff): ~ -159.592 MeV
(w/ UV-saturated data)
hω (MeV)
λsc (MeV)

Effective 2N force from 3N force

w/ M. Kohno

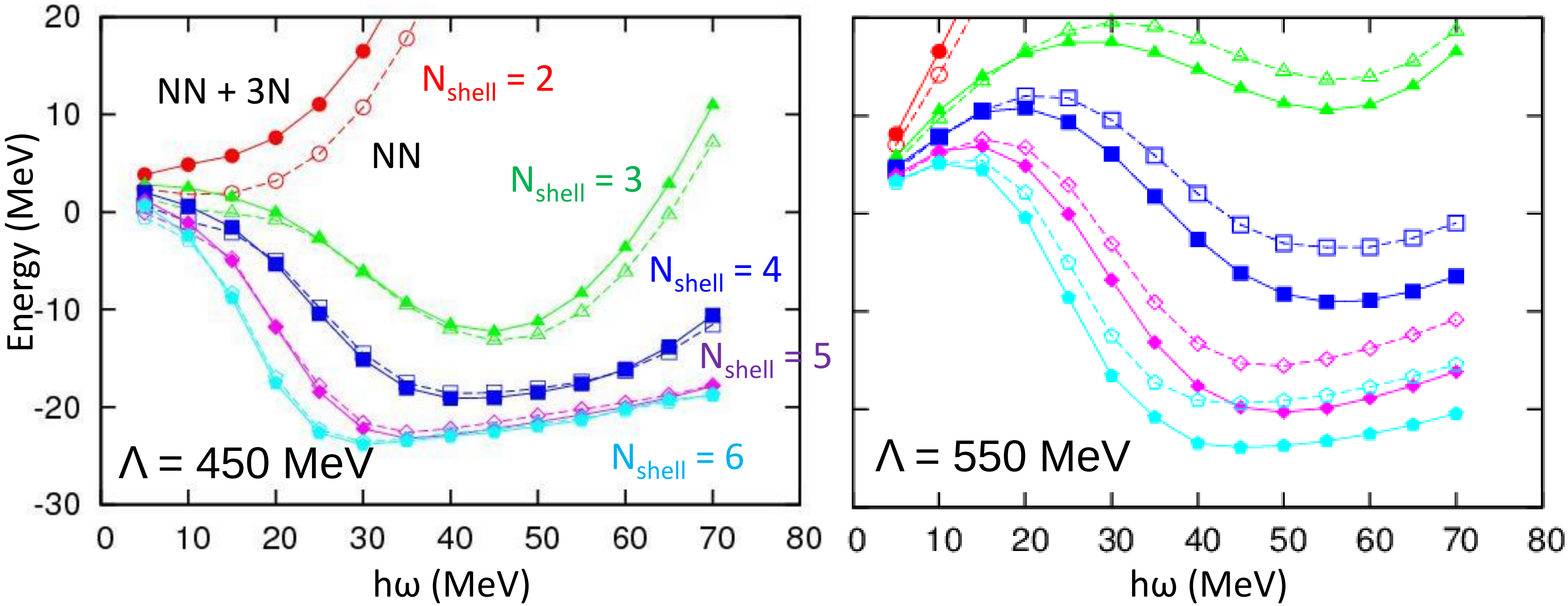
^{4}He 0^+ g.s. energy calculated by FCI & no-core MCSM w/ χEFT N3LO NN (+ "N2LO 3N") potential

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)

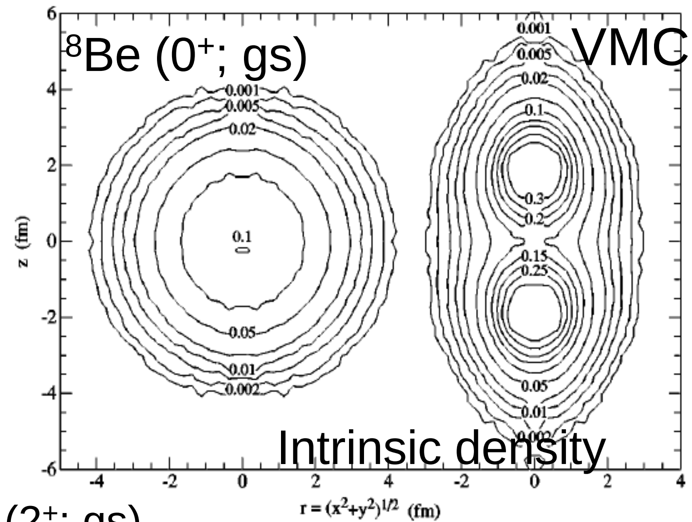
- Lattice EFT

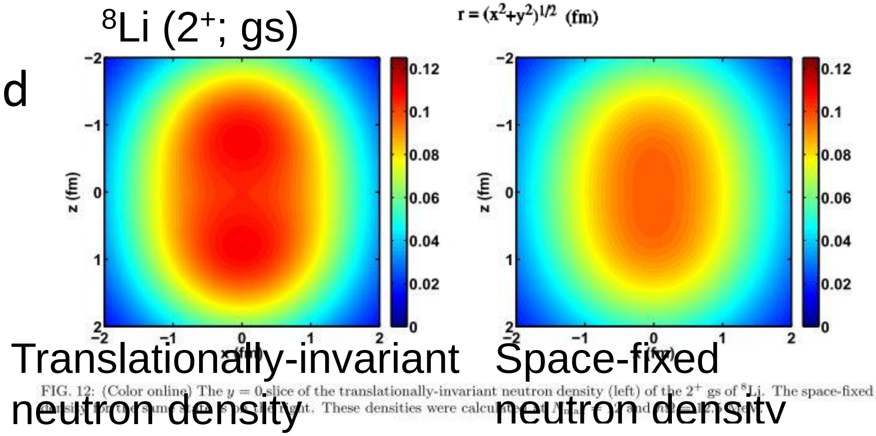
  - Triangle structure in carbon-12

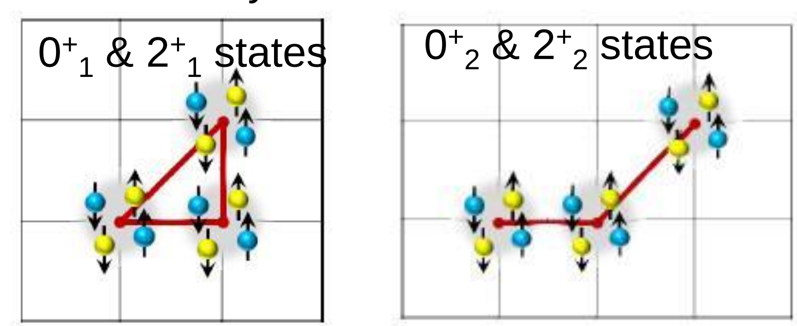
  E. Epelbaum, H. Krebs, T. A. Lahde,

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

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

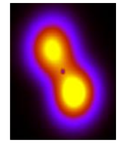
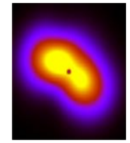
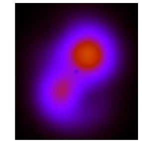
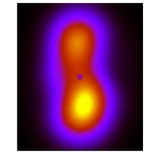






Density distribution in MCSM

T. Yoshida (CNS)

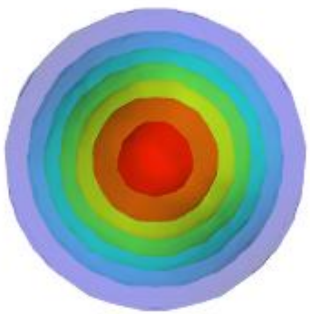
$$|\Phi\rangle = \sum_{i=1}^{N_{basis}} c_i|\Phi_i\rangle =$$ c_1  $+ c_2$  $+ c_3$  $+ c_4$  $+ \ldots$

Angular-momentum projection

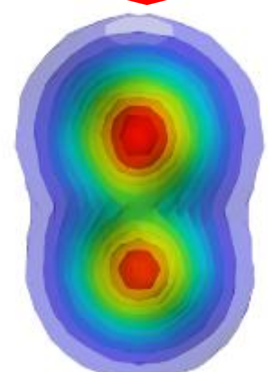
$$|\Psi\rangle = \sum_{i=1}^{N_{basis}} c_i P^J P^\pi |\Phi_i\rangle$$

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

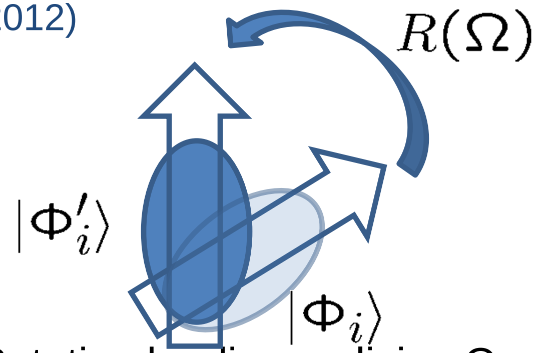
“Intrinsic” (body-fixed) frame

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)

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)

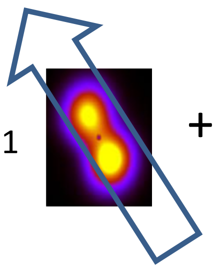
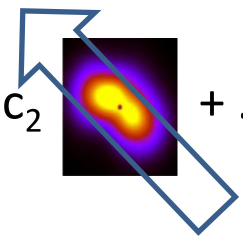
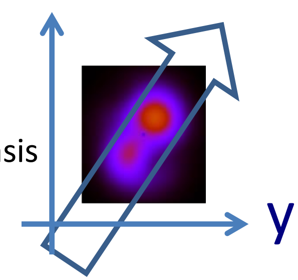


Rotation by diagonalizing Q-moment
($Q_{zz} > Q_{yy} > Q_{xx}$)

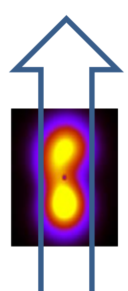
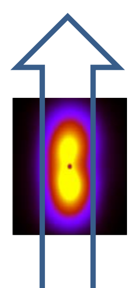
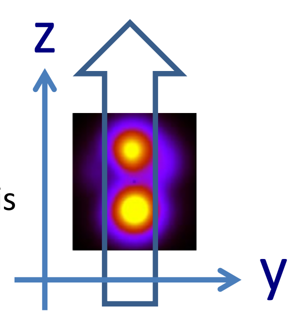
- MCSM wave function

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

- 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 g.s. of Be isotopes

(N$_{shell}$ = 4, hw = 25 MeV, β = 0, JISP16 NN w/o Coulomb)

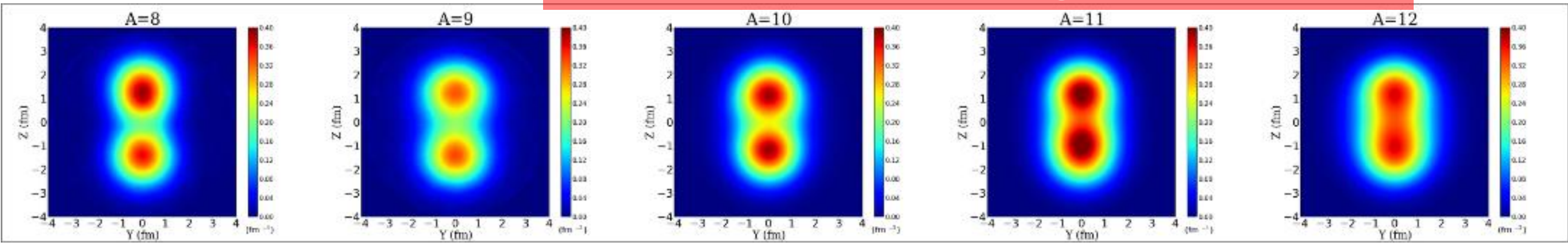
Preliminary

T. Yoshida (CNS)

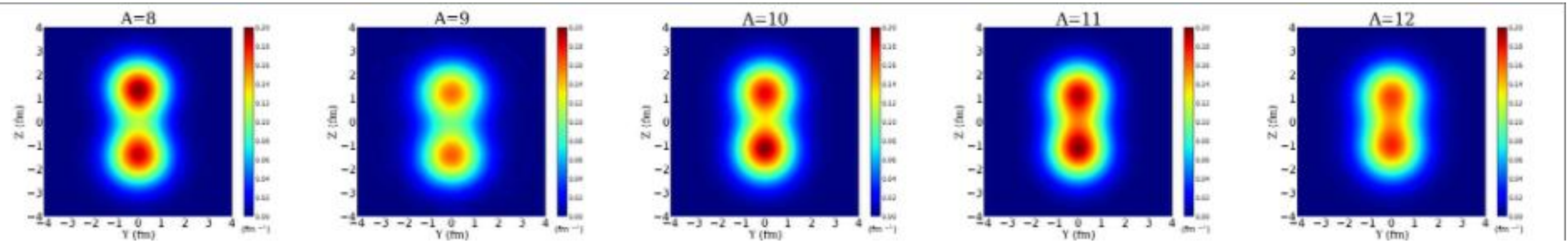
A = 8 A = 9 A = 10 A = 11 A = 12

Matter density

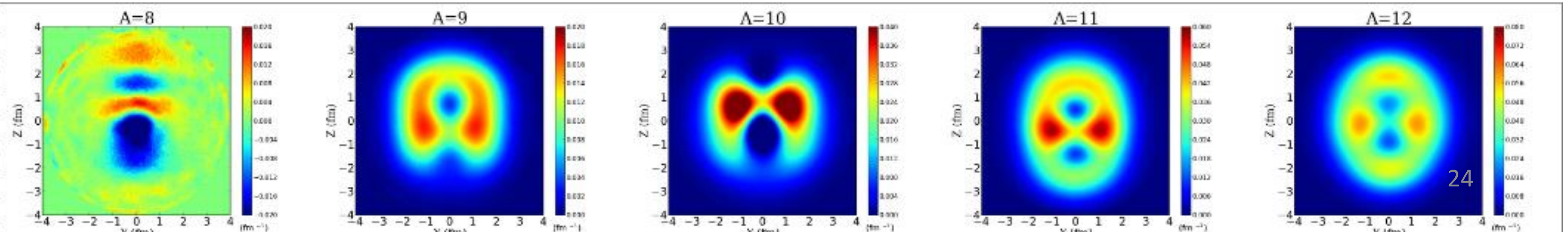
2-α structure is vanishing as A increases



Proton density



Neutron density – Proton density



Summary

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

  - Benchmarks for the p-shell nuclei have been performed and gave good agreements w/ FCI results. Some results are obtained only by MCSM.

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

Perspective

- MCSM algorithm/computation

  - Error estimates of the extrapolations

  - Inclusion of the full 3-body force

  - GPGPU

- Physics

  - 3-alpha cluster states in ^{12}C

  - sd-shell nuclei

Collaborators

- U of Tokyo
  - Takaharu Otsuka (Department of Physics & CNS)
  - Noritaka Shimizu (CNS)
  - Tooru Yoshida (CNS)
  - Yusuke Tsunoda (Department of Physics)
  - Takayuki Miyagi (Department of Physics)
- JAEA
  - Yutaka Utsuno
- Iowa State U
  - James P. Vary
  - Pieter Maris
- Kyushu Institute of Technology
  - Ryoji Okamoto
- RCNP, Osaka U
  - Michio Kohno