YIPQS long term workshop
``Computational Advances in Nuclear and Hadron Physics”
CANHP2015

Infinite basis-space extrapolation of ground-state energies of light nuclei in the no-core Monte Carlo shell model

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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)

"Ab initio" in low-energy nuclear structure physics

- Solve the non-relativistic 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.

- 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)

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

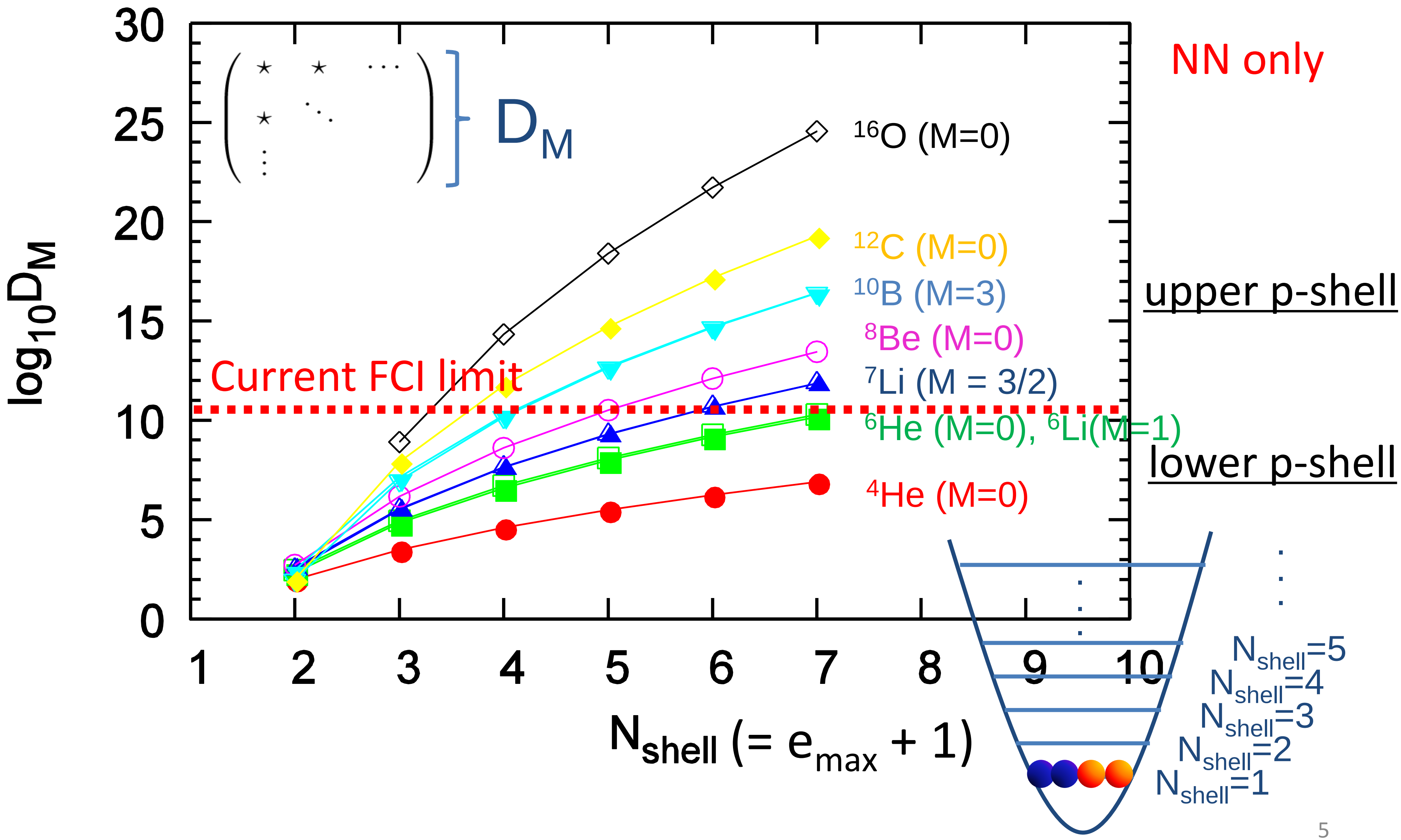
\# non-zero MEs $\sim \mathcal{O}(10^{13-14})$

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

M-scheme dimension in N_{shell} truncation

No-core calculations

NN only



Monte Carlo shell model (MCSM)

- Importance truncation

Standard shell model

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

Diagonalization

All Slater determinants

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

Monte Carlo shell model

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

Diagonalization

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)

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

- Eigenvalue problem

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

- MCSM many-body wave function & basis function

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

These coeff. are obtained by the diagonalization.

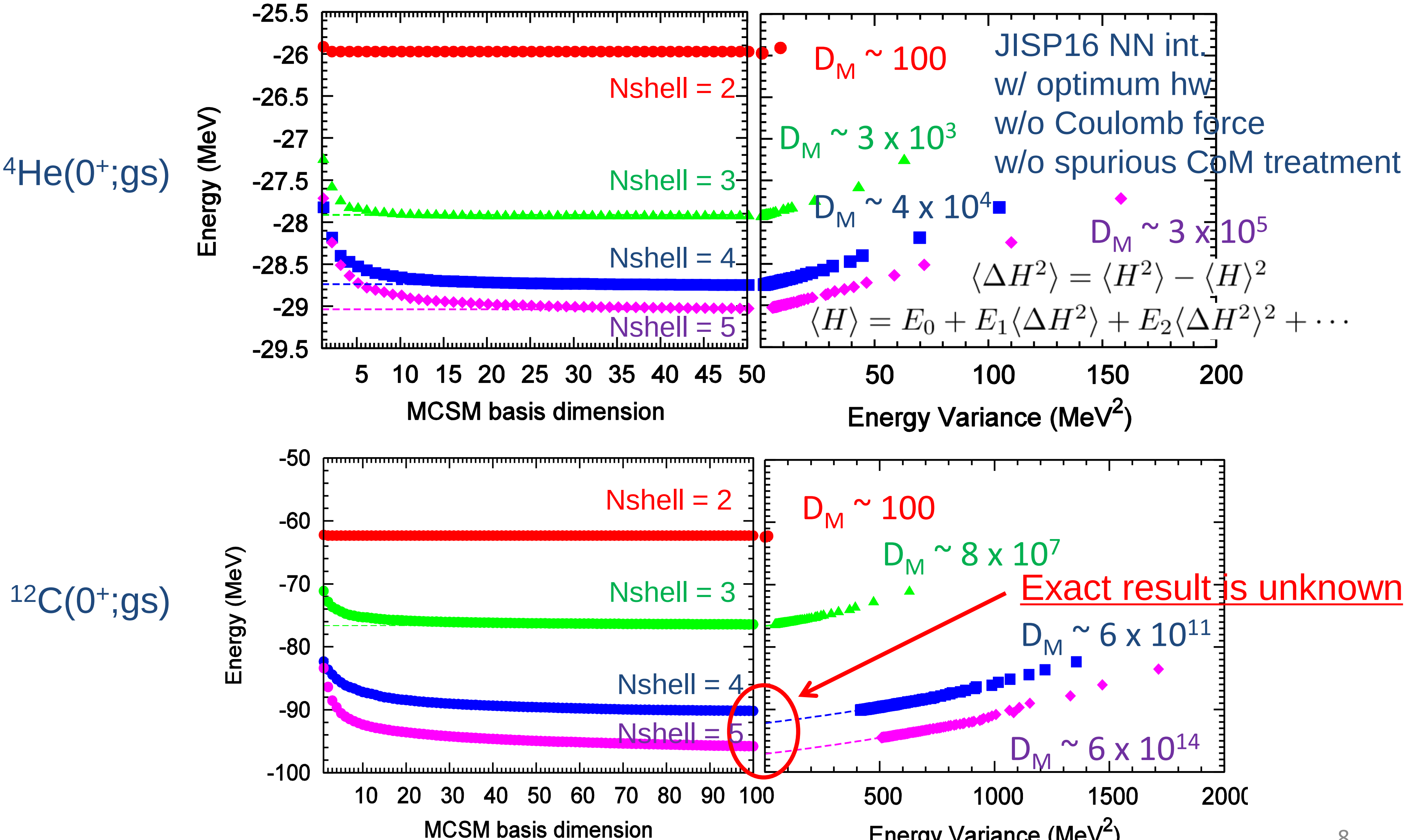
- Deformed SDs

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

$$|\phi\rangle = \prod_i^A a^\dagger_i |-\rangle \qquad a^\dagger_i = \sum_\alpha^{N_{sps}} c^\dagger_\alpha D_{\alpha i}$$

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

Energies wrt # of basis & energy variance



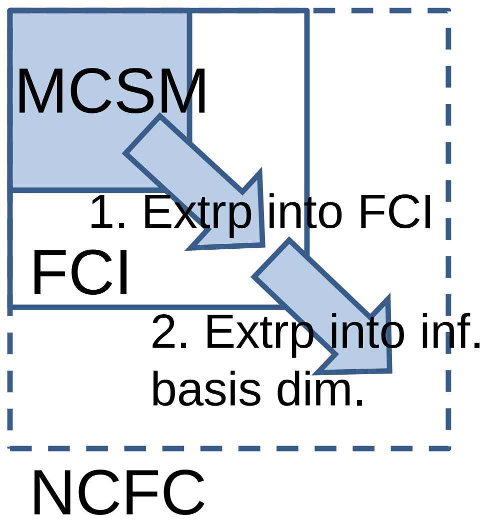
Extrapolations in the no-core MCSM

- 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_{max} in the NCFC
   - IR- & UV-cutoff extrapolations



Extrapolation to the infinite HO-basis space

- Background:
  Recent development of computational technologies
  (e.g., ~ 10 PFLOPS @ K computer)
  & quantum many-body techniques
  (e.g., shell model (CI), Lanczos diagonalization ~ 10^{10} x 10^{10})

- Purpose:
  Full ab initio solutions

- Methods:
  Extrapolations to the infinite HO-basis space motivated by an EFT idea

- Goal:
  Infinite basis-space extrapolation in the no-core MCSM

Extrapolation to the infinite basis space

- Two ways of the extrapolation to the infinite basis space
  1. Traditional exponential form (w/ fixed ħw)

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

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

  2. Cutoff extrapolations

(N, ħω) <-> (λ, Λ)

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

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

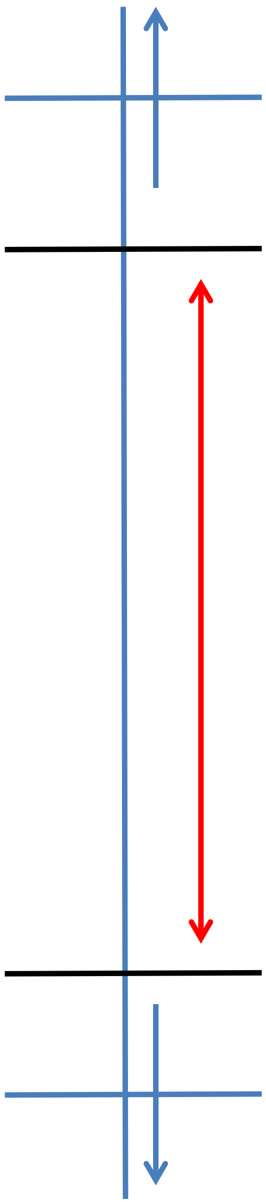
- IR- & UV-cutoff extrapolations (w/ any data, ideally)

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

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 (NTSE-2013 proceedings)

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, Phys. Rev. C89, 044301 (2014)
R. J. Furnstahl, G. Hagen, T. Papenbrock, K. A. Wendt, J. Phys. G: Nucl. Part. Phys. 42, 034032 (2015)
E. D. Jurgenson, P. Maris, R. J. Furnstahl, W. E. Ormand & J. P. Vary, Phys. Rev. C87, 054312 (2013)

Separation of the energy/momentum scale



Λ: UV cutoff -> + infinity

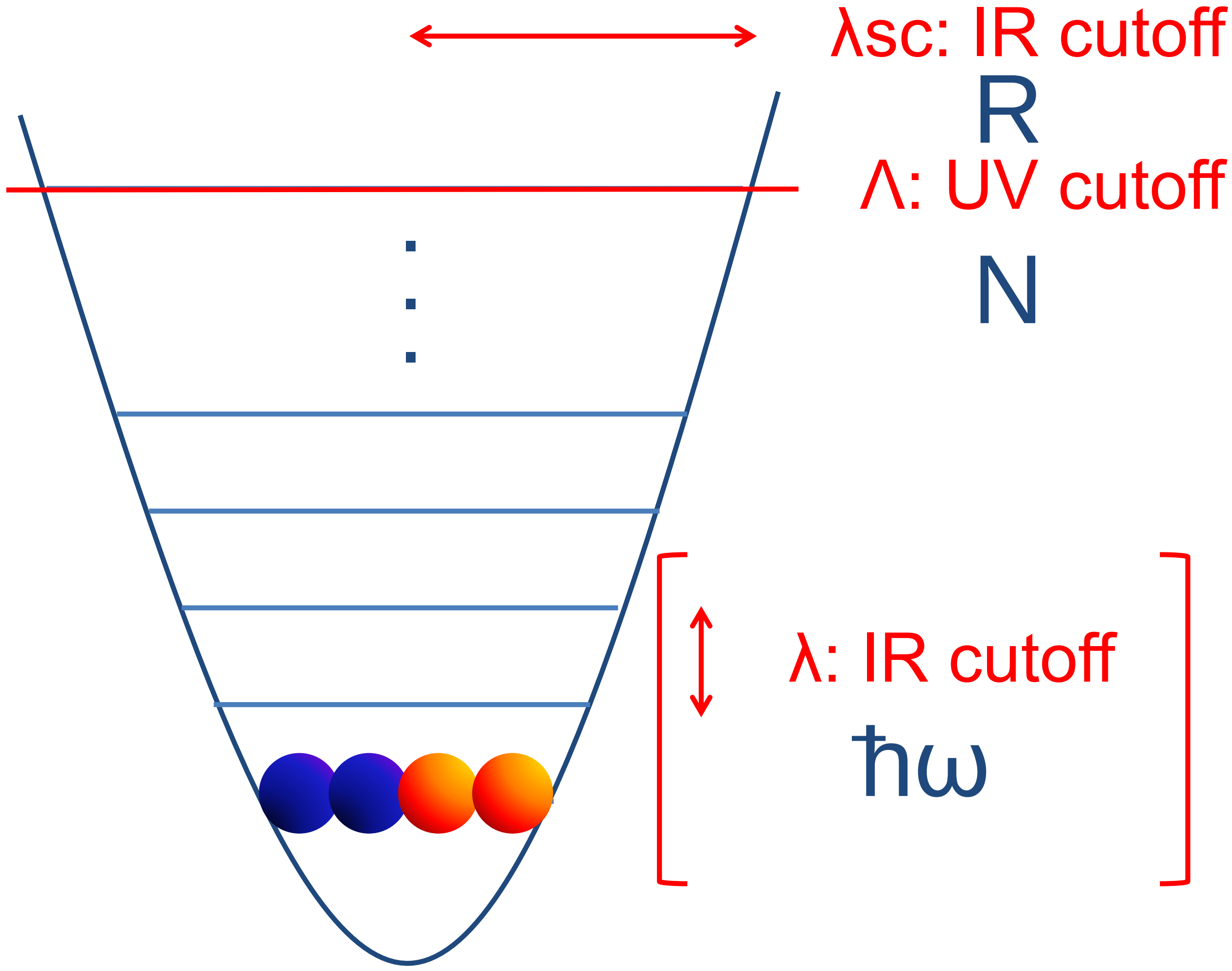
Λ^{NN}: UV cutoff of the NN interaction
~ 600 MeV (JISP16)

Low-energy physics

λ^{NN}: IR cutoff of the NN interaction
~ 60 MeV (JISP16)

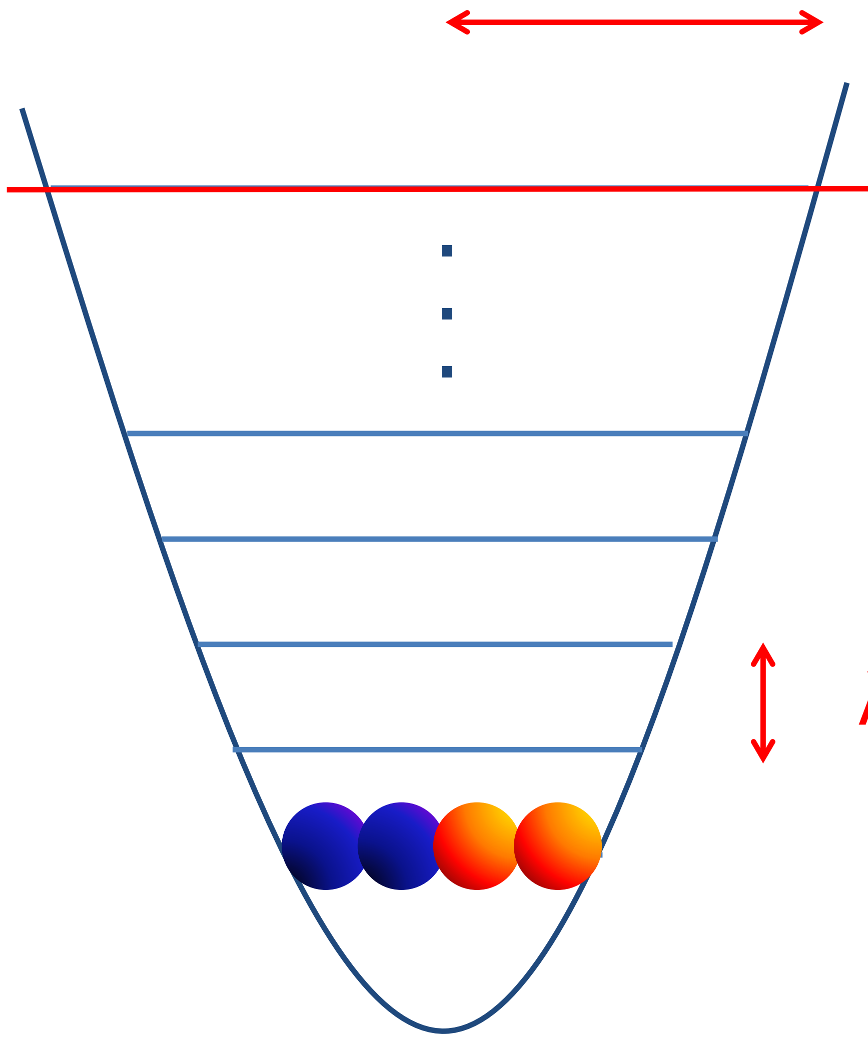
λ: IR cutoff -> 0

IR & UV cutoffs in HO basis



IR & UV cutoffs in HO basis

$$\lambda_{sc} = \sqrt{m\hbar\omega/(N+3/2)} = \lambda^2/\Lambda$$



λsc: IR cutoff

R $R = b\sqrt{N+3/2}$

Λ: UV cutoff

N $b = \sqrt{\hbar/(m\omega)}$

$$\Lambda = \sqrt{m(N+3/2)\hbar\omega}$$

λ: IR cutoff

ħω $\lambda = \sqrt{m\hbar\omega}$

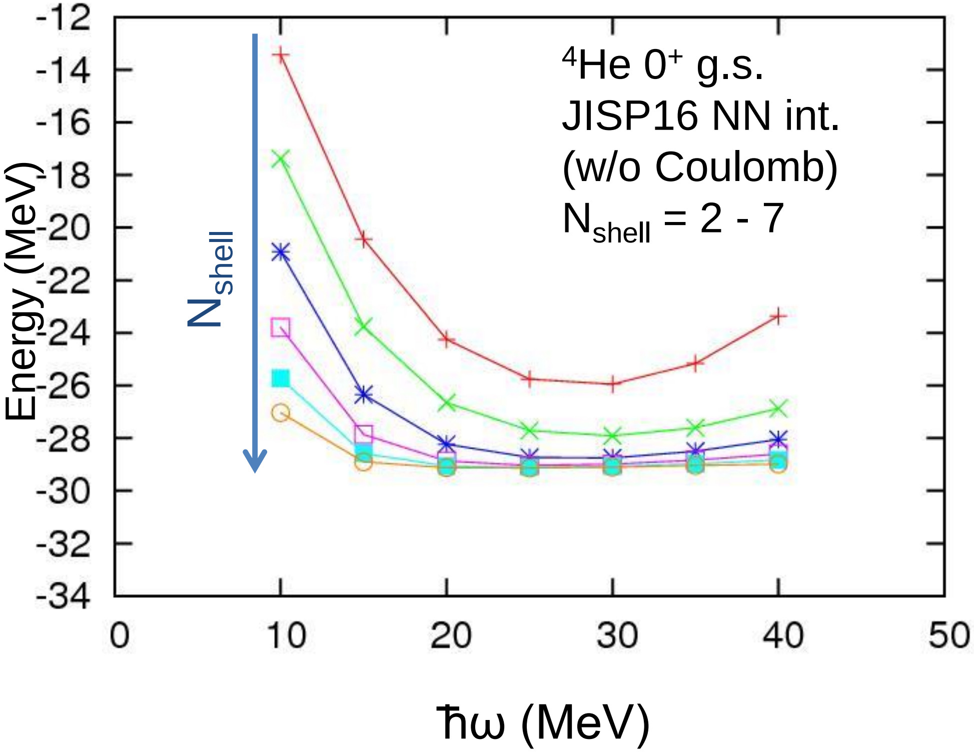
$$\lambda = \hbar/b$$

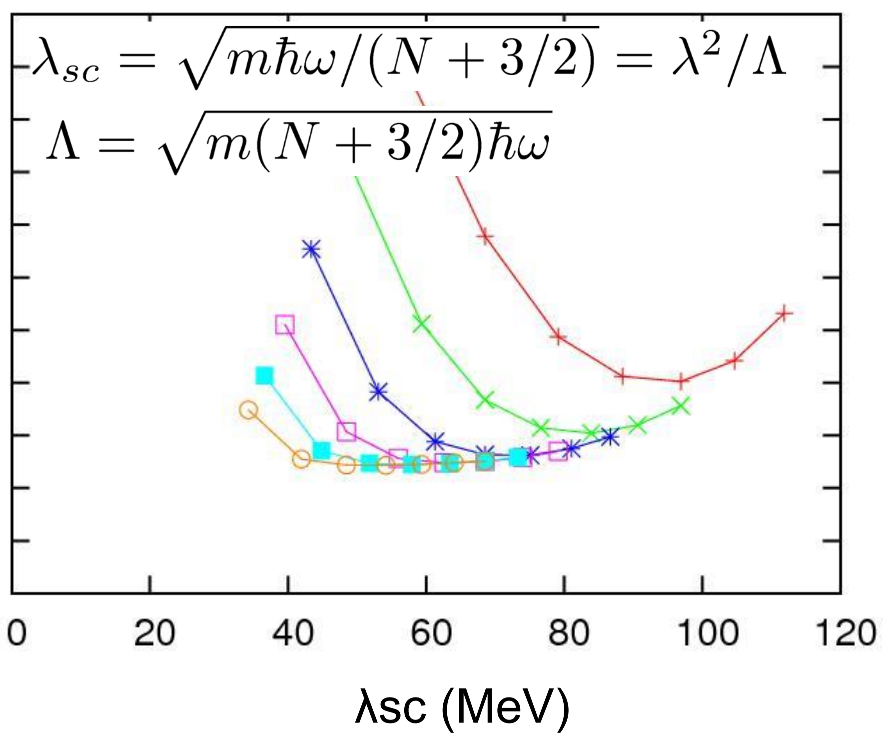
Traditional extrapolation

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

IR-cutoff extrapolation

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



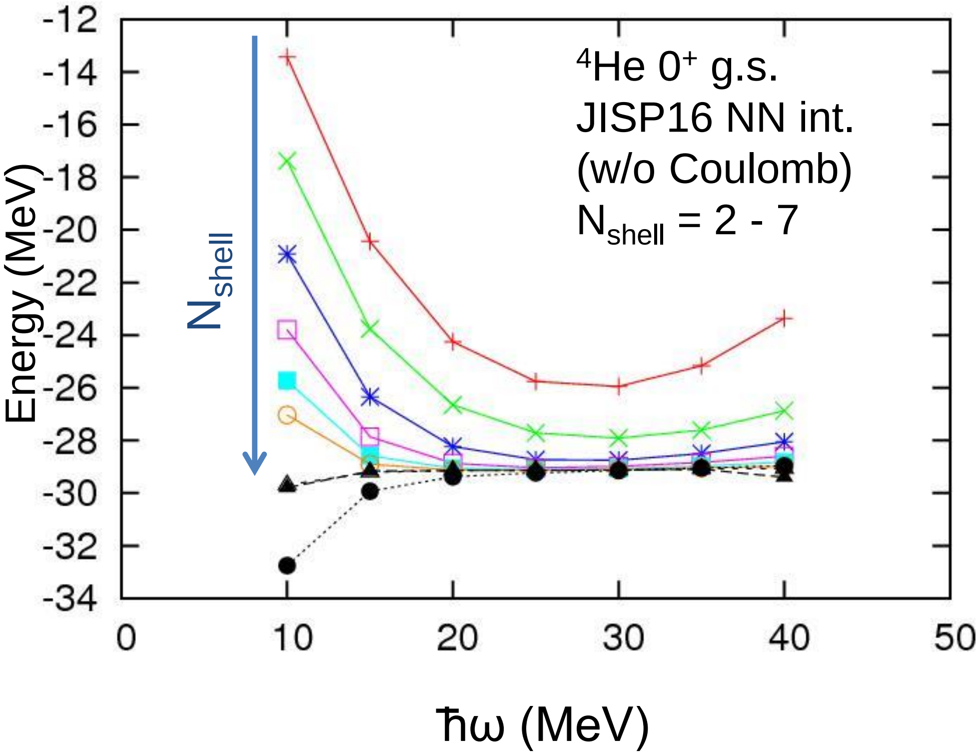


(N_{shell}, ħω) ⟷ (Λ, λsc)

Λ: UV cutoff   λsc: IR cutoff

Traditional extrapolation

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

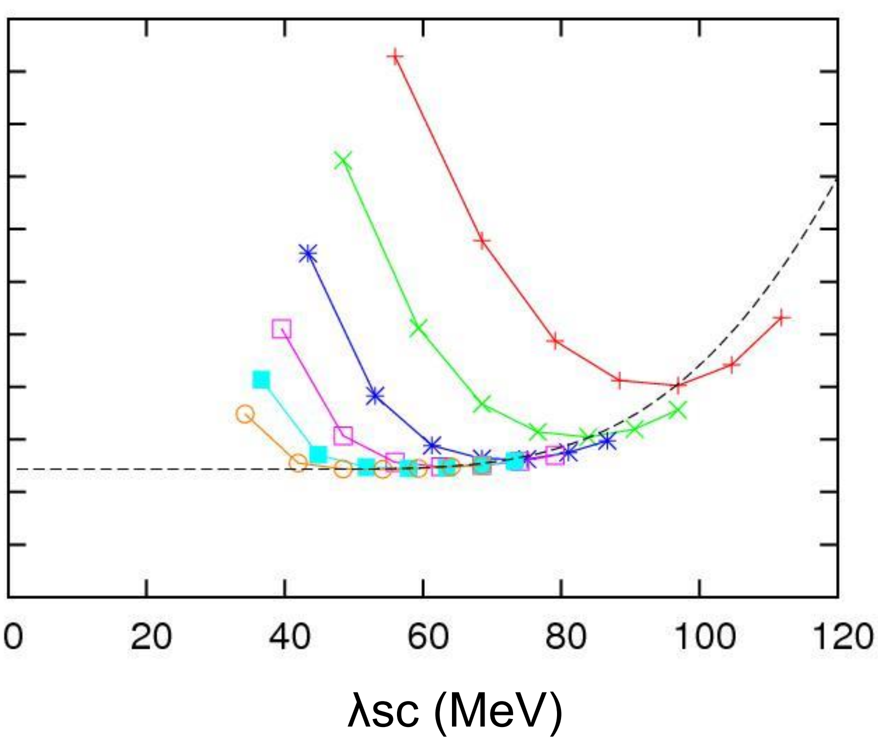


MCSM(empirical): -29.4 ~ -29.1 MeV
(N_{shell} = 3 - 7, hw = 15 - 35 MeV)

O(100) keV error

IR-cutoff extrapolation

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



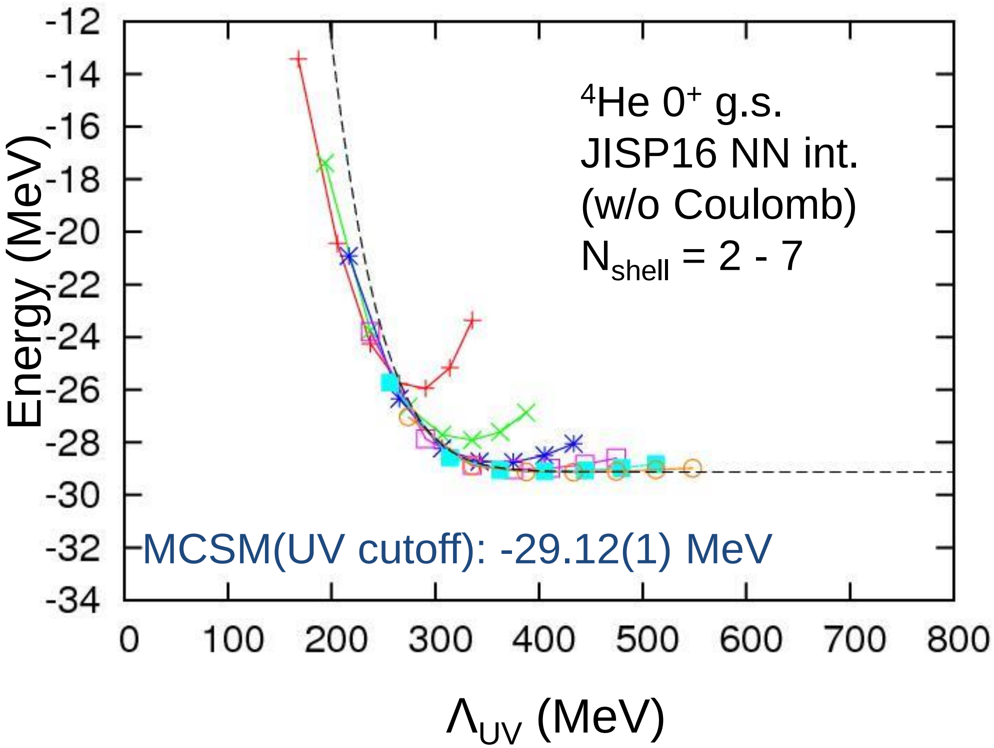
MCSM(IR cutoff): ~ -29.14(1) MeV

O(10) keV error

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

UV-cutoff extrapolation

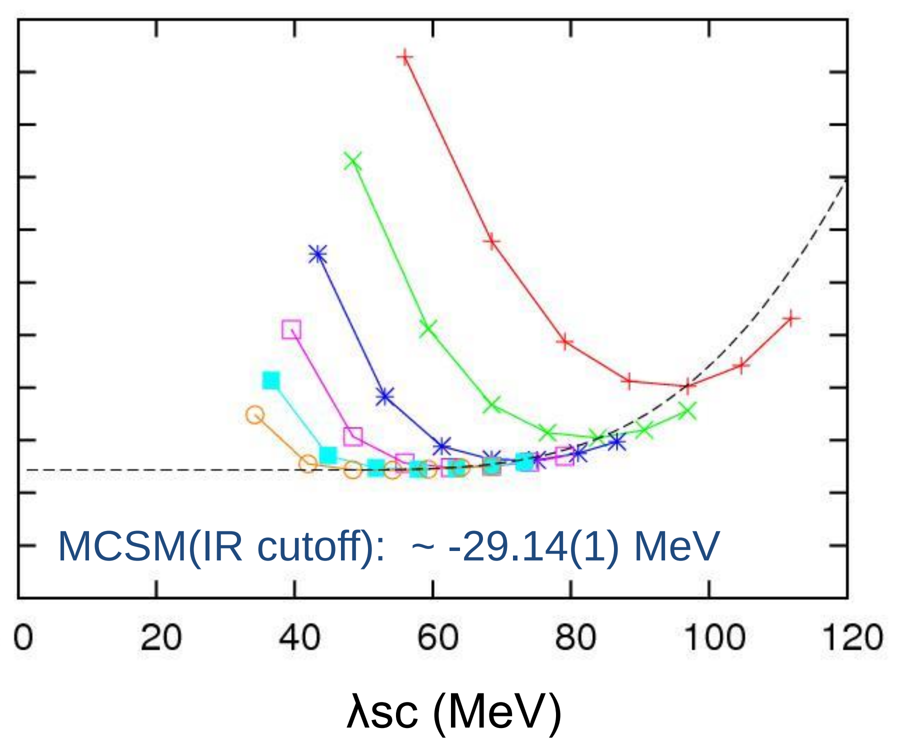
$$E(\Lambda) = E(\Lambda = \infty) + c \exp(-\Lambda^2/d^2)$$



O(10) keV error

IR-cutoff extrapolation

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

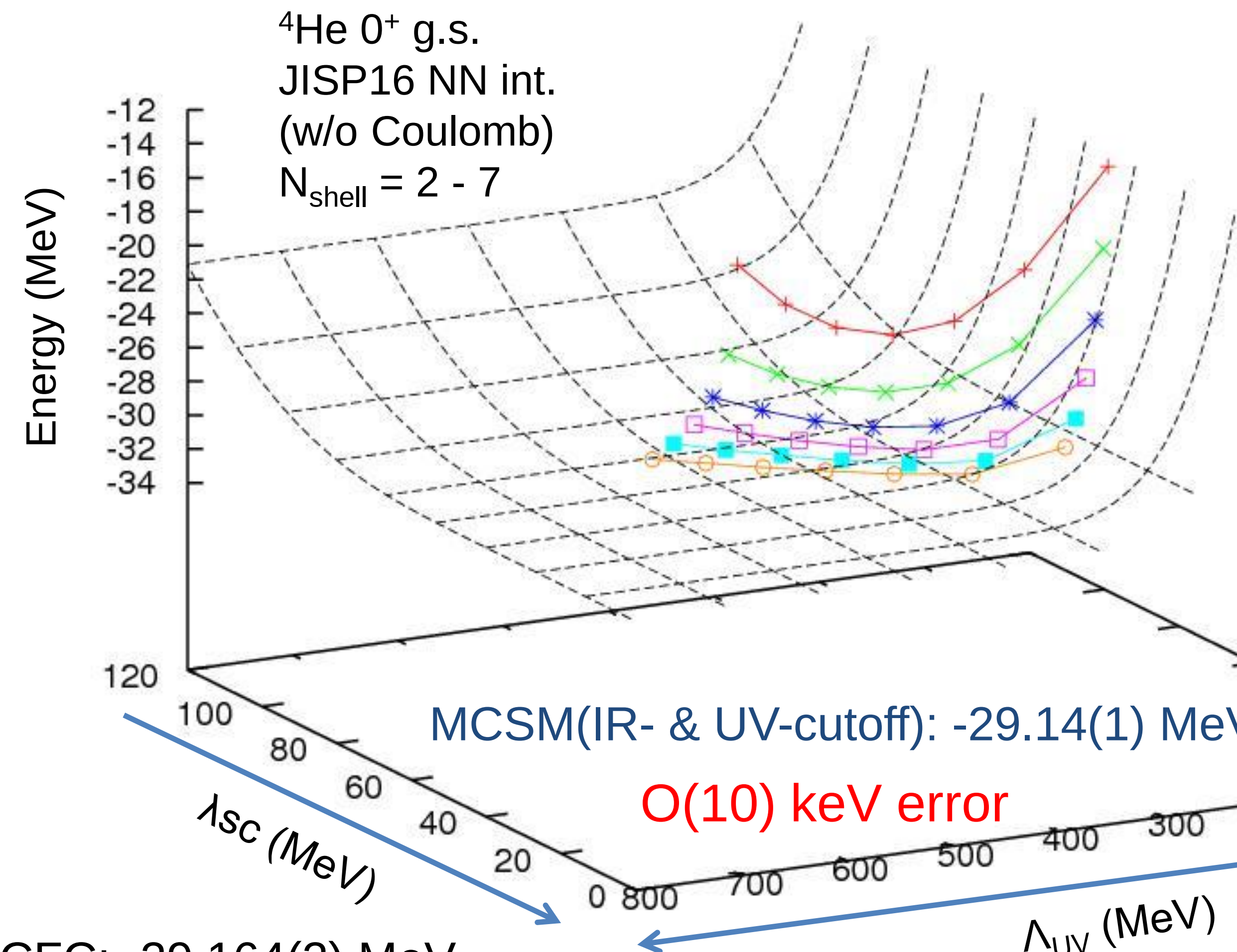


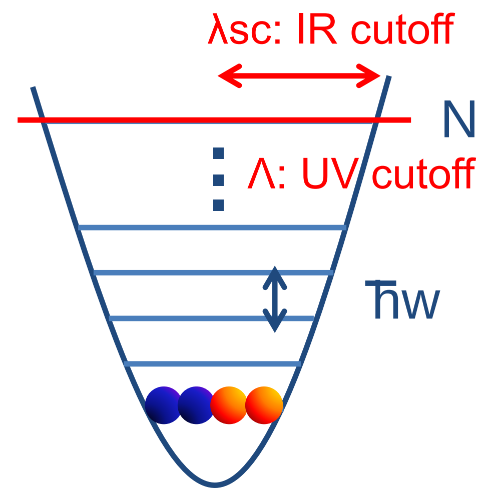
c.f.) NCFC: -29.164(2) MeV

Extrapolated results to infinite N_{max} space

IR- & UV-cutoff extrapolation

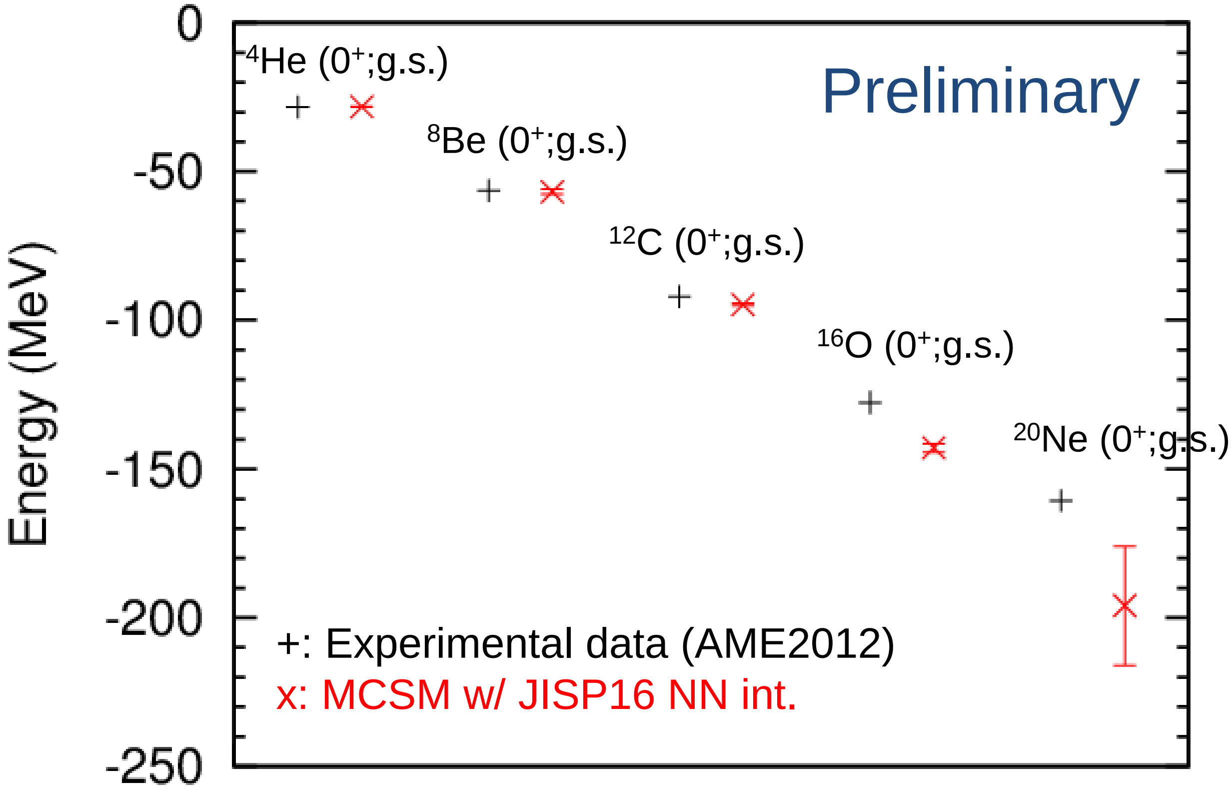
$$E(\lambda, \Lambda) = E(\lambda = 0, \Lambda = \infty) + a \exp(-b/\lambda) + c \exp(-\Lambda^2/d^2)$$





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

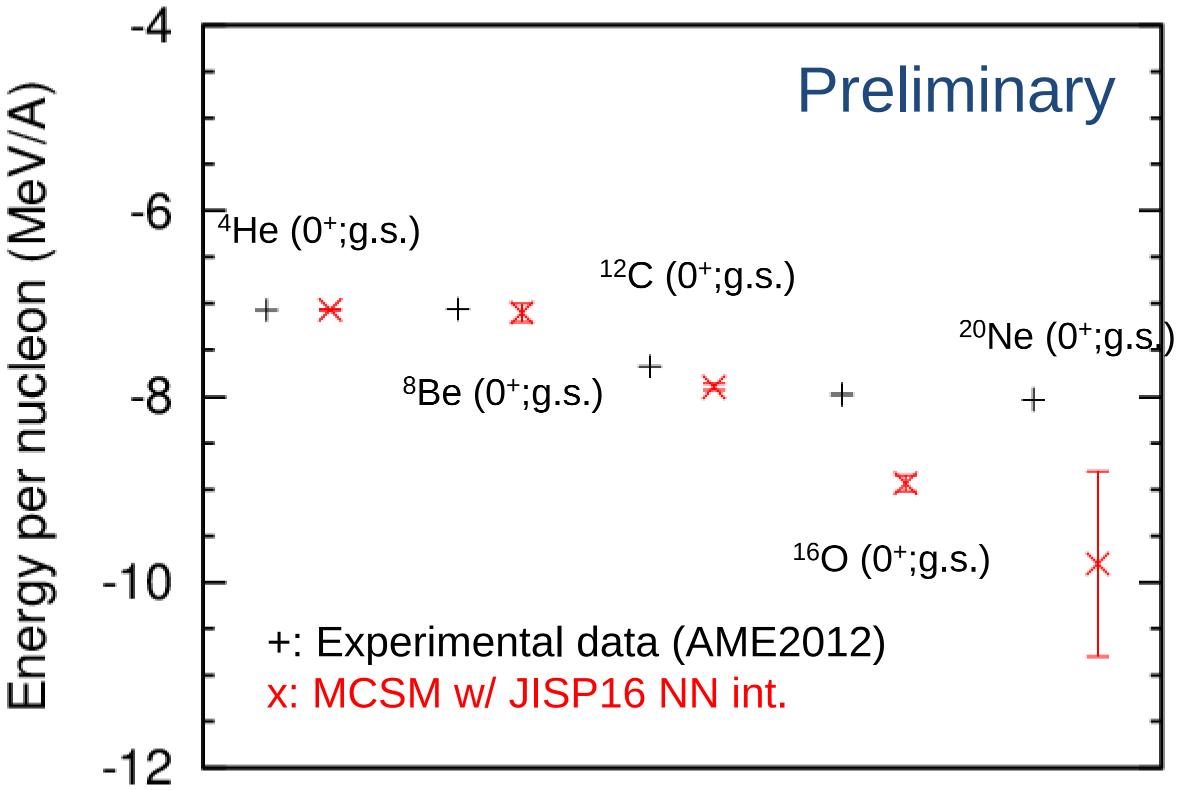
Comparison of MCSM results w/ experiments



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.

Comparison of MCSM results w/ experiments



MCSM results are obtained by traditional extrapolation w/ optimum harmonic oscillator energies.
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MCSM results show good agreements w/ experimental data up to ^{12}C, slightly overbound for ^{16}O, and clearly overbound for ^{20}Ne.

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.

Perspective

- MCSM algorithm/computation

  - Better error estimate for the extrapolations

  - Inclusion of the 3-body force
- Physics

  - Other observables (rms radius, …)

  - Other p- & sd-shell nuclei

Collaborators

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