Perspectives of the Ab Initio No-Core Shell Model

Recent development of the MCSM and its application to the no-core calculation

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in collaboration with
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Outline of this talk

- Motivation
- Monte Carlo Shell Model (MCSM)
- Benchmark results by the No-Core MCSM
- Summary & outlook

Current status of ab inito approaches

- Major challenge of the nuclear structure theory
  - Understand the nuclear structures from the first principle of quantum many-body theory by *ab-initio* calc w/ realistic nuclear forces

  - Standard approaches: GFMC, NCSM (up to A ~ 12-14), CC (closed shell +/- 1,2), SCGF theory, IM-SRG, Lattice EFT, …

→ demand for extensive computational resources

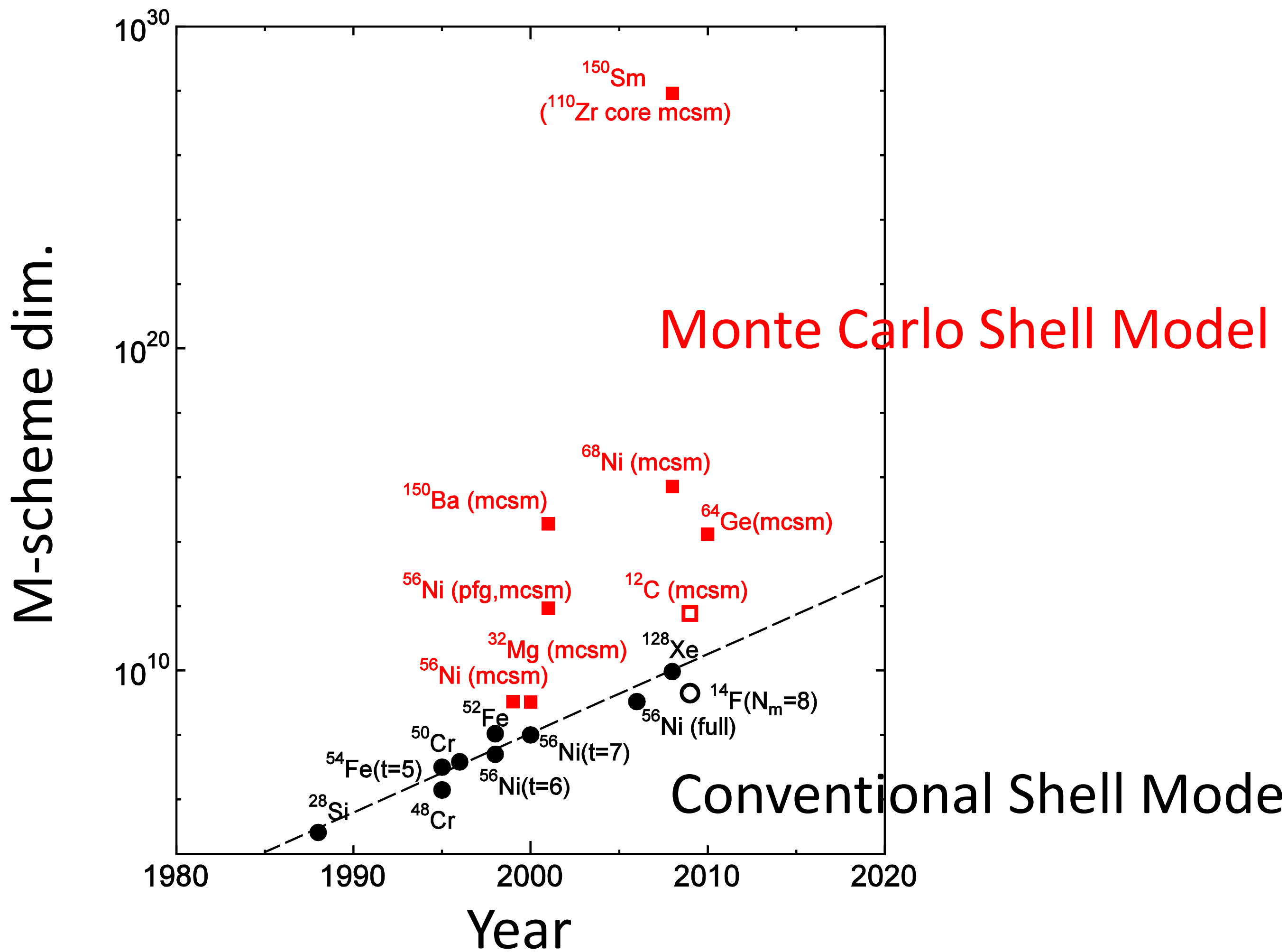
✓ *ab-initio*(-like) SM approaches (which attempt to go) beyond standard methods
  - IT-NCSM, IT-CI: R. Roth (TU Darmstadt), P. Navratil (TRIUMF)
  - Sp-NCSM: T. Dytrych, K.D. Sviratcheva, J.P. Draayer, C. Bahri, & J.P. Vary (Louisiana State U, Iowa State U)

→ - No-Core Monte Carlo Shell Model (MCSM)

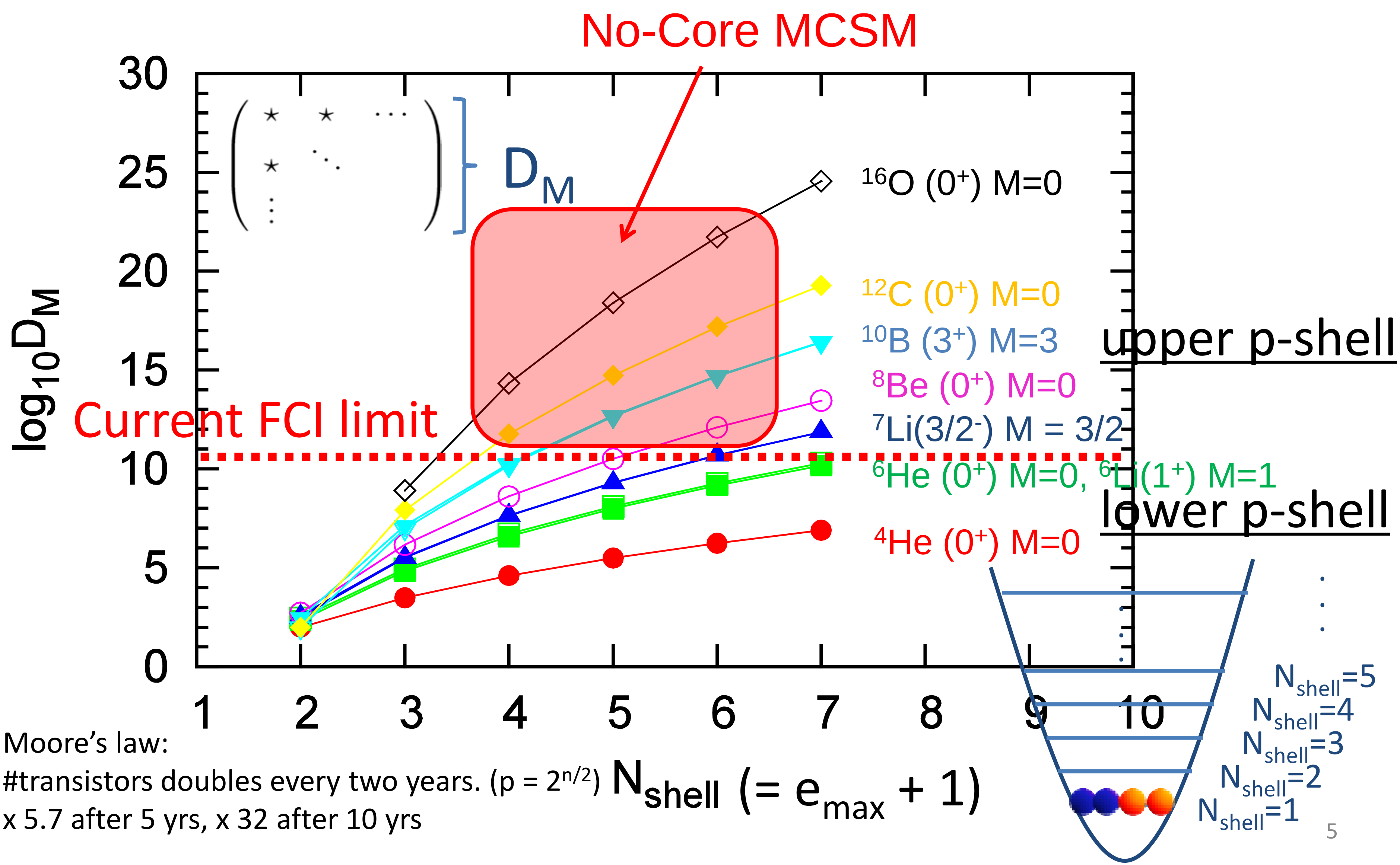
Review: T. Otsuka , M. Honma, T. Mizusaki, N. Shimizu, Y. Utsuno, Prog. Part. Nucl. Phys. 47, 319 (2001)

MCSM w/ a core

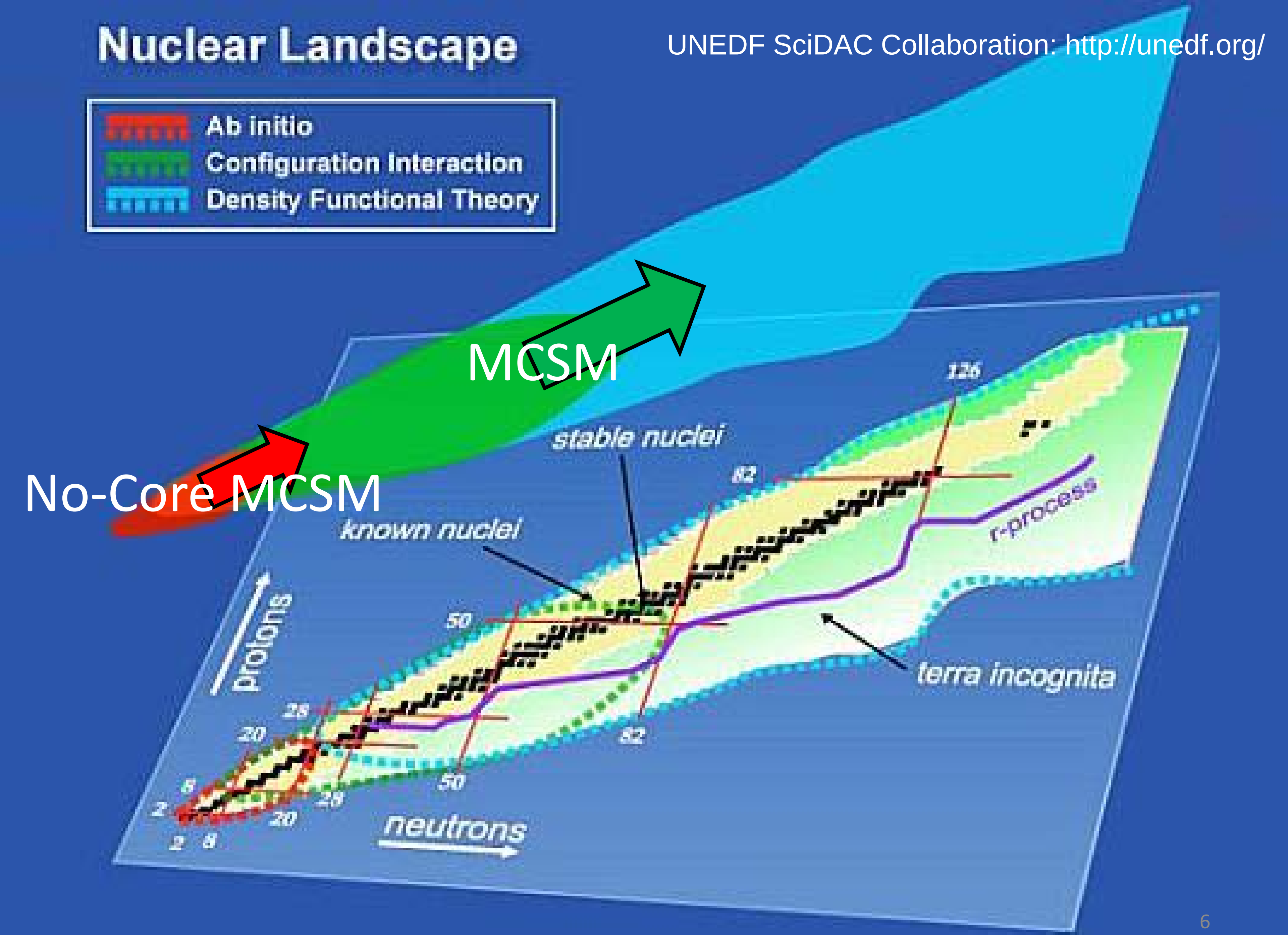
- MCSM (w/ a core) is one of the powerful shell model algorithms.



M-scheme dimension of p-shell nuclei



Moore's law:
#transistors doubles every two years. ($p = 2^{n/2}$)
x 5.7 after 5 yrs, x 32 after 10 yrs


Nuclear Landscape
UNEDF SciDAC Collaboration: http://unedf.org/
Ab initio
Configuration Interaction
Density Functional Theory
MCSM
No-Core MCSM
stable nuclei
known nuclei
terra incognita
r-process
protons
neutrons
126
82
50
28
20
8
2
82
50
28
20
8
2

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

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

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

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

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

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

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

These coeff. are obtained by Housholder/Lanczos methods.

- Deformed SDs

This coeff. is obtained by a stochastic sampling.

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

($c_\alpha^\dagger$ … HO basis)

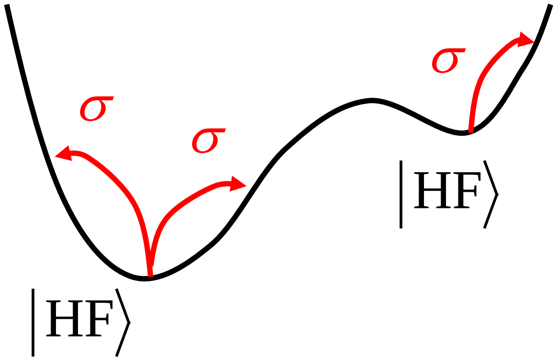
Sampling of basis functions in the MCSM

- Deformed Slater determinant basis

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

($c_\alpha^\dagger$ ... HO basis)

- Stochastic sampling of deformed SDs



$$|\phi(\sigma)\rangle = e^{-h(\sigma)}|\phi\rangle$$

$$h(\sigma) = h_{HF} + \sum_i^{N_{AF}} s_i V_i \sigma_i O_i$$

c.f.) Imaginary-time evolution & Hubbard-Stratonovich transf.

$$|\phi(\sigma)\rangle = \prod_{N_\tau} e^{-\Delta\beta h(\sigma)}|\phi\rangle$$

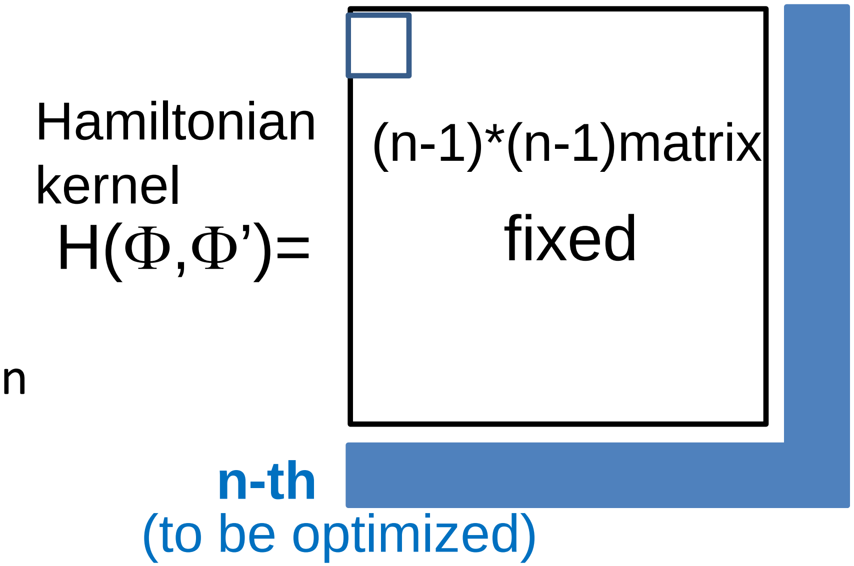
$$e^{-\beta H} = \int_{-\infty}^{+\infty} \prod_i d\sigma_i \sqrt{\frac{\beta|V_i|}{2\pi}} e^{-\frac{\beta}{2}|V_i|\sigma_i^2} e^{-\beta h(\vec{\sigma})}$$

$$h(\sigma) = \sum_i^{N_{AF}} (\epsilon_i + s_i V_i \sigma_i) O_i$$

$$H = \sum_i \epsilon_i O_i + \frac{1}{2}\sum_i V_i O_i^2$$

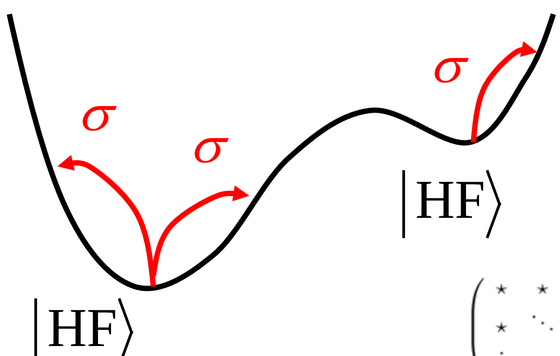
Rough image of the search steps

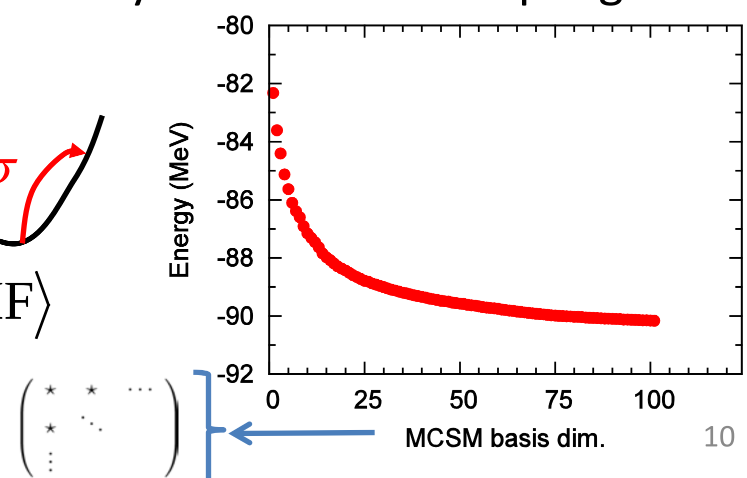
- Basis search
  - HF solution is taken as the 1st basis
  - Fix the n-1 basis states already taken
  - Requirement for the new basis: atopt the basis which makes the energy (of a many-body state) as low as possible by a stochastic sampling



$$|\phi(\sigma)\rangle = \prod_n e^{-\Delta\beta h(\vec{\sigma}_n)}|\phi\rangle$$

$$h(\vec{\sigma}_n) = h_{HF} + \sum_\alpha \sigma_{\alpha n} O_\alpha$$





Recent developments in MCSM

- Acceleration of the computation of two-body matrix elements

$$\langle \phi | \hat{V} | \phi' \rangle = \frac{1}{2} \sum_{i,k} \rho_{ki} \left(\sum_{j,l} v_{ijkl} \rho_{lj} \right) = \frac{1}{2} \sum_{(ki)} \rho_{(ki)} \left(\sum_{jl} v_{(ki),(lj)} \rho_{(lj)} \right)$$

Matrix product is performed w/ bundled density matrices by DGEMM subroutine in BLAS level-3 library

Y. Utsuno, N. Shimizu, T. Otsuka, and T. Abe, arXiv:1202.2957 [nucl-th] (submitted to Comp. Phys. Comm.)

- Extrapolation method by the energy variance

$$\langle H \rangle = E_0 + E_1 \langle \Delta H^2 \rangle + E_2 \langle \Delta H^2 \rangle^2 + \cdots \qquad \langle \Delta H^2 \rangle = \langle H^2 \rangle - \langle H \rangle^2$$

$$\frac{\langle \phi | \hat{H}^2 | \psi \rangle}{\langle \phi | \psi \rangle} = \sum_{i<j,\alpha<\beta} \left(\sum_{k<l} v_{ijkl} ((1-\rho)_{k\alpha}(1-\rho)_{l\beta} - (1-\rho)_{l\alpha}(1-\rho)_{k\beta}) \right) \left(\sum_{\gamma<\delta} v_{\alpha\beta\gamma\delta} (\rho_{\gamma i}\rho_{\delta j} - \rho_{\delta i}\rho_{\gamma j}) \right)$$

$$+\mathrm{Tr}((t+\Gamma)(1-\rho)(t+\Gamma)\rho) + \left(\mathrm{Tr}(\rho(t+\frac{1}{2}\Gamma)) \right)^2 \qquad \Gamma_{ik} = \sum_{jl} v_{ijkl} \rho_{lj}$$

(naively) 8-fold loops -> (effectively) 6-fold loops by the factorization

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

Hot spot of the MCSM calculation

- Evaluation of the Hamiltonian kernel btw. non-orthogonal SDs

$$\mathcal{H}(q', q) = \mathcal{N}(q', q) \left(\sum_{l_1 l_2}^{N_s} t_{l_1 l_2} \rho_{l_2 l_1} + \frac{1}{2} \sum_{l_1 l_2 l_3 l_4}^{N_s} \rho_{l_3 l_1} \bar{v}_{l_1 l_2, l_3 l_4} \rho_{l_4 l_2} \right)$$

$$\langle V \rangle \equiv \sum_{l_1 l_2 l_3 l_4}^{N_s} \rho_{l_3 l_1} \bar{v}_{l_1 l_2, l_3 l_4} \rho_{l_4 l_2}$$

Computation of the TBMEs

- hot spot: Computation of the TBMEs

(w/o projections, for simplicity)

$$\frac{\langle \Phi' | V | \Phi \rangle}{\langle \Phi' | \Phi \rangle} = \frac{1}{2} \sum_{ijkl} \bar{v}_{ijkl} \rho_{ki} \rho_{lj}$$

c.f.) Indirect-index method (list-vector method)

- Utilization of the symmetry

$$j_z(i) + j_z(j) = j_z(k) + j_z(l) \rightarrow j_z(i) - j_z(k) = -(j_z(j) - j_z(l)) \equiv \Delta m$$

$$\sum_{ijkl} \bar{v}_{ijkl} \rho_{ki} \rho_{lj} = \sum_{\Delta m} \left[\sum_{a \in J_z(a) = -\Delta m} \tilde{\rho}_a \left(\sum_{b \in J_z(b) = \Delta m} \tilde{v}_{ab} \tilde{\rho}_b \right) \right]$$

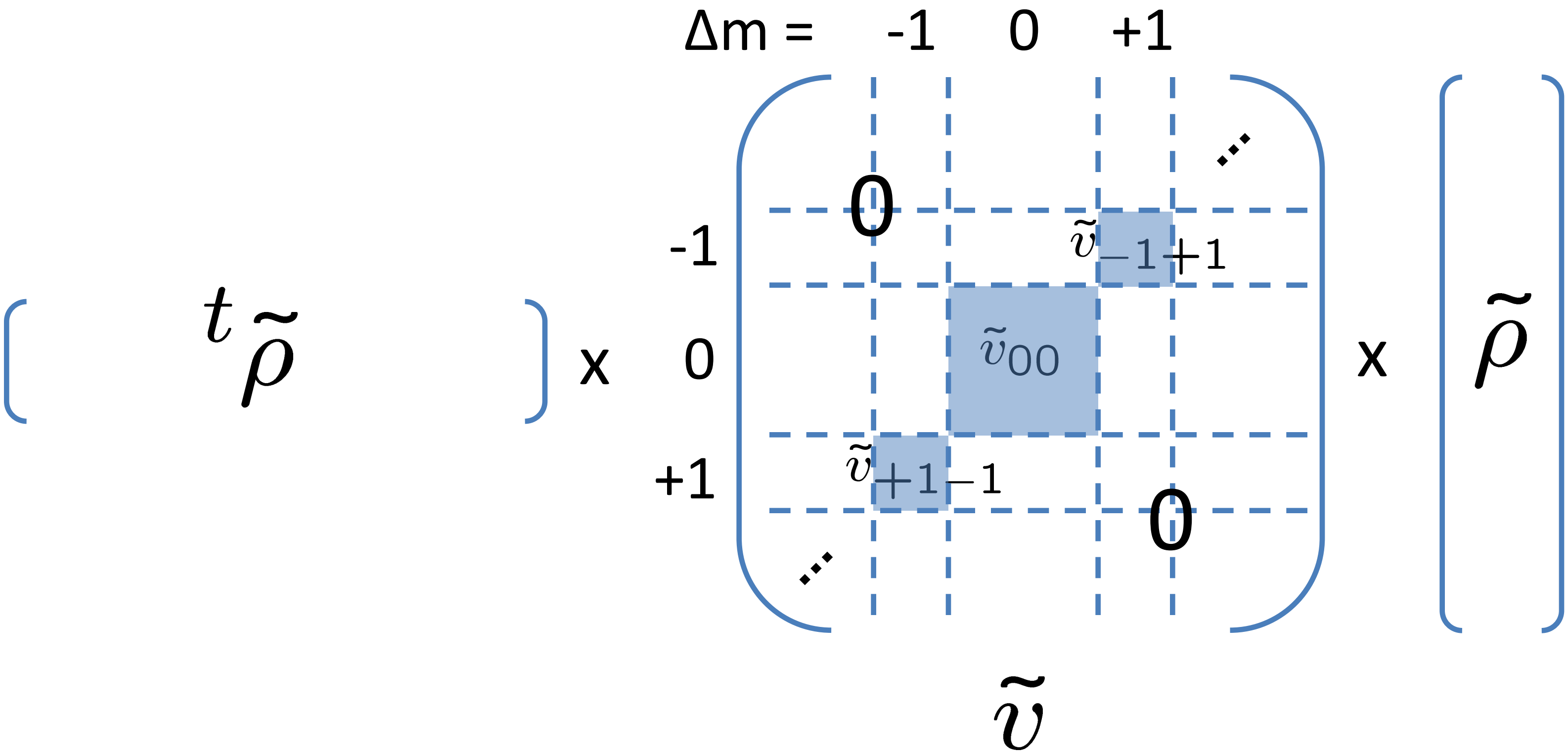
$\bar{v}_{ijkl} \rightarrow \tilde{v}_{ab}$ $\qquad$ $\rho_{ki} \rightarrow \tilde{\rho}_a$ $\qquad$ $\rho_{lj} \rightarrow \tilde{\rho}_b$

sparse $\qquad$ dense

Schematic illustration of the computation of TBMEs

- Matrix-vector method

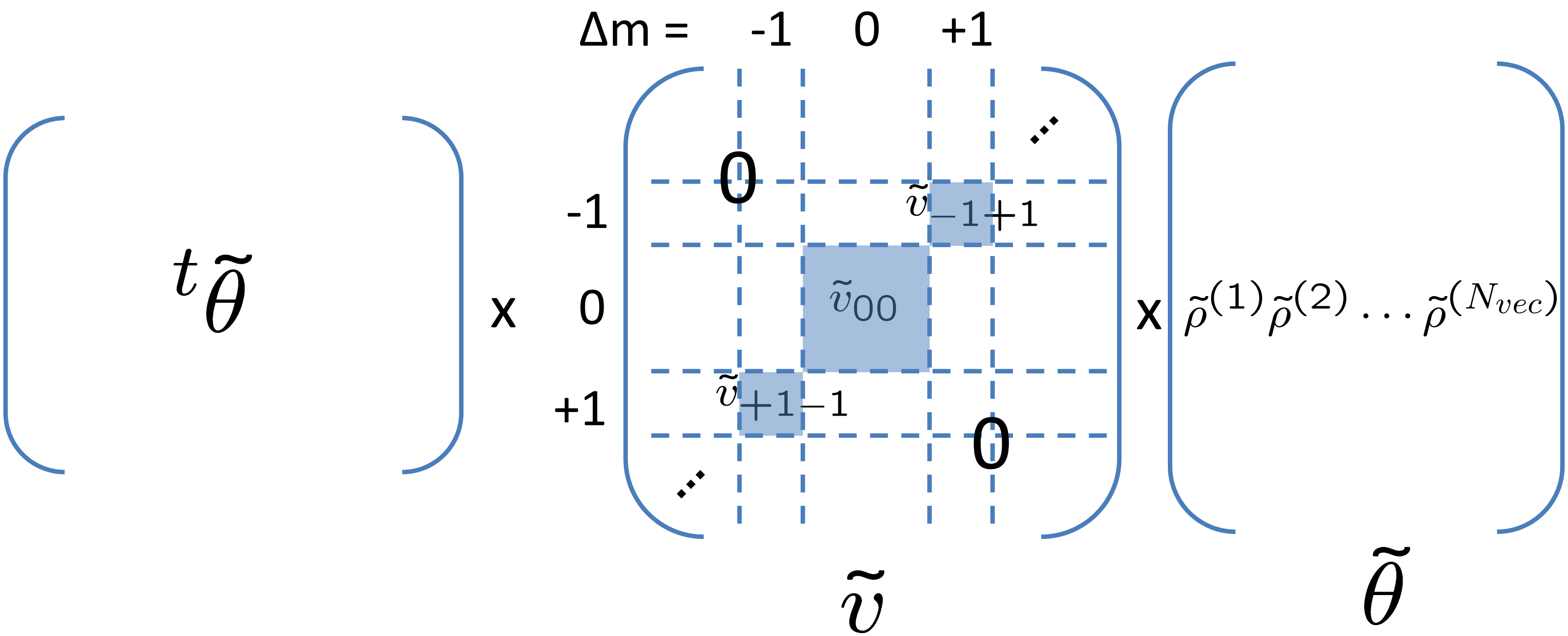
$$\sum_{ijkl} \bar{v}_{ijkl}\rho_{ki}\rho_{lj} = \sum_{\Delta m}\left[\sum_{a\in J_z(a)=-\Delta m}\tilde{\rho}_a\left(\sum_{b\in J_z(b)=\Delta m}\tilde{v}_{ab}\tilde{\rho}_b\right)\right]$$



Schematic illustration of the computation of TBMEs

- Matrix-matrix method

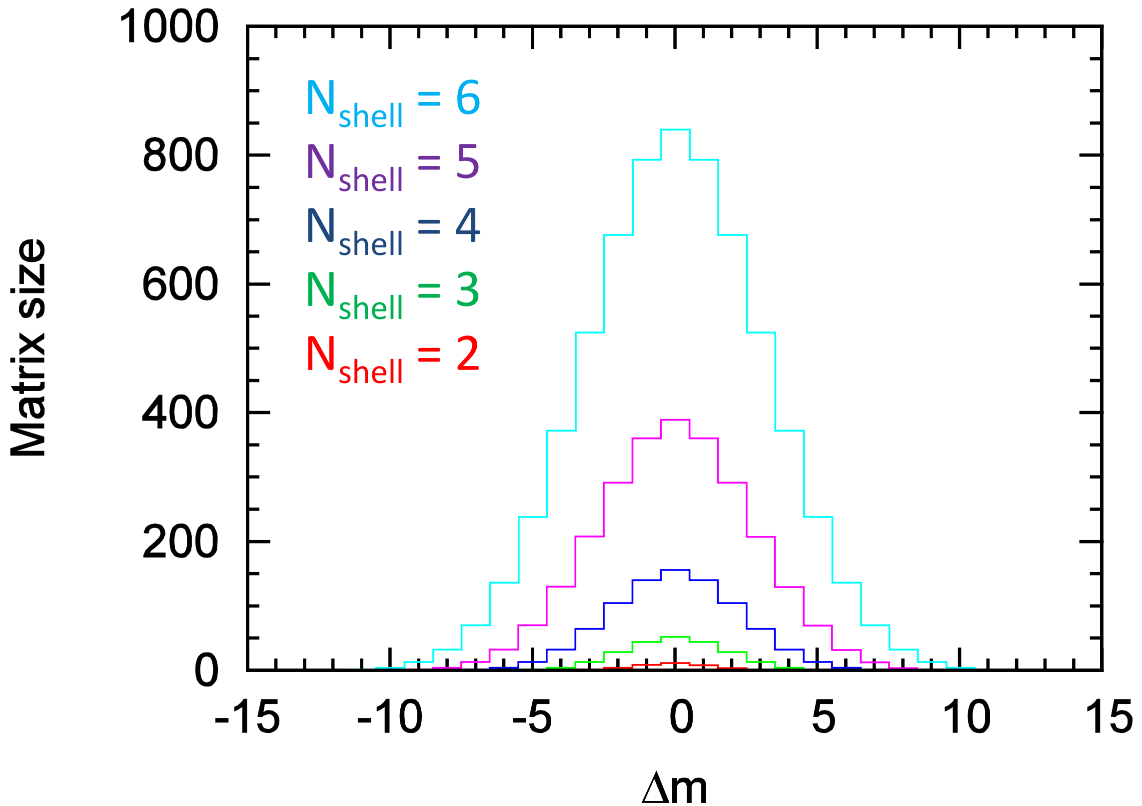
$$\sum_{ijkl} \bar{v}_{ijkl}\rho_{ki}\rho_{lj} = \sum_{\Delta m}\left[\sum_{a\in J_z(a)=-\Delta m}\tilde{\rho}_a\left(\sum_{b\in J_z(b)=\Delta m}\tilde{v}_{ab}\tilde{\rho}_b\right)\right]$$

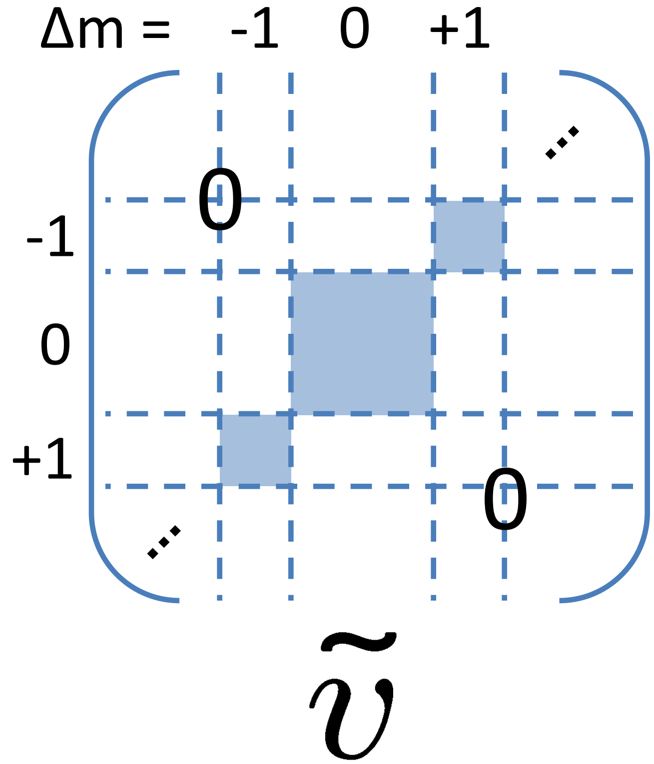


⟶ BLAS Level 3

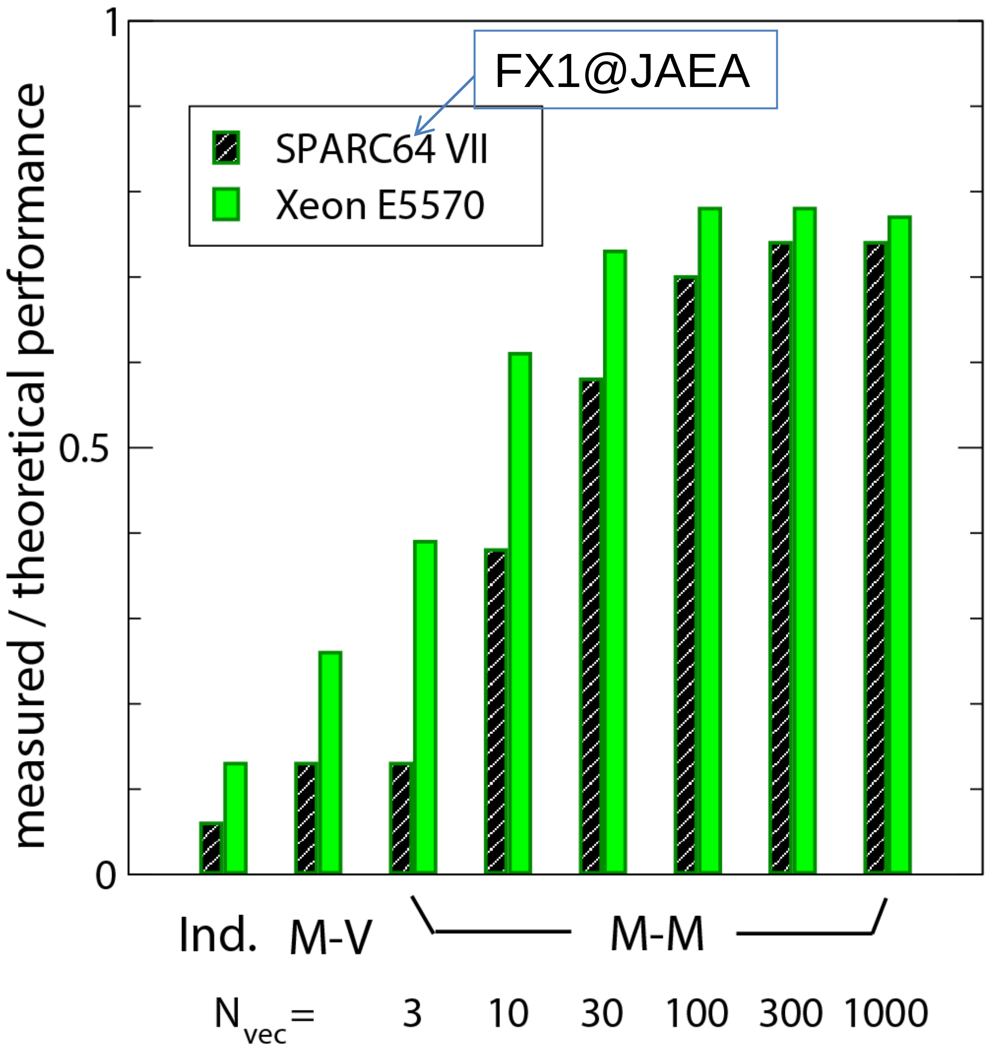
Size of the off-diagonal dense matrix

$$\sum_{ijkl} \bar{v}_{ijkl}\rho_{ki}\rho_{lj} = \sum_{\Delta m}\left[\sum_{a\in J_z(a)=-\Delta m}\tilde{\rho}_a\left(\sum_{b\in J_z(b)=\Delta m}\tilde{v}_{ab}\tilde{\rho}_b\right)\right]$$





Tuning of the density matrix product



Nshell = 5

The performance reaches 80% of the theoretical peak at hot spot.

SPARC64 requires large N_{bunch} in comparison to Xeon

Matrix product e.g.
(390 x 390) x (390 x $2N_{bunch}$)

N_{bunch} controllable tuning parameter
chunk size

Courtesy of Y. Utsuno

Extrapolations in the MCSM

- Two steps of the extrapolation

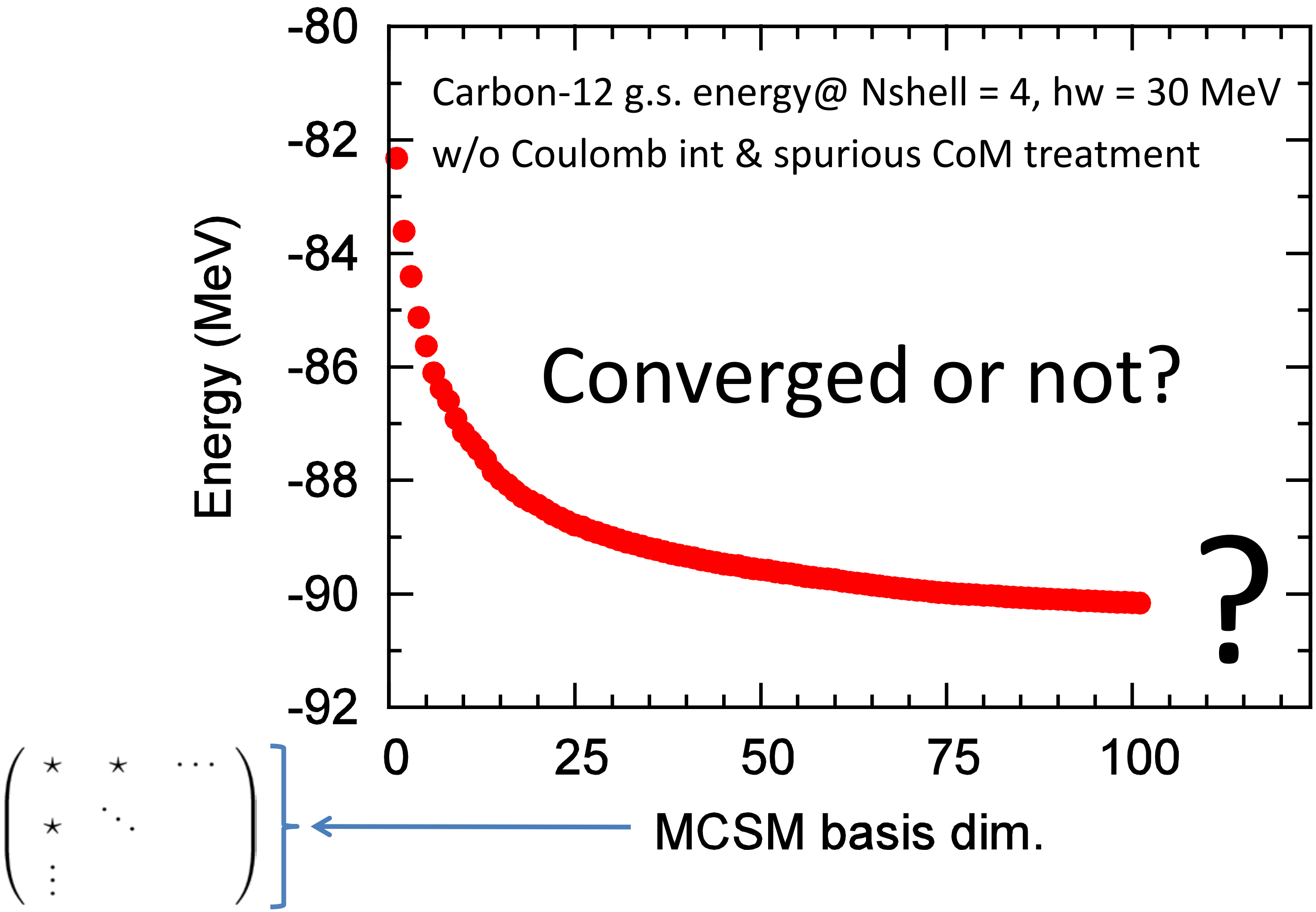
  1. Extrapolation of our MCSM (approx.) results to the FCI (exact) results in fixed model space

     Energy-variance extrapolation

  2. Extrapolation into the infinite model space

     Not applied in the MCSM, so far…

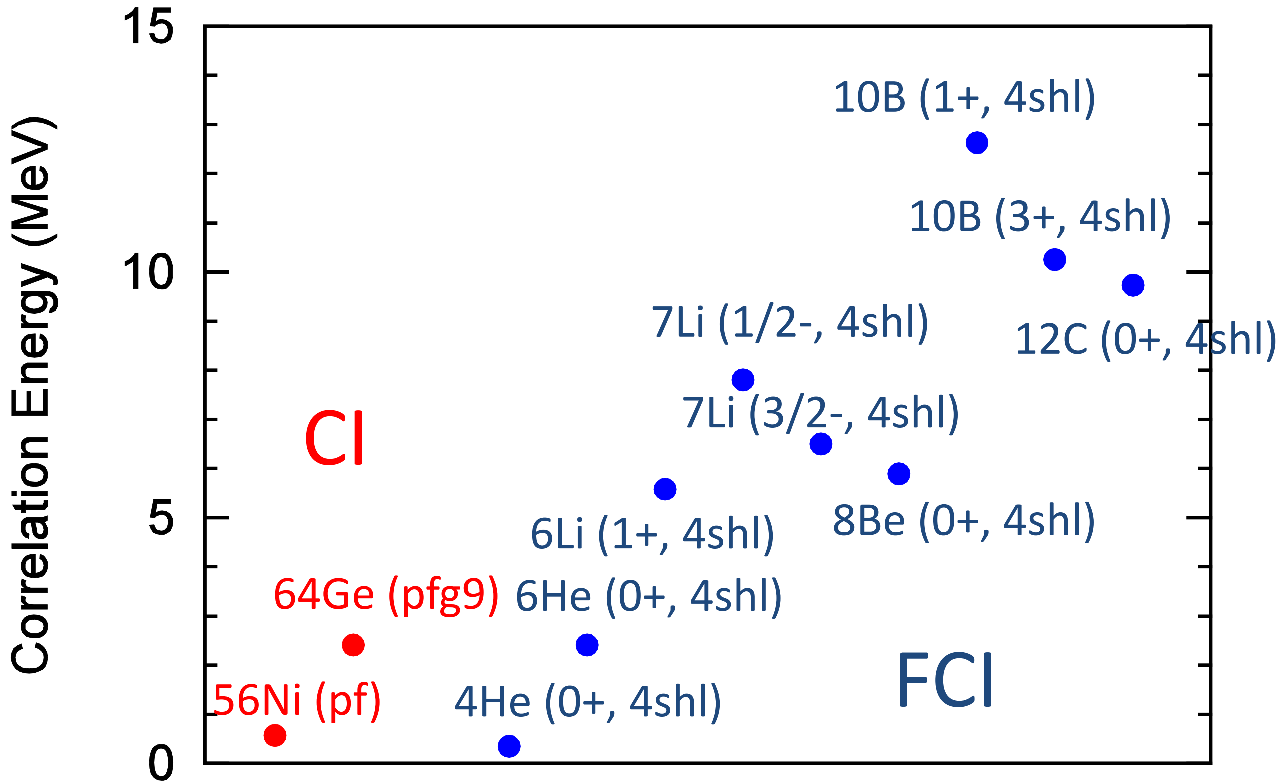
Energy-variance extrapolation



$D_M \sim 6 \times 10^{11}$

Why we need to extrapolate the energies

- Definition: (Correlation Energy) $\equiv \langle\Psi|H|\Psi\rangle_{\mathrm{JHF}} - \langle\Psi|H|\Psi\rangle_{\mathrm{Exact}}$



NCSM wf w/ realistic NN int is more correlated (complicated) than SSM wf w/ effective int

Need energy-variance extrapolation for No-Core MCSM calc

Energy-variance extrapolation

- Originally proposed in condensed matter physics

  Path Integral Renormalization Group method

  M. Imada and T. Kashima, J. Phys. Soc. Jpn 69, 2723 (2000)

- Imported to nuclear physics

  Lanczos diagonalization with particle-hole truncation

  T. Mizusaki and M. Imada Phys. Rev. C65 064319 (2002)

  T. Mizusaki and M. Imada Phys. Rev. C68 041301 (2003)

  single deformed Slater determinant

  T. Mizusaki, Phys. Rev. C70 044316 (2004)

  → Apply to the MCSM (multi deformed SDs)

Numerical effort

8-folded loop
~O(Nsps^8)

$$\frac{\langle\Phi'|\hat{V}^2|\Phi\rangle}{\langle\Phi'|\Phi\rangle} = \sum_{ijkl\alpha\beta\gamma\delta}\bar{v}_{ijkl}\bar{v}_{\alpha\beta\gamma\delta}\left[\frac{1}{4}(1-\rho)_{k\alpha}(1-\rho)_{l\beta}\rho_{\gamma i}\rho_{\delta j} + \rho_{\gamma\alpha}(1-\rho)_{l\beta}\rho_{ki}\rho_{\delta j} + \frac{1}{4}\rho_{ki}\rho_{lj}\rho_{\gamma\alpha}\rho_{\delta\beta}\right]$$

$$= \frac{1}{4}\sum_{ij\alpha\beta}\left(\sum_{kl}\bar{v}_{ijkl}(1-\rho)_{k\alpha}(1-\rho)_{l\beta}\right)\left(\sum_{\gamma\delta}\bar{v}_{\alpha\beta\gamma\delta}\rho_{\gamma i}\rho_{\delta j}\right) + \mathrm{Tr}(\Gamma(1-\rho)\Gamma\rho) + \frac{1}{4}[\mathrm{Tr}(\rho\Gamma)]^2$$

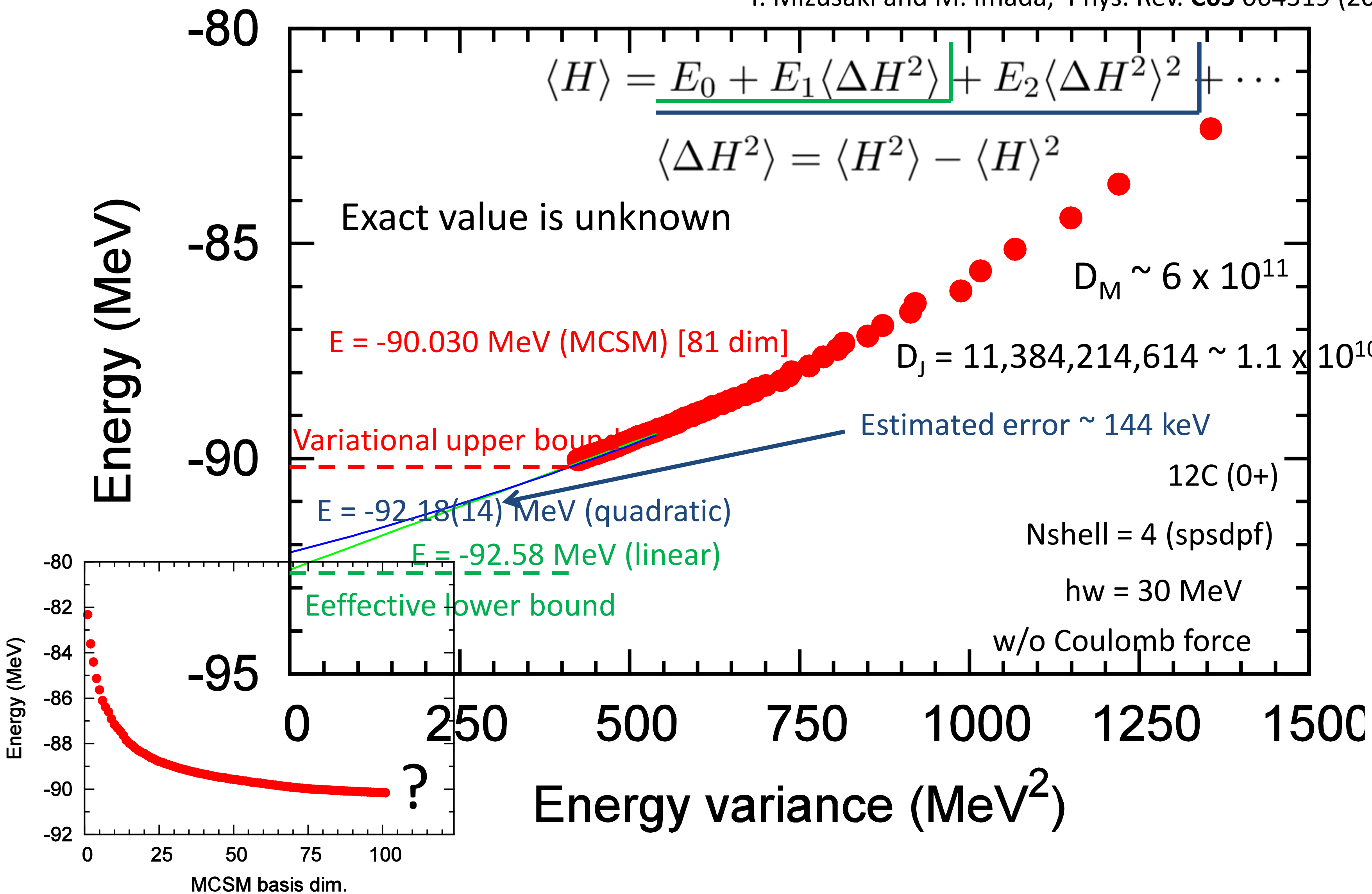
6-folded loop
~O(Nsps^6)

$$\rho_{\beta\alpha} = \frac{\langle\Phi'|c^\dagger_\alpha c_\beta|\Phi\rangle}{\langle\Phi'|\Phi\rangle} \quad \Gamma_{ik} = \sum_{jl}\bar{v}_{ijkl}\rho_{lj} \quad \frac{\langle\Phi'|V|\Phi\rangle}{\langle\Phi'|\Phi\rangle} = \frac{1}{2}\sum_{\alpha\beta\gamma\delta}\bar{v}_{\alpha\beta\gamma\delta}\rho_{\gamma\alpha}\rho_{\delta\beta}$$

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

Extrapolation of 12C Energy

T. Mizusaki and M. Imada, Phys. Rev. **C65** 064319 (2002)



Benchmark results

- Energy
- RMS
- Q-moment
- μ-moment

What we have calculated as Benchmark

- Comparison btw MCSM & FCI (exact diag.) calc
- Nuclei (JP): s- & p-shell nuclei:
  - 4He(0+)
  - 6He(0+)
  - 6Li(1+)
  - 7Li(1/2-, 3/2-)
  - 8Be(0+)
  - 10B(1+, 3+)
  - 12C(0+)
- Observables:
  - BE
  - Point-particle RMS radius (matter)
  - Electromagnetic moments (Q, μ)

Our test set up:
- NN interaction: JISP16
- model space: Nshell = 2, 3, 4, (5)
- optimal hw selected for states & Nshell's
- w/o Coulomb
- w/o Gloeckner-Lawson prescription

MCSM: Abe, Otsuka, Shimizu, Utsuno (Tokyo)
T2K (Tokyo, Tsukuba), BX900 (JAEA)

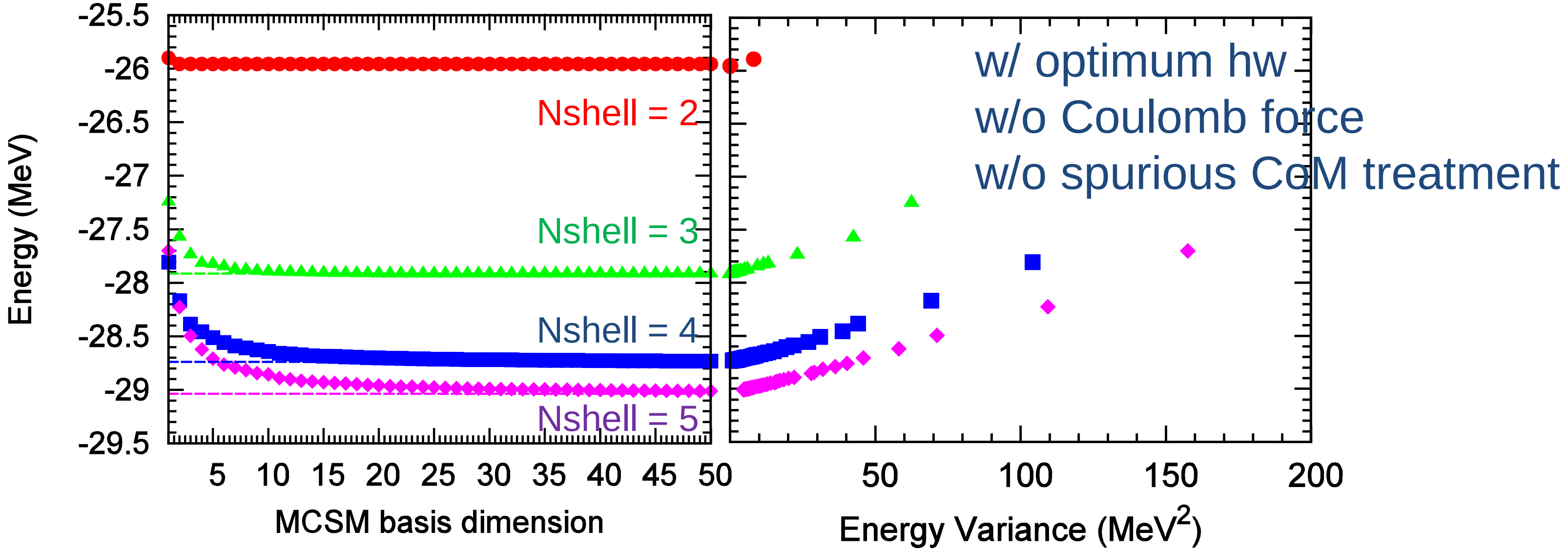
FCI: Maris, Vary (Iowa)
Jaguar, Franklin (NERSC, DOE)

JISP16:
A.M. Shirokov, J.P. Vary, A. I. Mazur, T.A. Weber,
Phys. Lett. B644, 33 (2007)

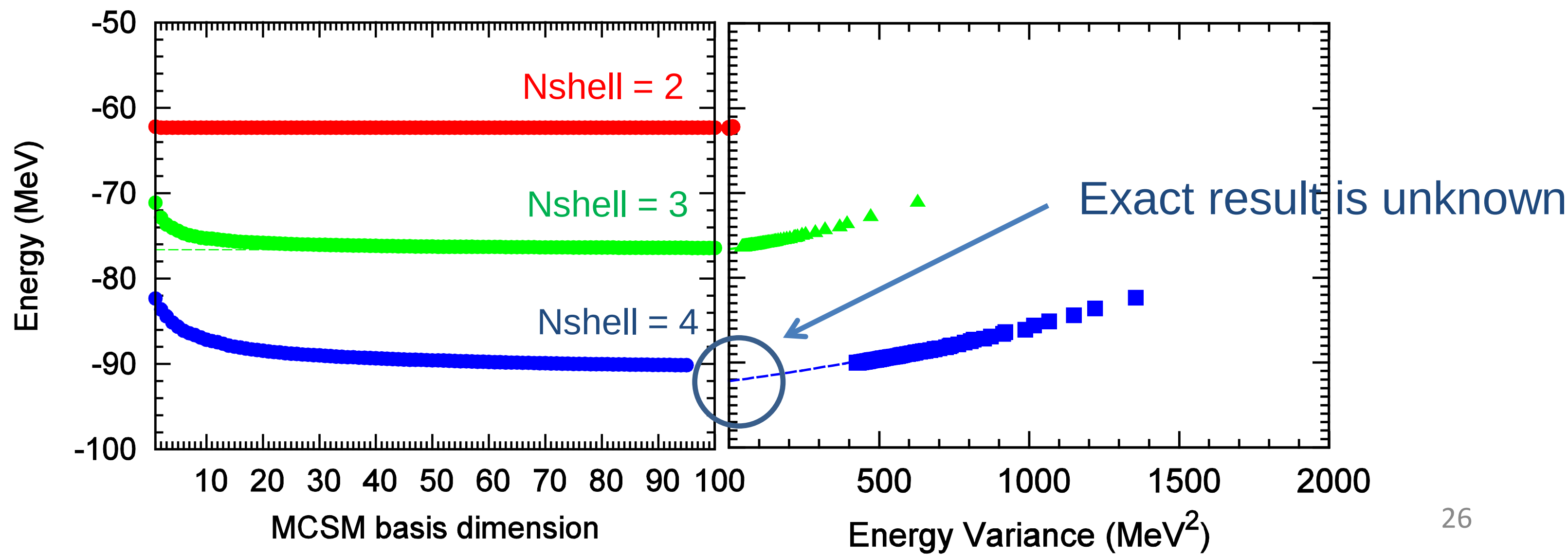
NCFC calc of light nuclei w/ JISP16:
P. Maris, J.P. Vary, A.M. Shirokov,
Phys. Rev. C 79, 014308 (2009)

Helium-4 & carbon-12 gs energies

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

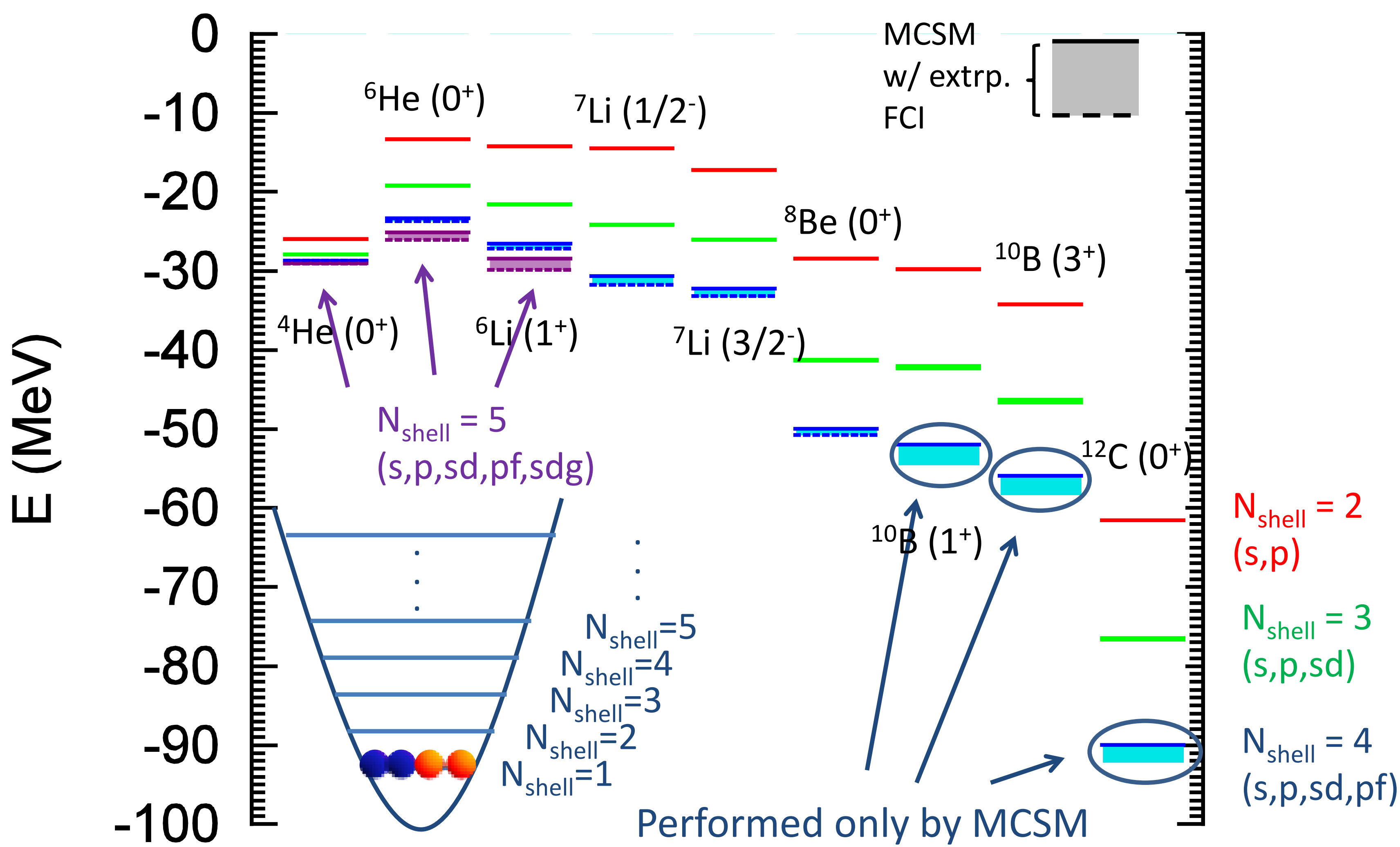


^{12}C(0$^+$;gs)



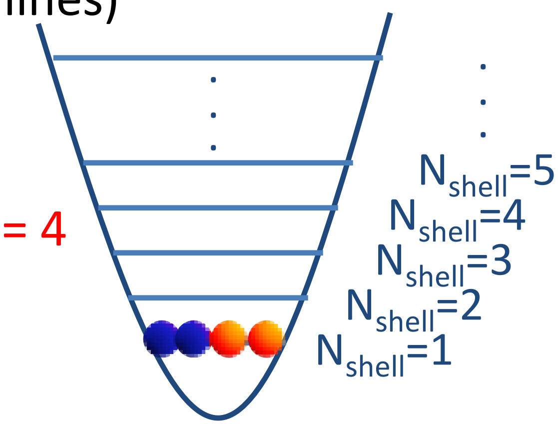
T. Abe, P. Maris, T. Otsuka, N. Shimizu, Y. Utsuno, J. P. Vary

Energies of the Light Nuclei



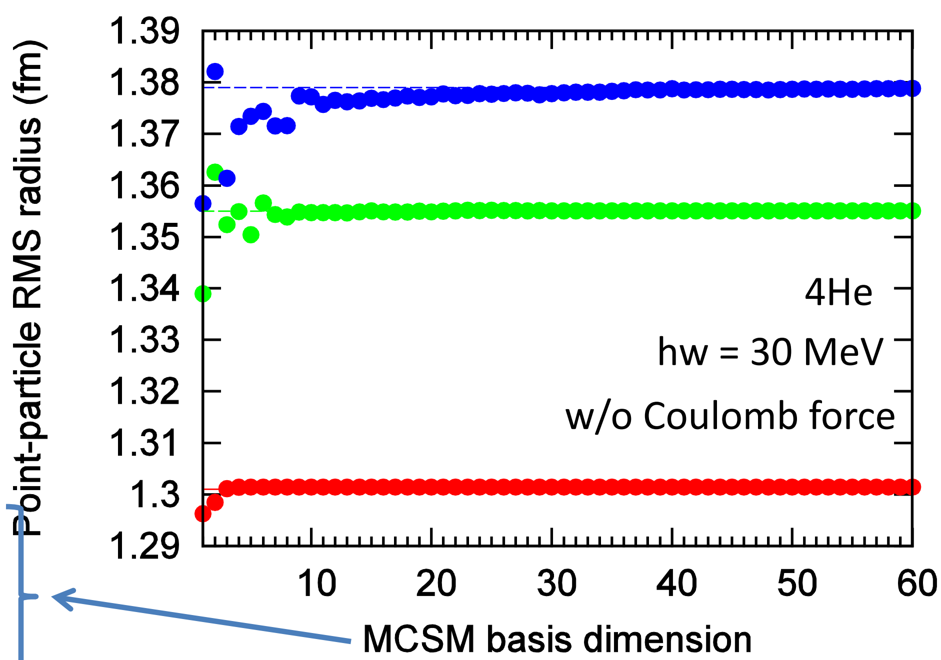
Convergence pattern of the 4He point-particle RMS radius w.r.t. MCSM basis dimension

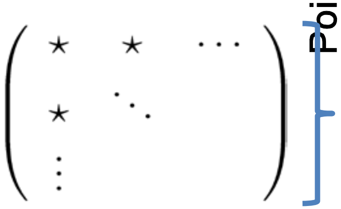
- Comparison of MCSM (solid symbols) w/ FCI (dashed lines) @ Nshell = 2 (sp), 3 (spsd), & 4 (spsdpf)



Good agreement w/ FCI within 0.001 fm up to Nshell = 4

H = Hint + β Hcm, (β = 0)





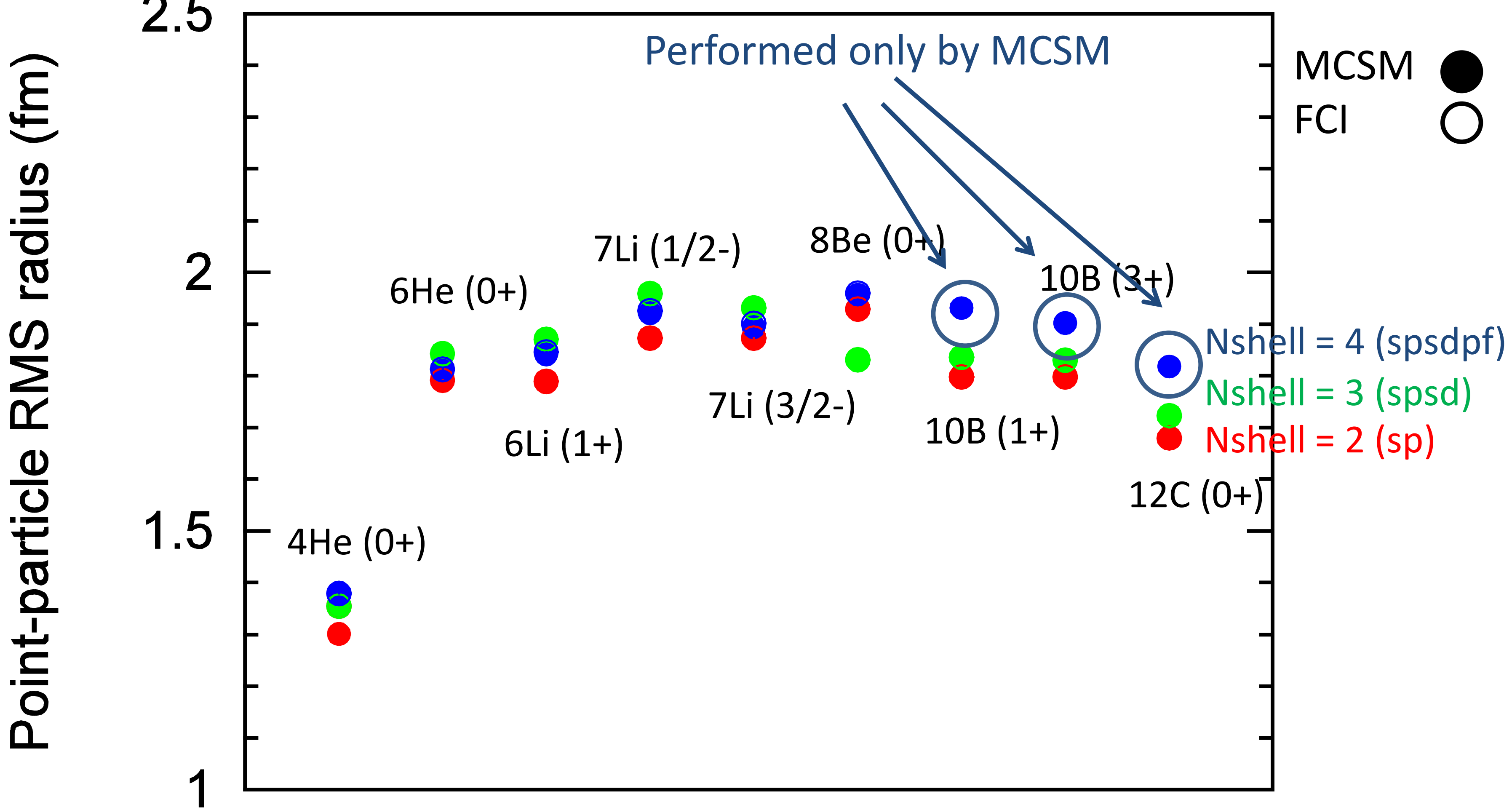
Nshell = 4 (spsdpf)
1.379 fm (MCSM)
1.379 fm (FCI)

Nshell = 3 (spsd)
1.355 fm (MCSM)
1.355 fm (FCI)

Nshell = 2 (sp)
1.301 fm (MCSM)
1.301 fm (FCI)

Point-particle RMS matter Radius

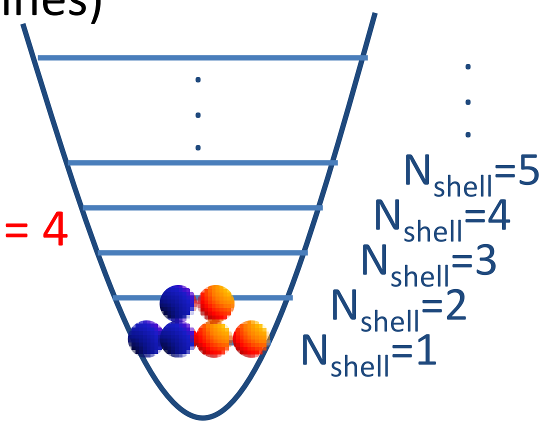
w/ energy-variance extrapolation
by 1st-order polynomial



MCSM & FCI results are consistent within the size of symbols

Convergence pattern of the 6Li Q-moment w.r.t. MCSM basis dimension

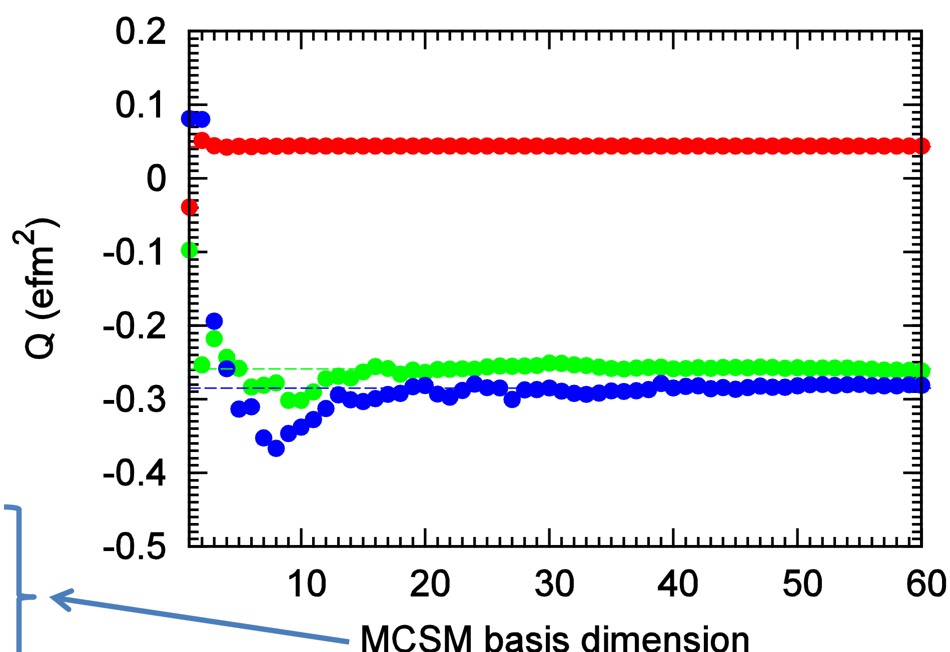
- Comparison of MCSM (solid symbols) w/ FCI (dashed lines) @ Nshell = 2 (sp), 3 (spsd), & 4 (spsdpf)



Good agreement w/ FCI within 0.01 efm^2 up to Nshell = 4

H = Hint + β Hcm, (β = 0)

w/o Coulomb force



N_{shell} = 2 (s,p)
0.044 efm^2 (MCSM)
0.043 efm^2 (FCI)

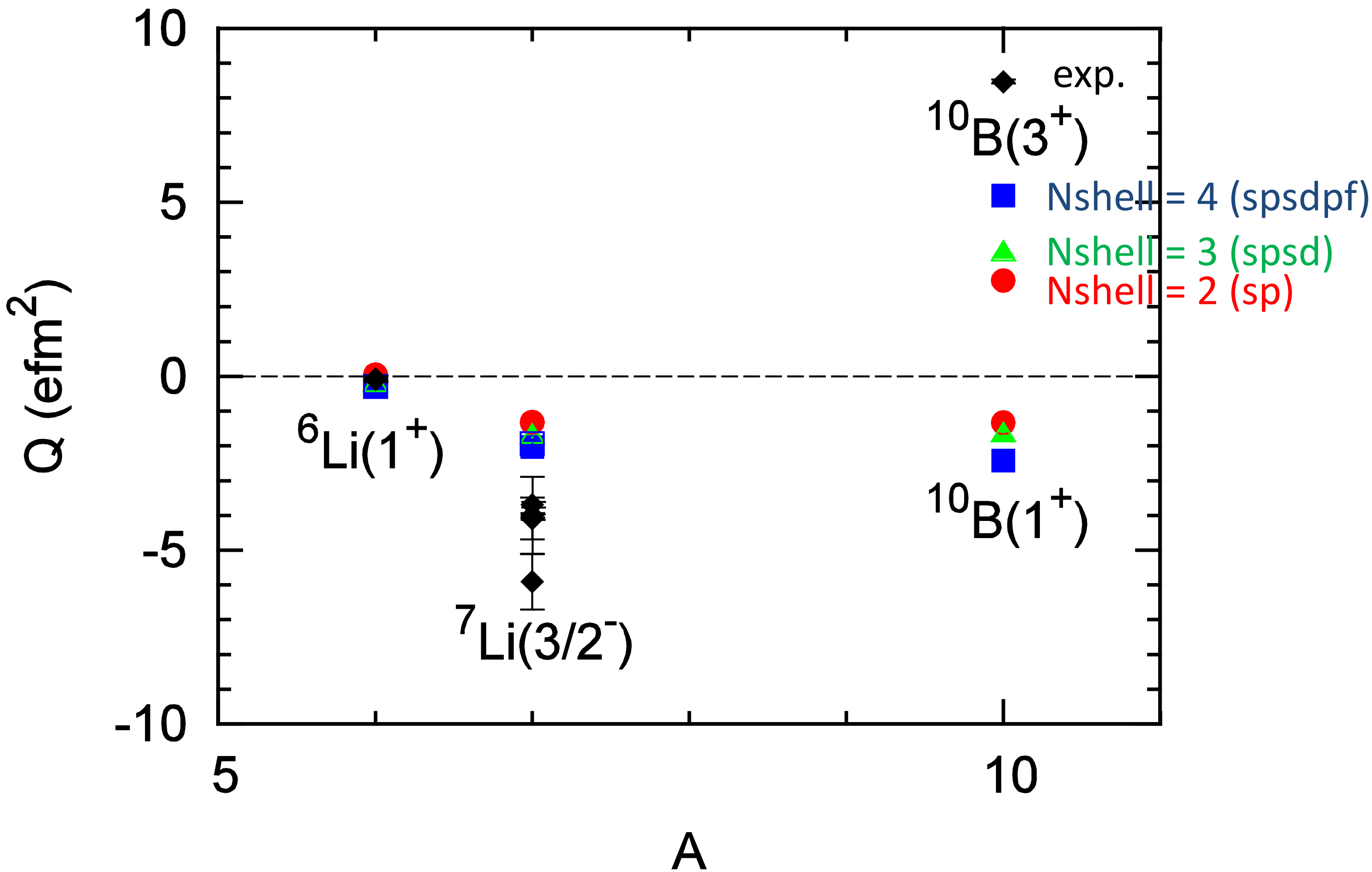
N_{shell} = 3 (s,p,sd)
-0.260 efm^2 (MCSM)
-0.259 efm^2 (FCI)

N_{shell} = 4 (s,p,sd,pf)
-0.280 efm^2 (MCSM)
-0.285 efm^2 (FCI)

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

Q moment

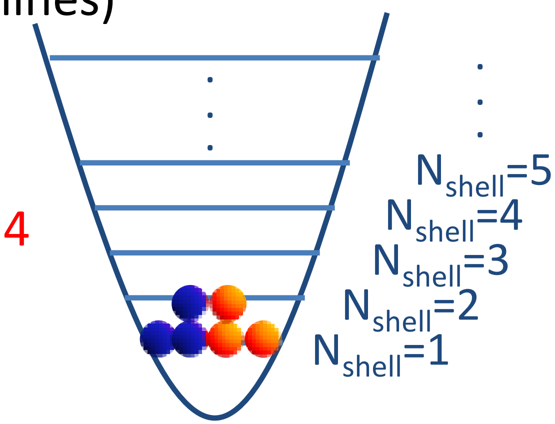
MCSM ●
FCI ○



MCSM & FCI results are consistent within the size of symbols

Convergence pattern of the 6Li μ-moment w.r.t. MCSM basis dimension

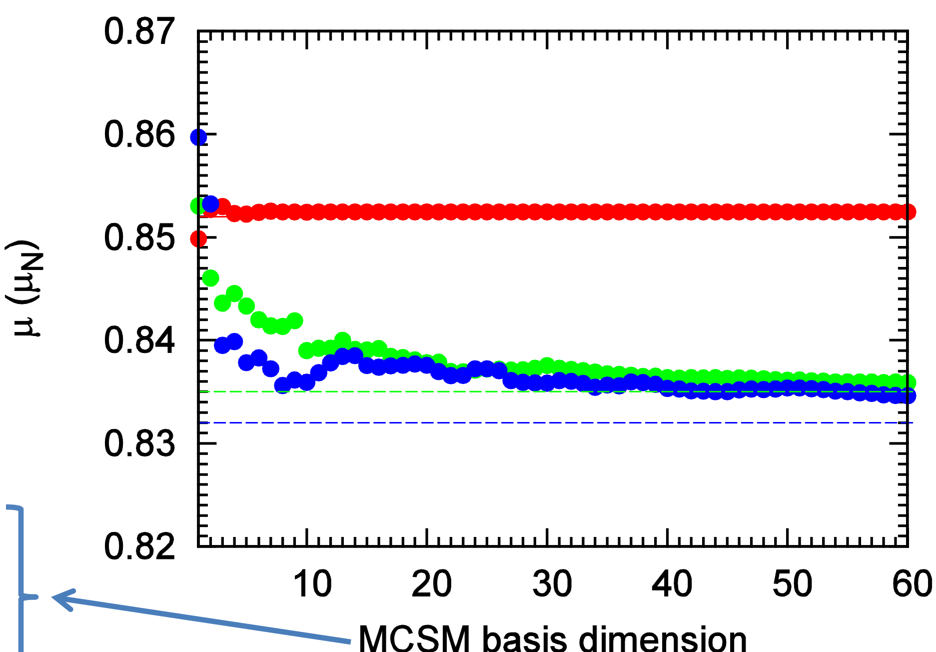
- Comparison of MCSM (solid symbols) w/ FCI (dashed lines) @ Nshell = 2 (s,p), 3 (s,p,sd), & 4 (s,p,sd,pf)



Good agreement w/ FCI within 0.01 μ_N up to Nshell = 4

H = Hint + β Hcm, (β = 0)

w/o Coulomb force



Nshell = 2 (sp)

0.852 μN (MCSM)

0.852 μN (FCI)

Nshell = 3 (spsd)

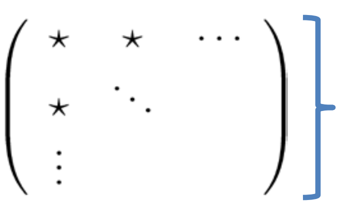
-0.836 μN (MCSM)

-0.833 μN (FCI)

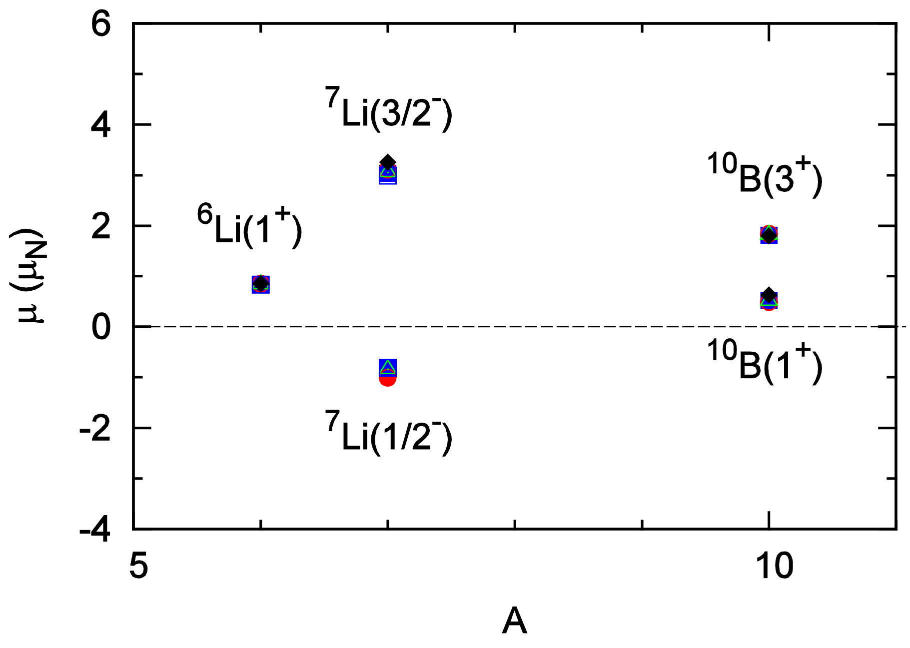
Nshell = 4 (spsdpf)

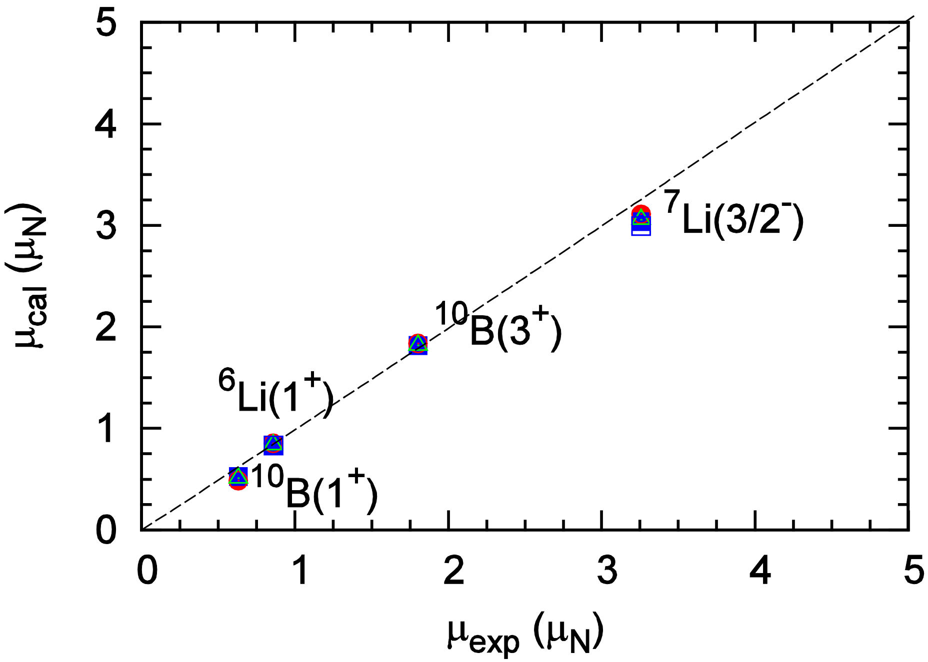
-0.835 μN (MCSM)

-0.832 μN (FCI)



μ moment





MCSM & FCI results are consistent with each other, and μ moments are well-reproduced even at small Nshell.

Summary

- MCSM can be applied to the no-core calculations
  & the benchmarks for the p-shell nuclei have been performed.
  - MCSM & FCI results are consistent with each other.

Outlook

- MCSM algorithm
  - ✓ Spurious CoM (Gloeckner-Lawson prescription)
  - ✓ Coulomb force
  - Larger model spaces (Nshell = 5, 6, …), Nshell vs Nmax?
  - Inclusion of the 3-body force
  - Coupling to the continuum states
- Physics
  - Cluster(-like) states (12C Hoyle state, …)
  - Un-natural parity states
- Tuning of the MCSM code on the K Computer

END