International Workshop
"Nuclear Theory in the Supercomputing Era"

Application of the Monte Carlo shell model to the ab initio no core calculations

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in collaboration with
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Pacific National University, Khabarovsk, Russia
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Outline of this talk

- Motivation
- Monte Carlo Shell Model (MCSM)
- Benchmark s in p-shell nuclei
- Tests in sd-shell nuclei
- Application to K-computer
- Summary & perspective

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

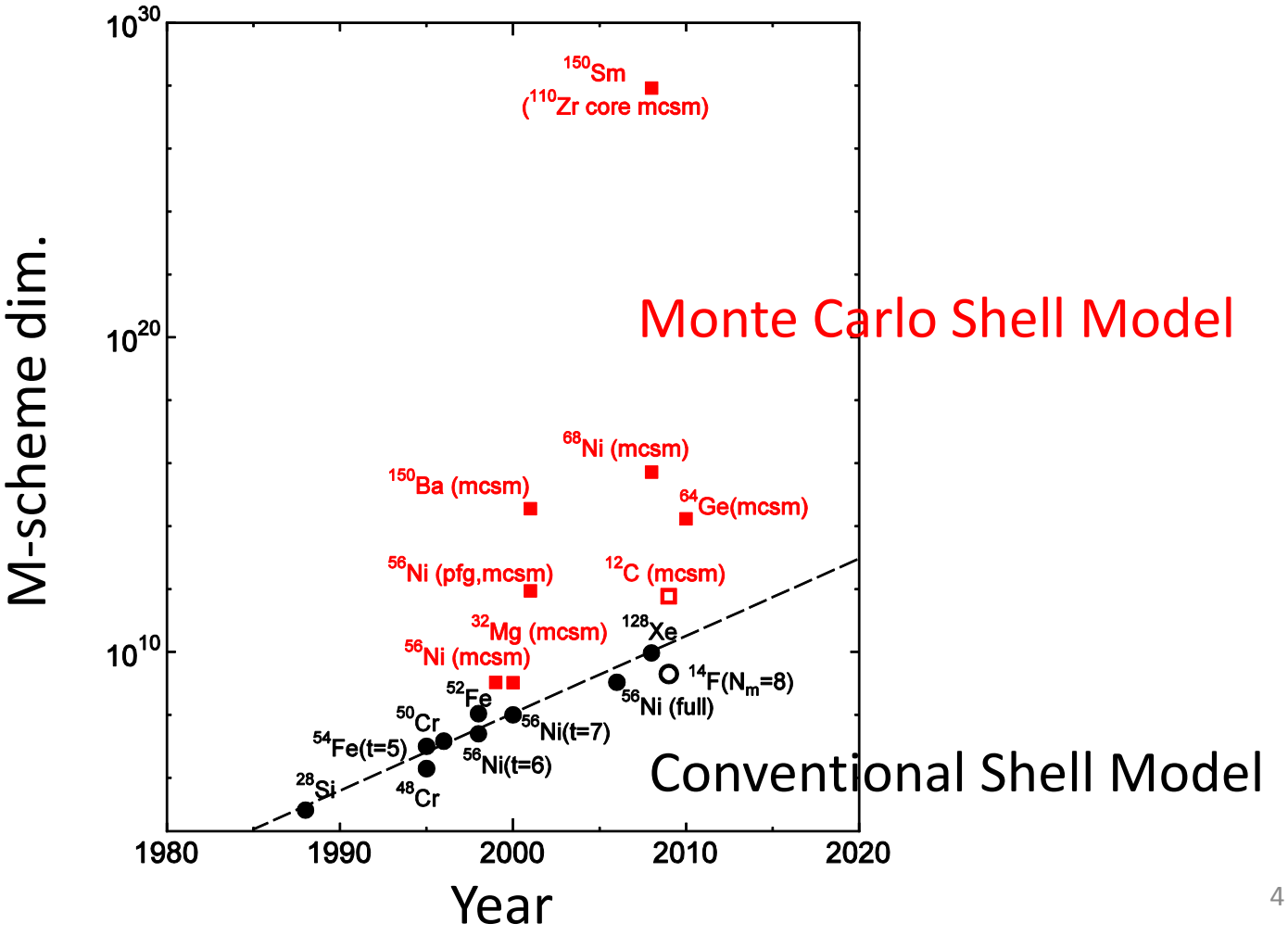
- IT-NCSM, IT-CI: R. Roth (TU Darmstadt), P. Navratil (TRIUMF)
- Sp-NCSM: T. Dytrych, K.D. Sviratcheva, J.P. Draayer, C. Bahri, & J.P. Vary (Louisiana State U, Iowa State U)

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

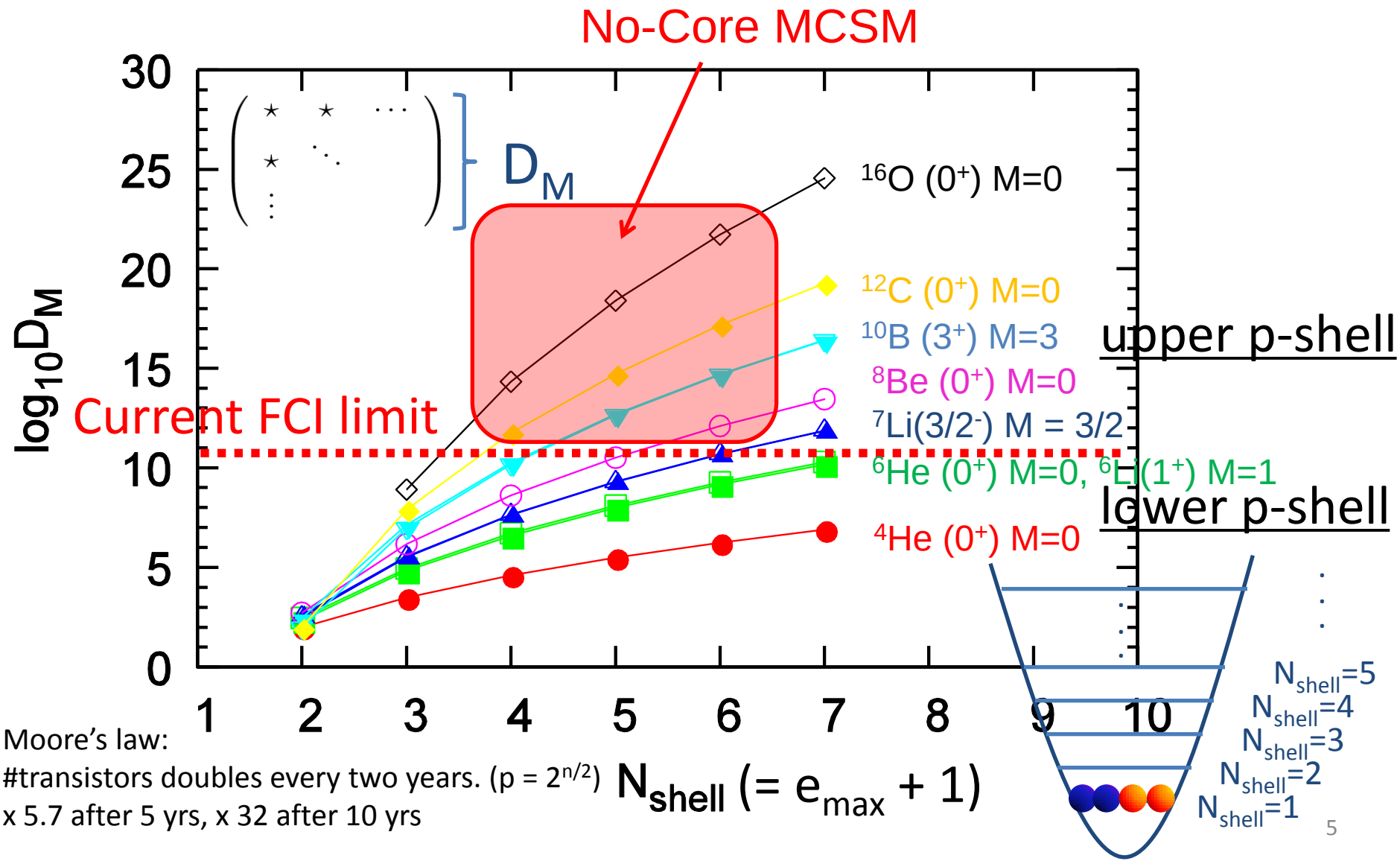
Review: T. Otsuka , M. Honma, T. Mizusaki, N. Shimizu, Y. Utsuno, Prog. Part. Nucl. Phys. 47, 319 (2001)

MCSM w/ a core

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



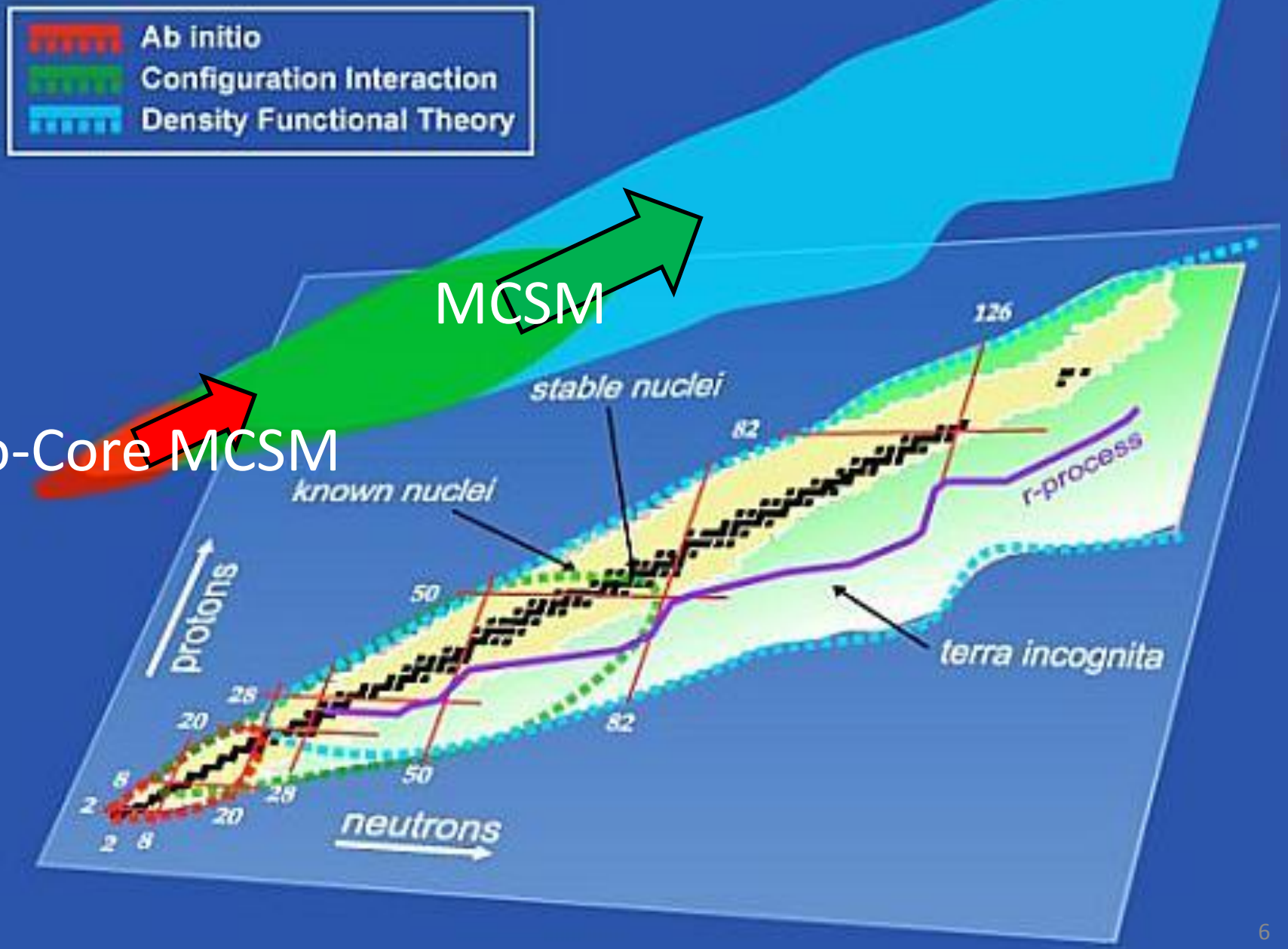
M-scheme dimension of p-shell nuclei



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/



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

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

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} <~ 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

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

This coeff. is obtained by a stochastic sampling.

($c_\alpha^\dagger$ … HO basis)

Sampling of basis functions in the MCSM

- Deformed Slater determinant basis

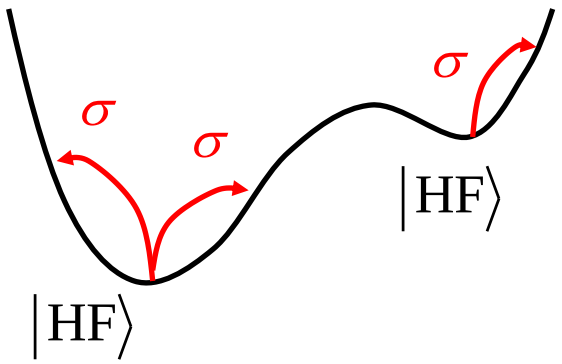
$$|\phi\rangle = \prod_i^A a_i^\dagger |-\rangle \qquad a_i^\dagger = \sum_\alpha^{N_{sps}} c_\alpha^\dagger D_{\alpha i}$$

($c_\alpha^\dagger$ … 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.

$$|\phi(\sigma)\rangle = \prod_{N_\tau} e^{-\Delta\beta h(\sigma)}|\phi\rangle \qquad e^{-\beta H} = \int_{-\infty}^{+\infty} \prod_i d\sigma_i \sqrt{\frac{\beta|V_i|}{2\pi}} e^{-\frac{\beta}{2}|V_i|\sigma_i^2} e^{-\beta h(\vec{\sigma})}$$

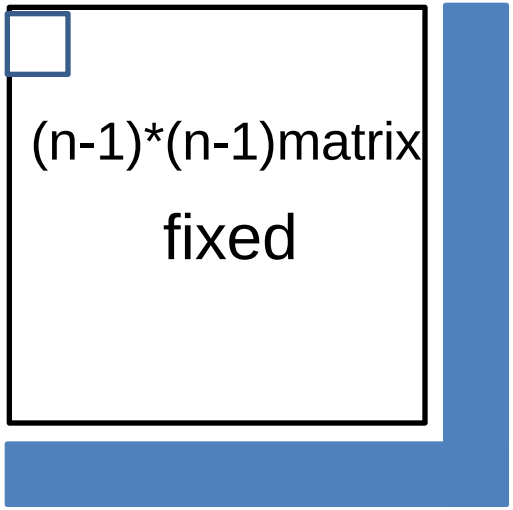
$$h(\sigma) = \sum_i^{N_{AF}} (\epsilon_i + s_i V_i \sigma_i) O_i \qquad H = \sum_i \epsilon_i O_i + \frac{1}{2}\sum_i V_i O_i^2$$

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

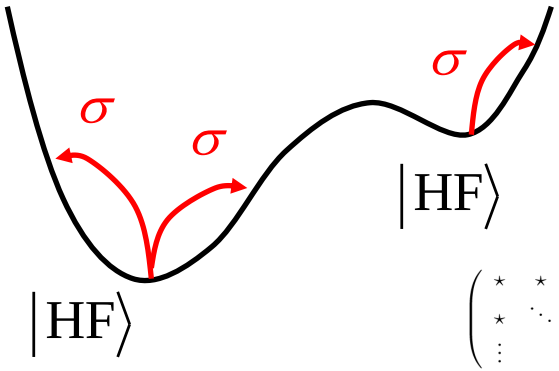
Hamiltonian kernel

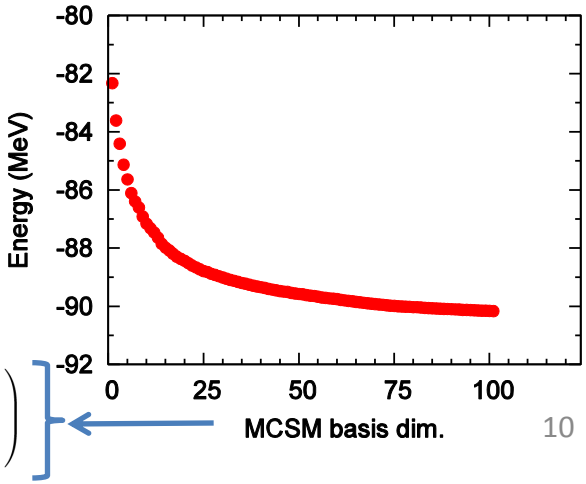
$H(\Phi,\Phi')=$



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

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





Energy minimization by Conjugate Gradient method

Evaluation of the energy variance is time consuming due to the four-body interaction.

$$\left|\Psi(D)\right\rangle = \sum_{n=1}^{N_B} c_i \sum_{K=-J}^{J} g_K P^{J,\Pi}_{MK} \left|\phi(D^{(n)})\right\rangle \quad \left|\phi(D^{(n)})\right\rangle = \prod_{\alpha=1}^{N_p} \left(\sum_{i=1}^{N_{sp}} c_i^{\dagger} D_{i\alpha}^{(n)} \right) \left|-\right\rangle$$

$$E(D) = \left\langle \Psi(D) \middle| H \middle| \Psi(D) \right\rangle$$

Minimize $E(D)$ as a function of D utilizing Conjugate Gradient method

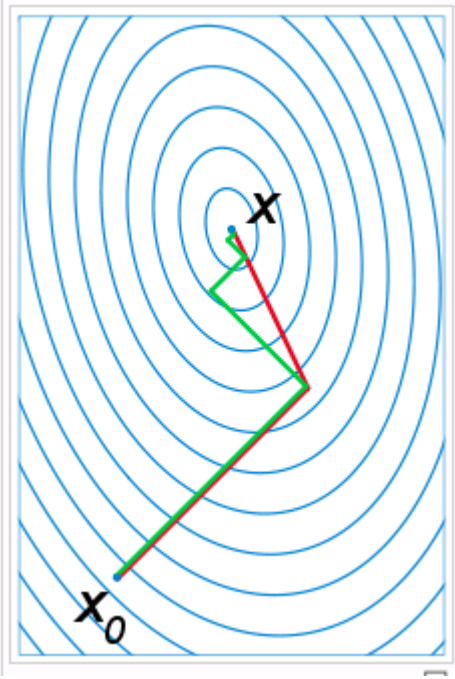
Step1 : Generate basis candidate by auxiliary field technique stochastically

$$\left|\phi(\sigma)\right\rangle = \prod e^{\Delta\beta \cdot h(\sigma)} \cdot \left|\phi^{(0)}\right\rangle$$

and select basis which lowers the energy

Step 2 : Energy expectation value is taken as a function of D, and optimize it using Conjugate Gradient method (VAP)

Iterate these steps every basis till the energy converges



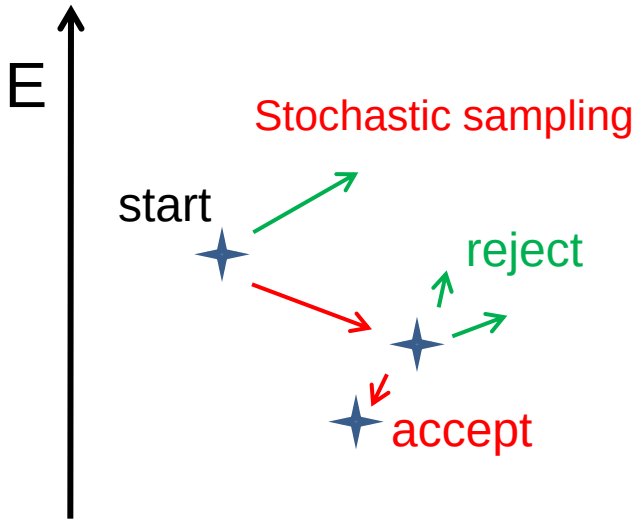
Conjugate gradient taken from wikipedia

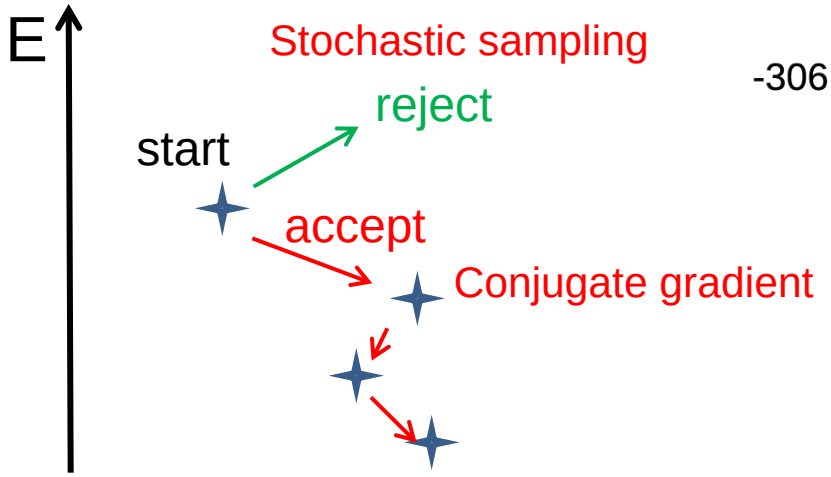
Few Determinant Approximation
M. Honma, B.A.Brown, T. Mizusaki, and T. Otsuka
Nucl. Phys. A 704, 134c (2002)

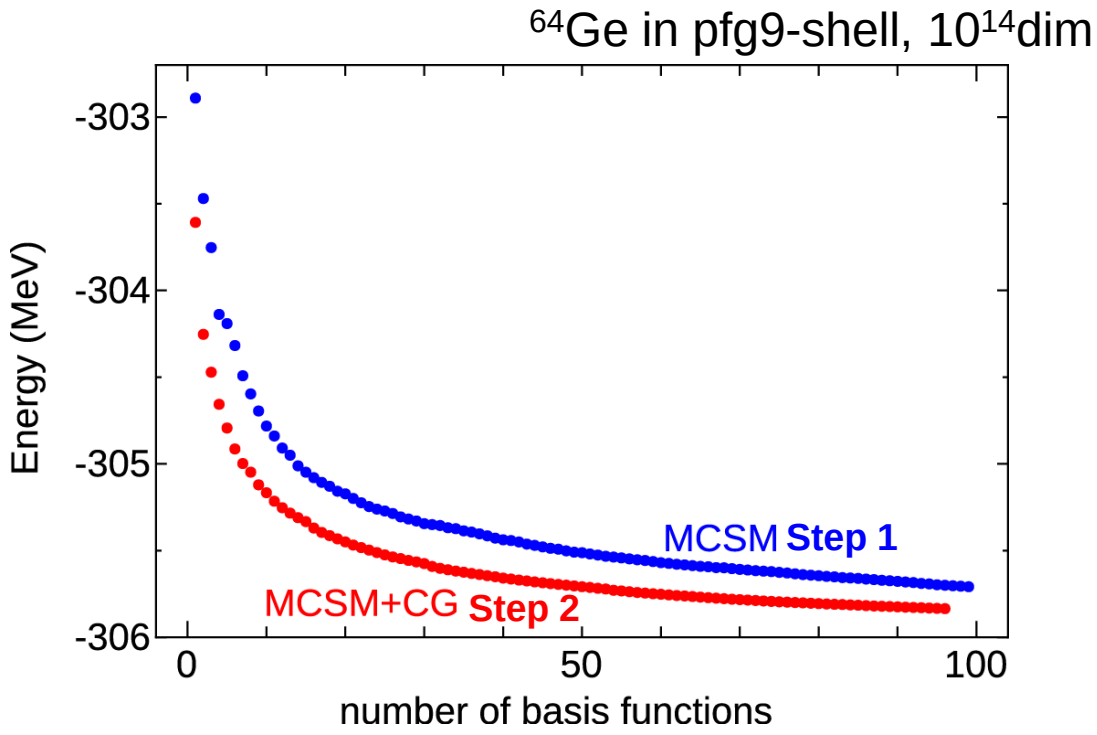
Hybrid Multi-Determinant
G. Puddu, Acta Phys. Polon. B42, 1287 (2011)

VAMPIR
K.W. Schmid, F. Glummer, M. Kyotoku, and A. Faessler
Nucl. Phys. A 452, 493 (1986)

Energy minimization by Conjugate Gradient method







Stochastic sampling before conjugate gradient to minimize the expectation value energy

reduce the number of basis function roughly 30%

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

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

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

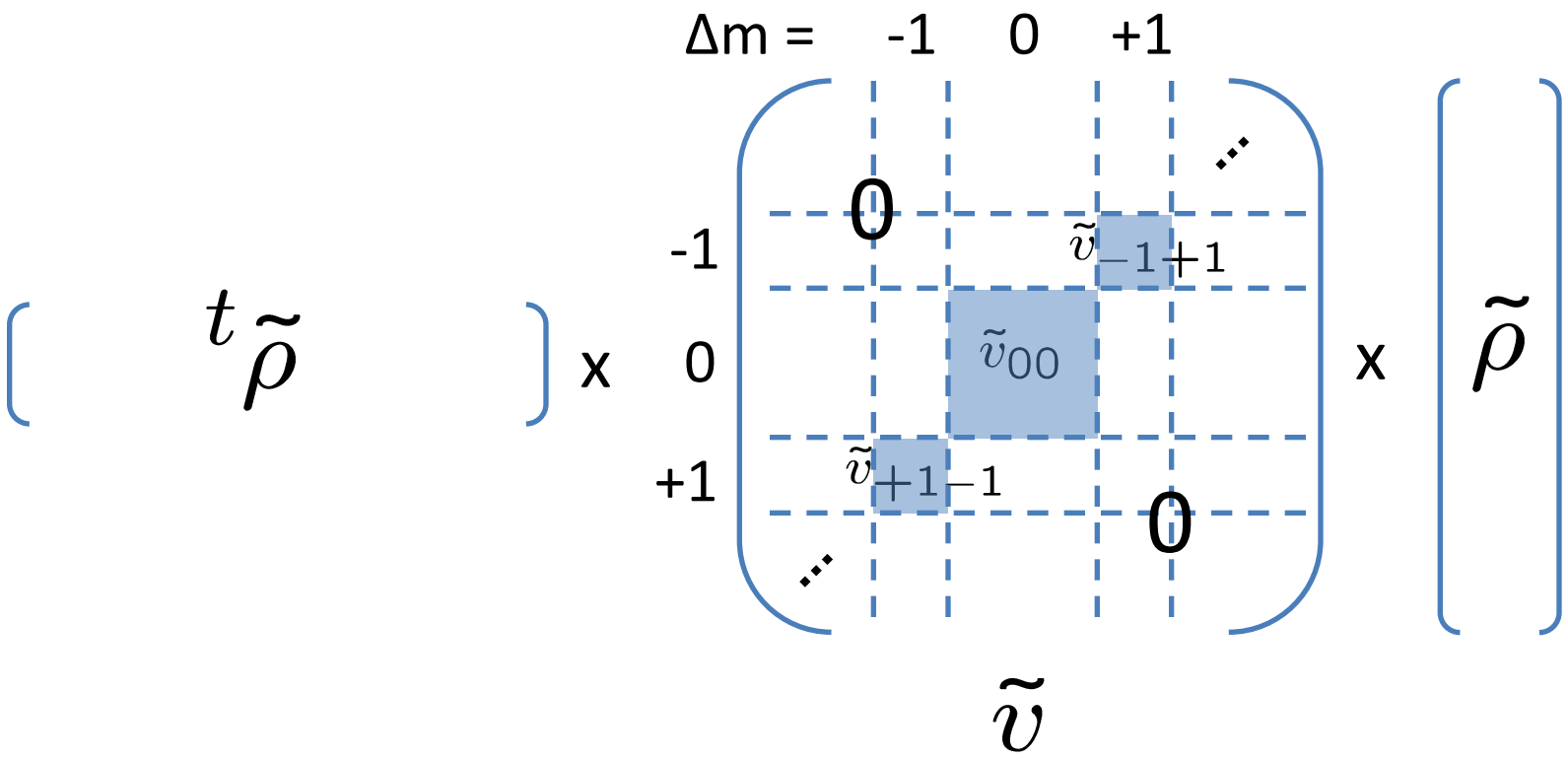
$\bar{v}_{ijkl} \rightarrow \tilde{v}_{ab}$ (sparse → dense)

$\rho_{ki} \rightarrow \tilde{\rho}_a$ $\quad \rho_{lj} \rightarrow \tilde{\rho}_b$

Schematic illustration of the computation of TBMEs

- Matrix-vector method

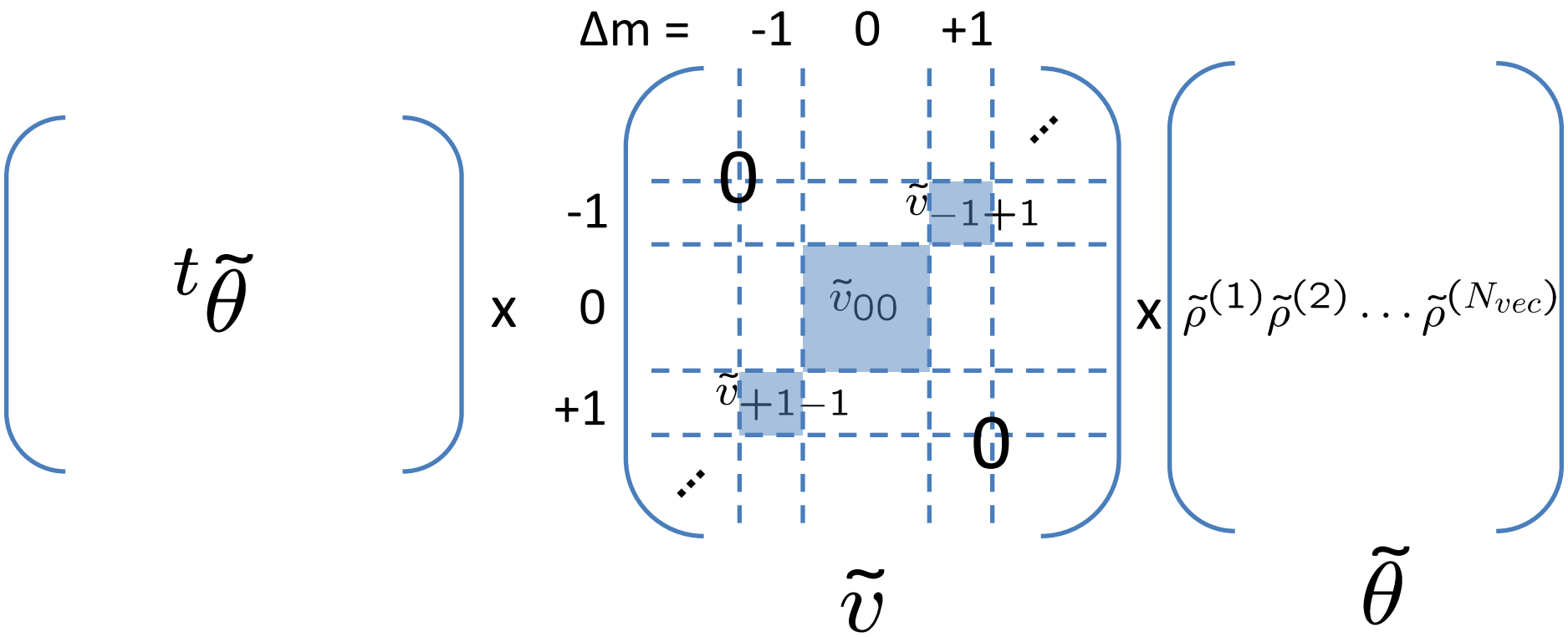
$$\sum_{ijkl} \bar{v}_{ijkl}\rho_{ki}\rho_{lj} = \sum_{\Delta m}\left[\sum_{a\in J_z(a)=-\Delta m} \tilde{\rho}_a \left(\sum_{b\in J_z(b)=\Delta m} \tilde{v}_{ab}\tilde{\rho}_b\right)\right]$$



Schematic illustration of the computation of TBMEs

- Matrix-matrix method

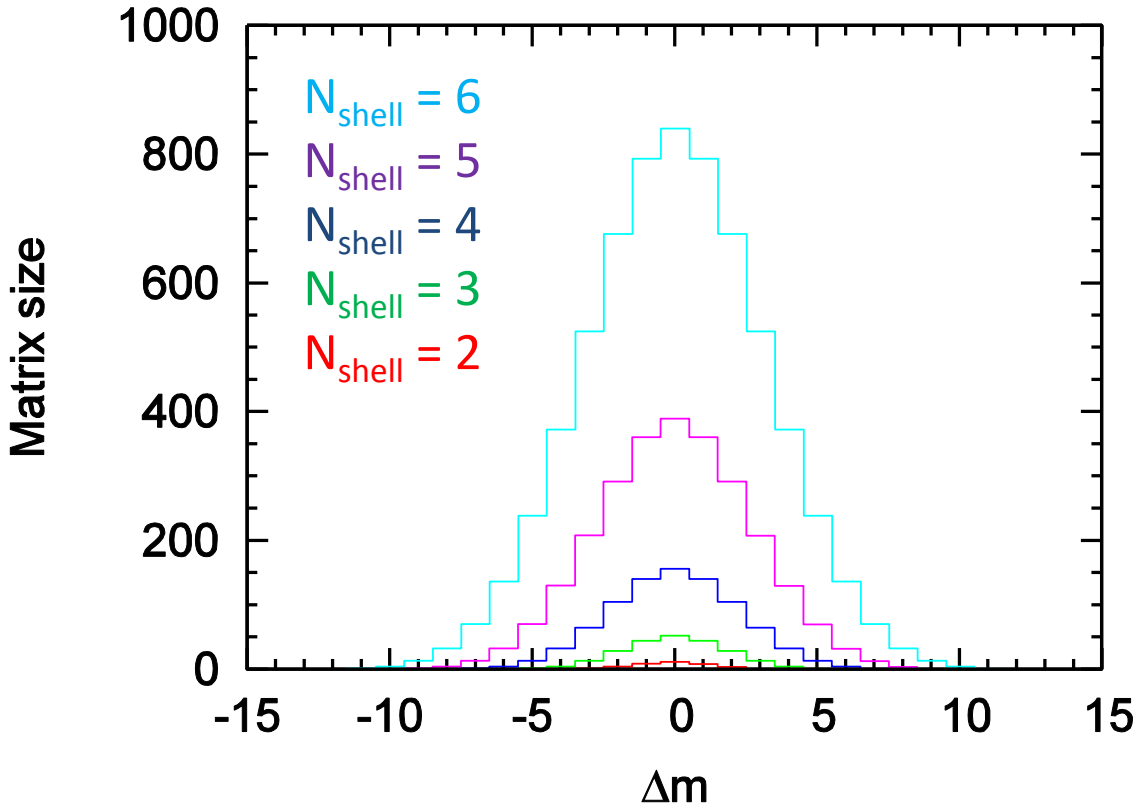
$$\sum_{ijkl} \bar{v}_{ijkl}\rho_{ki}\rho_{lj} = \sum_{\Delta m}\left[\sum_{a\in J_z(a)=-\Delta m} \tilde{\rho}_a \left(\sum_{b\in J_z(b)=\Delta m} \tilde{v}_{ab}\tilde{\rho}_b\right)\right]$$

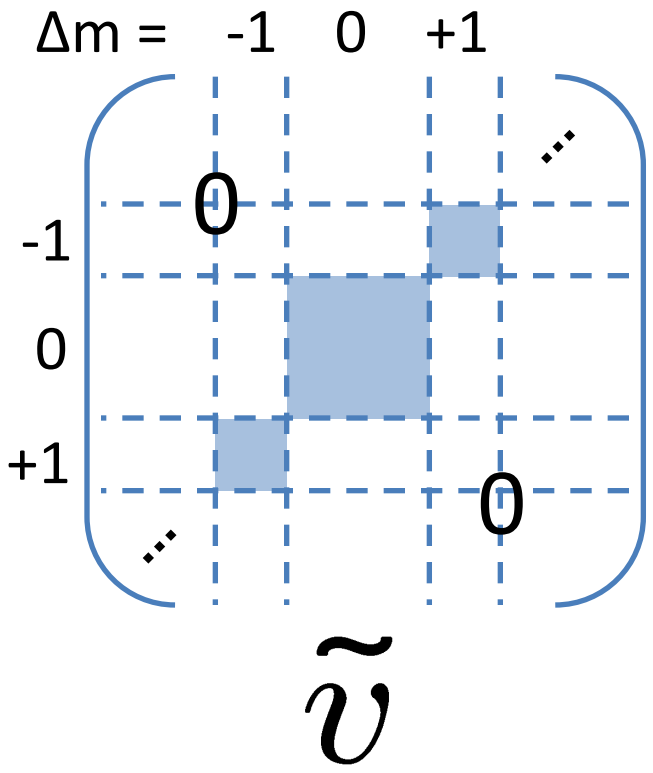


⟶ BLAS Level 3

Size of the off-diagonal dense matrix

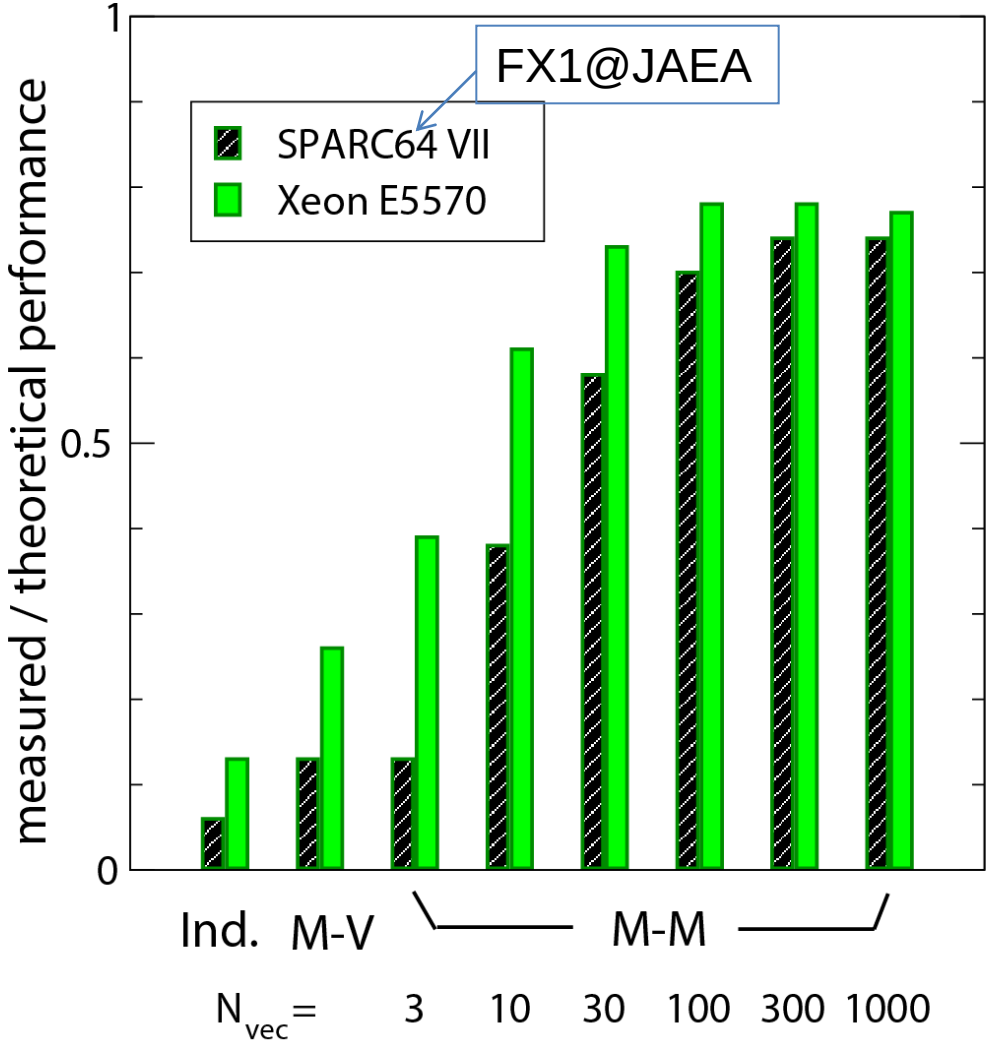
$$\sum_{ijkl} \bar{v}_{ijkl}\rho_{ki}\rho_{lj} = \sum_{\Delta m}\left[\sum_{a\in J_z(a)=-\Delta m} \tilde{\rho}_a \left(\sum_{b\in J_z(b)=\Delta m} \tilde{v}_{ab}\tilde{\rho}_b\right)\right]$$





Y. Utsuno, N. Shimizu, T. Otsuka, T. Abe, arXiv:1202.2957

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

Extrapolations in the MCSM

- Two steps of the extrapolation

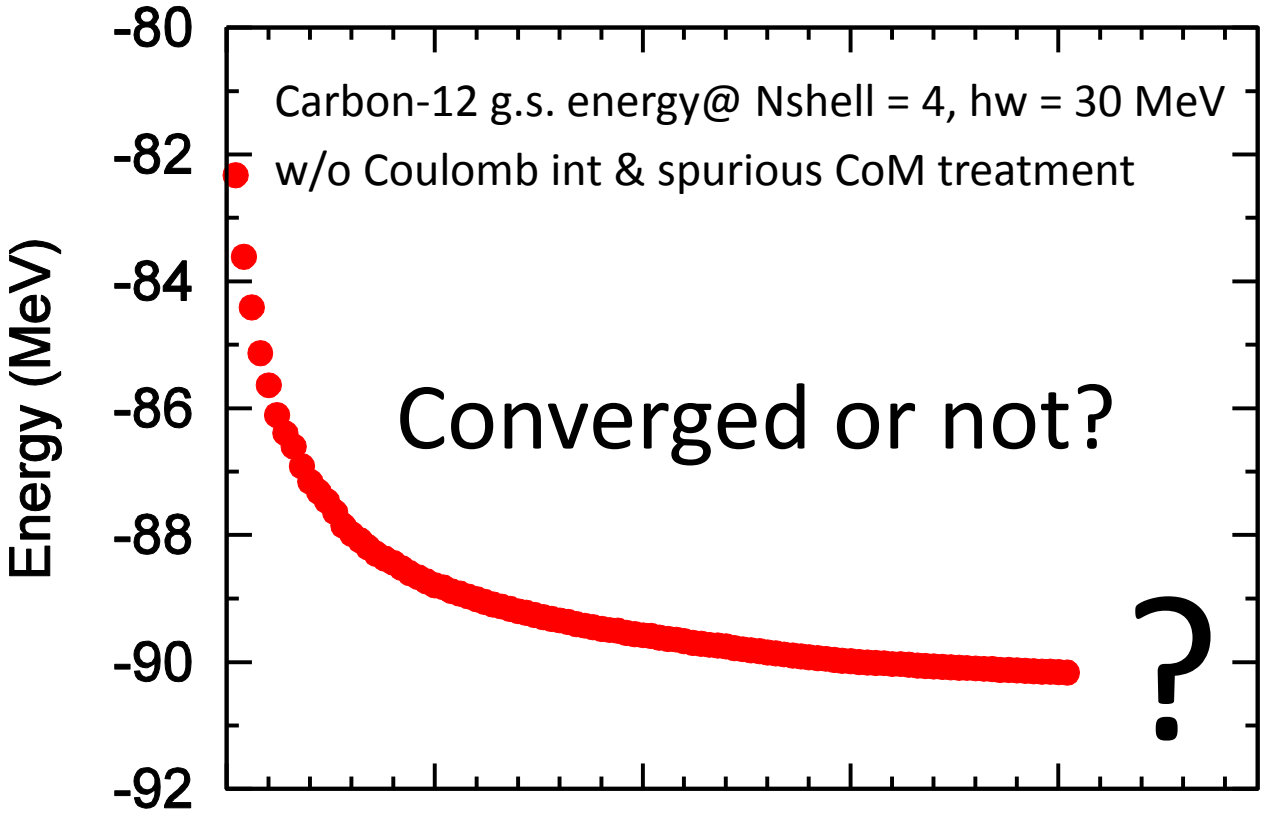
  1. Extrapolation of our MCSM (approx.) results to the FCI (exact) results in fixed model space

     Energy-variance extrapolation

  2. Extrapolation into the infinite model space

     Not applied in the MCSM, so far…

Energy-variance extrapolation

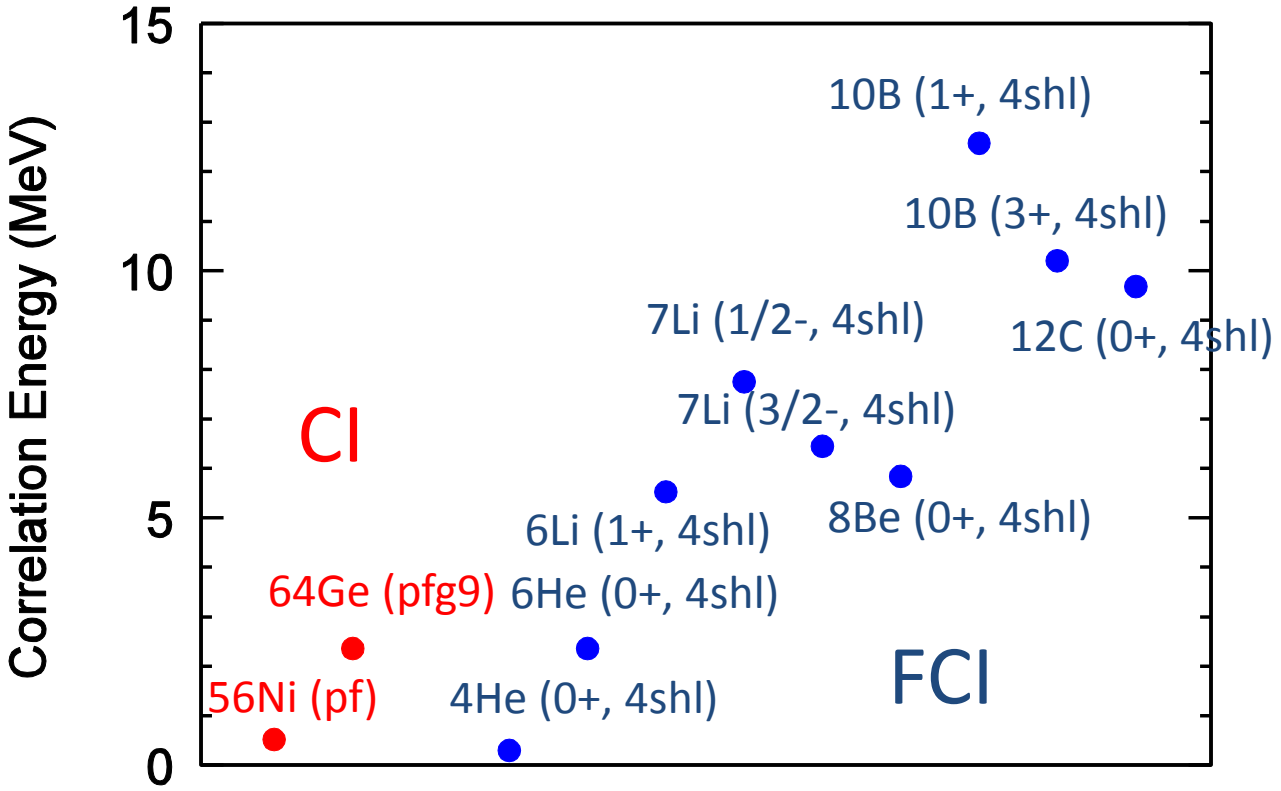


$D_M \sim 6 \times 10^{11}$

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

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)

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

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

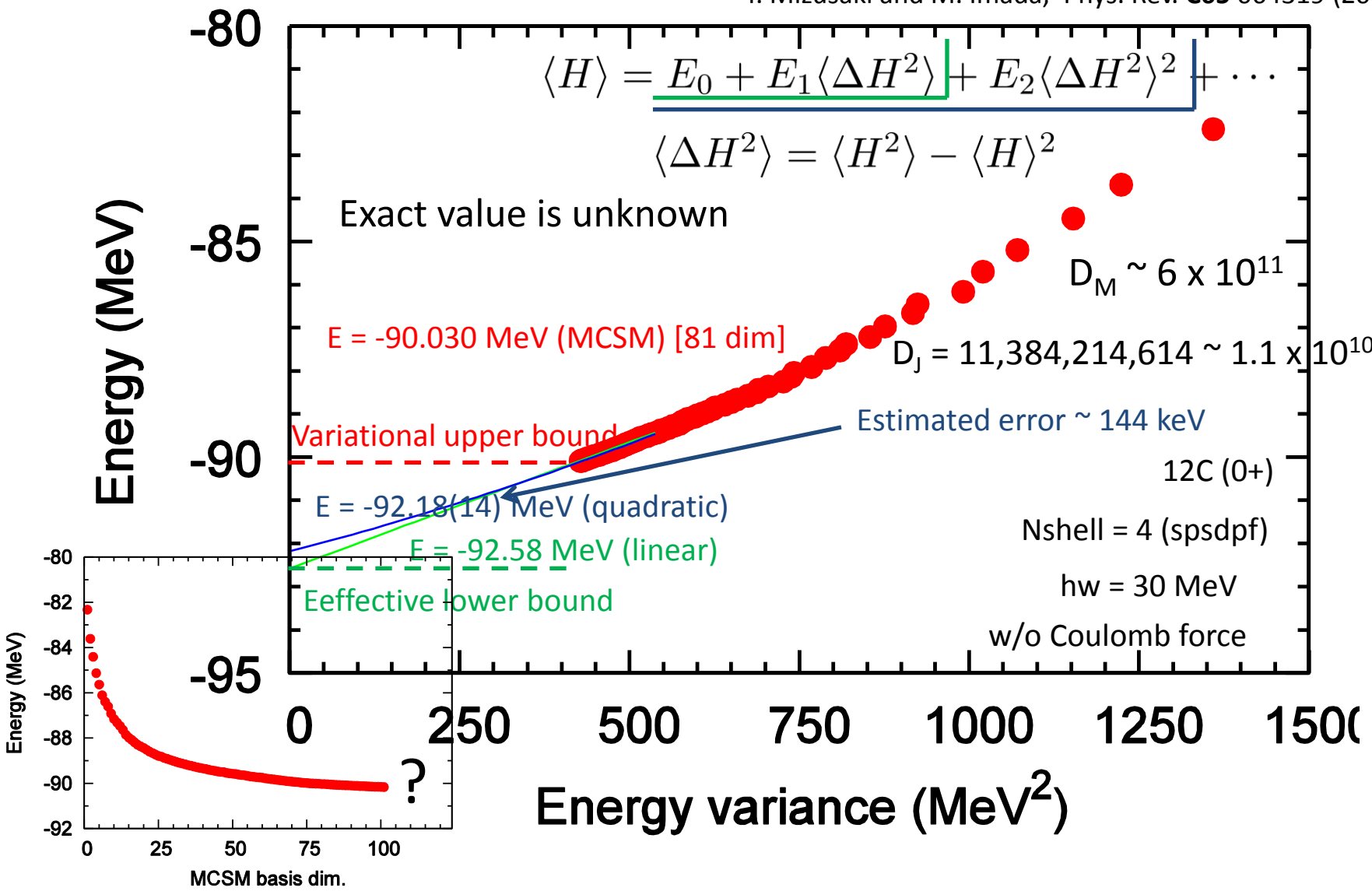
6-folded loop
~O(Nsps^6)

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

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

T. Abe, P. Maris, T. Otsuka, N. Shimizu, Y. Utsuno, J. P. Vary, arXiv:1204.1755

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)

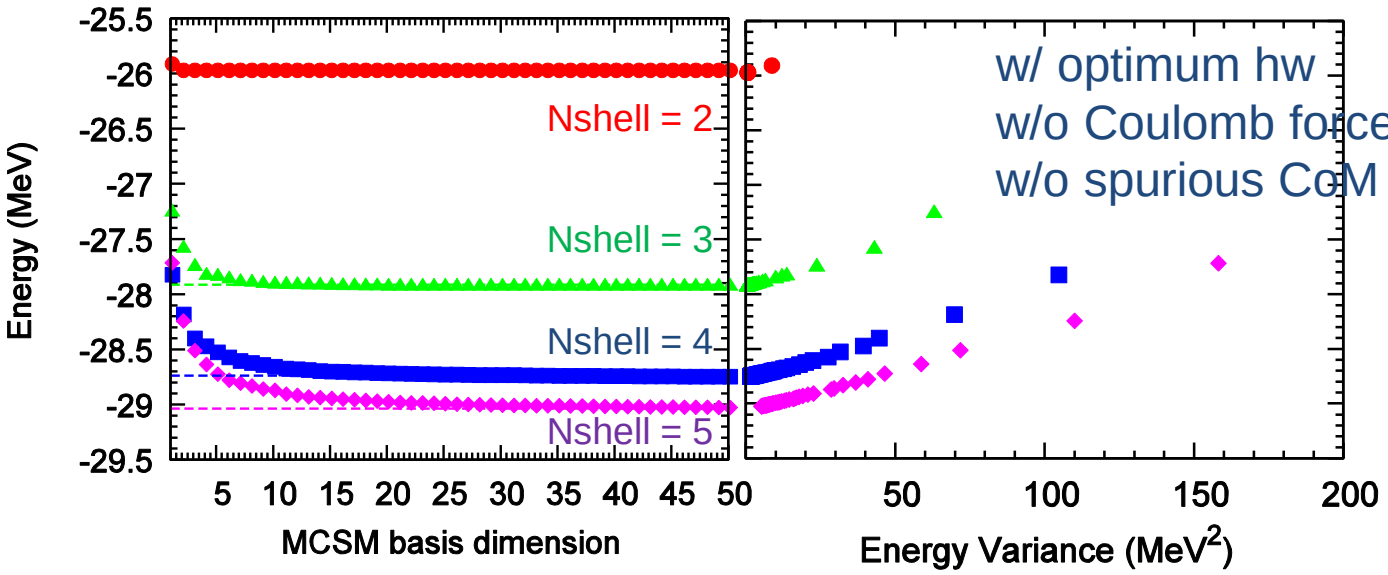
Our test set up:
- NN interaction: JISP16
- model space: Nshell = 2, 3, 4, (5)
- optimal hw selected for states & Nshell's
- w/o Coulomb
- w/o Gloeckner-Lawson prescription

MCSM: Abe, Otsuka, Shimizu, Utsuno (Tokyo)
T2K (Tokyo, Tsukuba), BX900 (JAEA)
FCI: Maris, Vary (Iowa)
Jaguar, Franklin (NERSC, DOE)

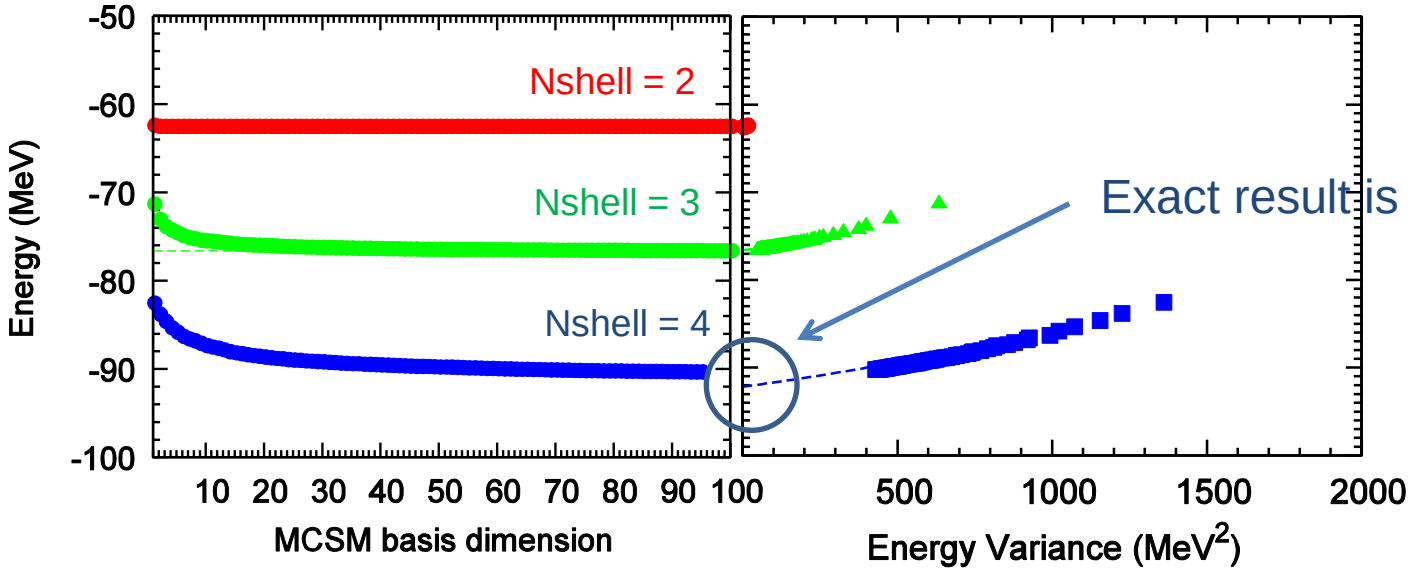
JISP16:
A.M. Shirokov, J.P. Vary, A. I. Mazur, T.A. Weber, Phys. Lett. B644, 33 (2007)
NCFC calc of light nuclei w/ JISP16:
P. Maris, J.P. Vary, A.M. Shirokov, Phys. Rev. C 79, 014308 (2009)

Helium-4 & carbon-12 gs energies

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

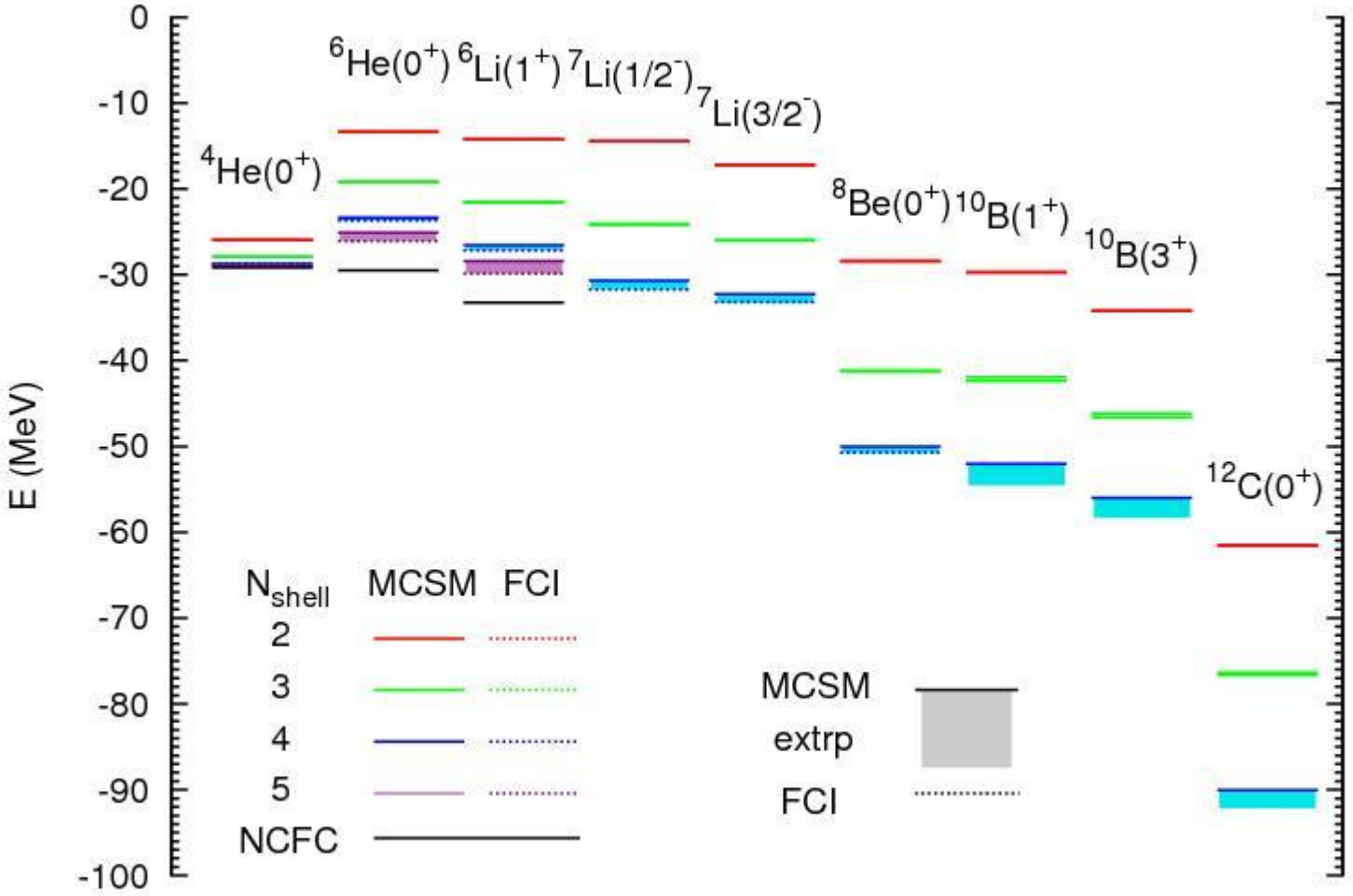


$^{12}C(0^+;gs)$



T. Abe, P. Maris, T. Otsuka, N. Shimizu, Y. Utsuno, J. P. Vary, arXiv:1204.1755

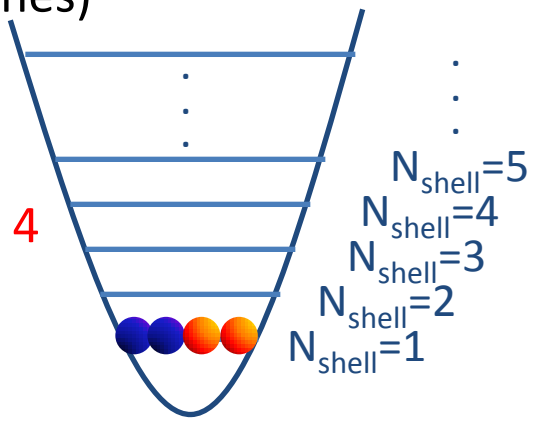
Energies of the Light Nuclei



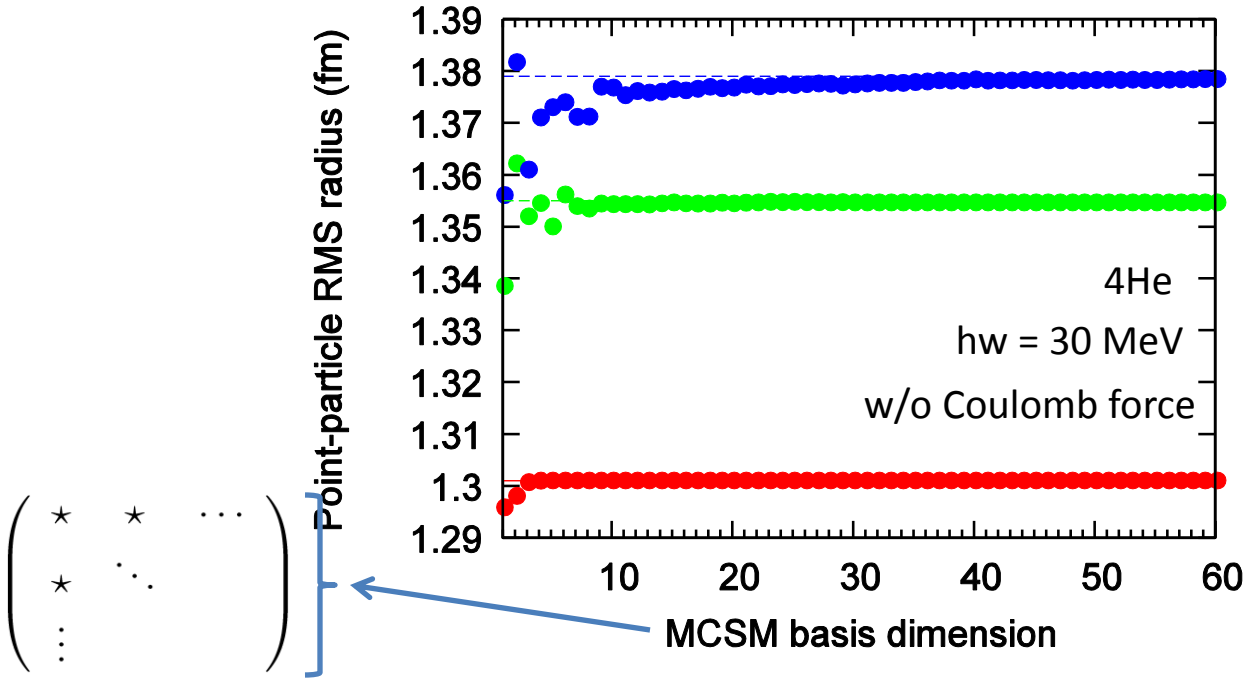
Convergence pattern of the 4He point-particle RMS radius w.r.t. MCSM basis dimension

- 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)

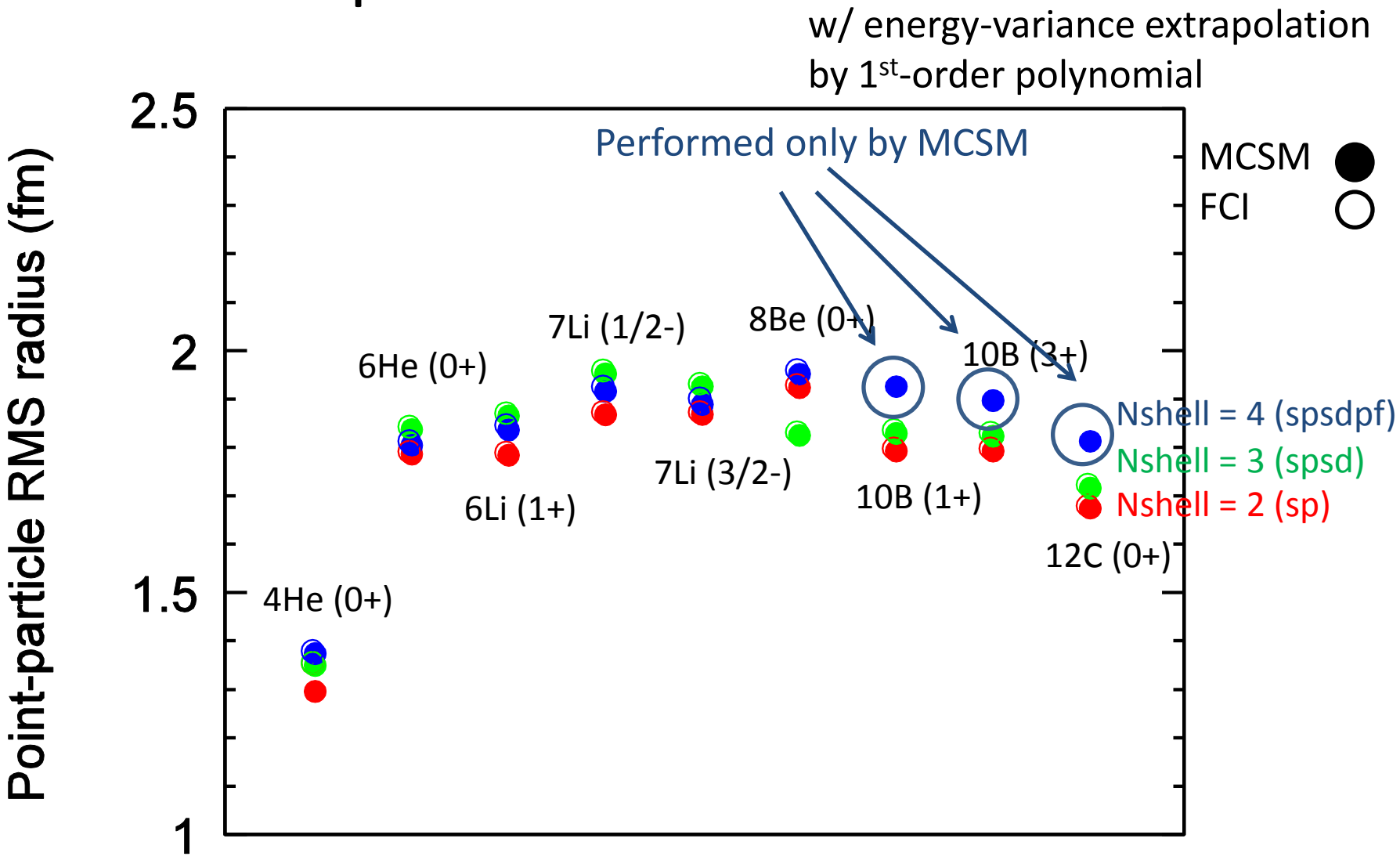


Nshell = 4 (spsdpf)
1.379 fm (MCSM)
1.379 fm (FCI)

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

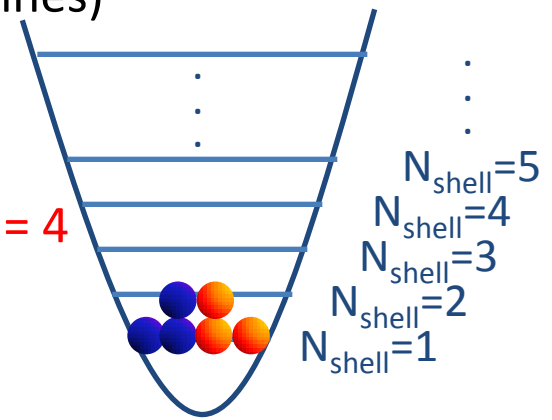


MCSM & FCI results are consistent within the size of symbols

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

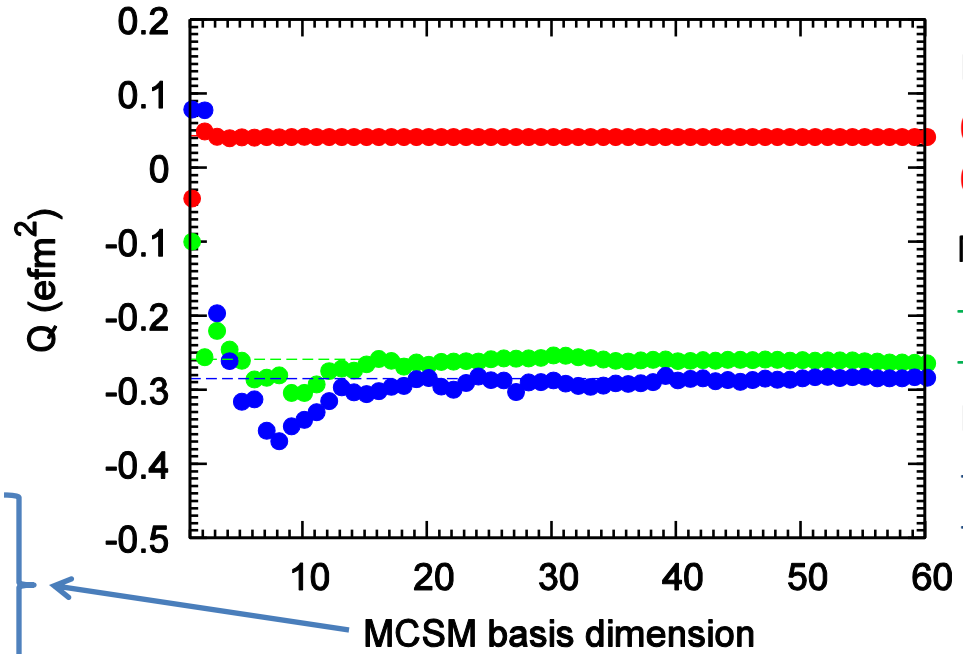
- Comparison of MCSM (solid symbols) w/ FCI (dashed lines)
  @ Nshell = 2 (sp), 3 (spsd), & 4 (spsdpf)

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



H = Hint + β Hcm, (β = 0)

w/o Coulomb force



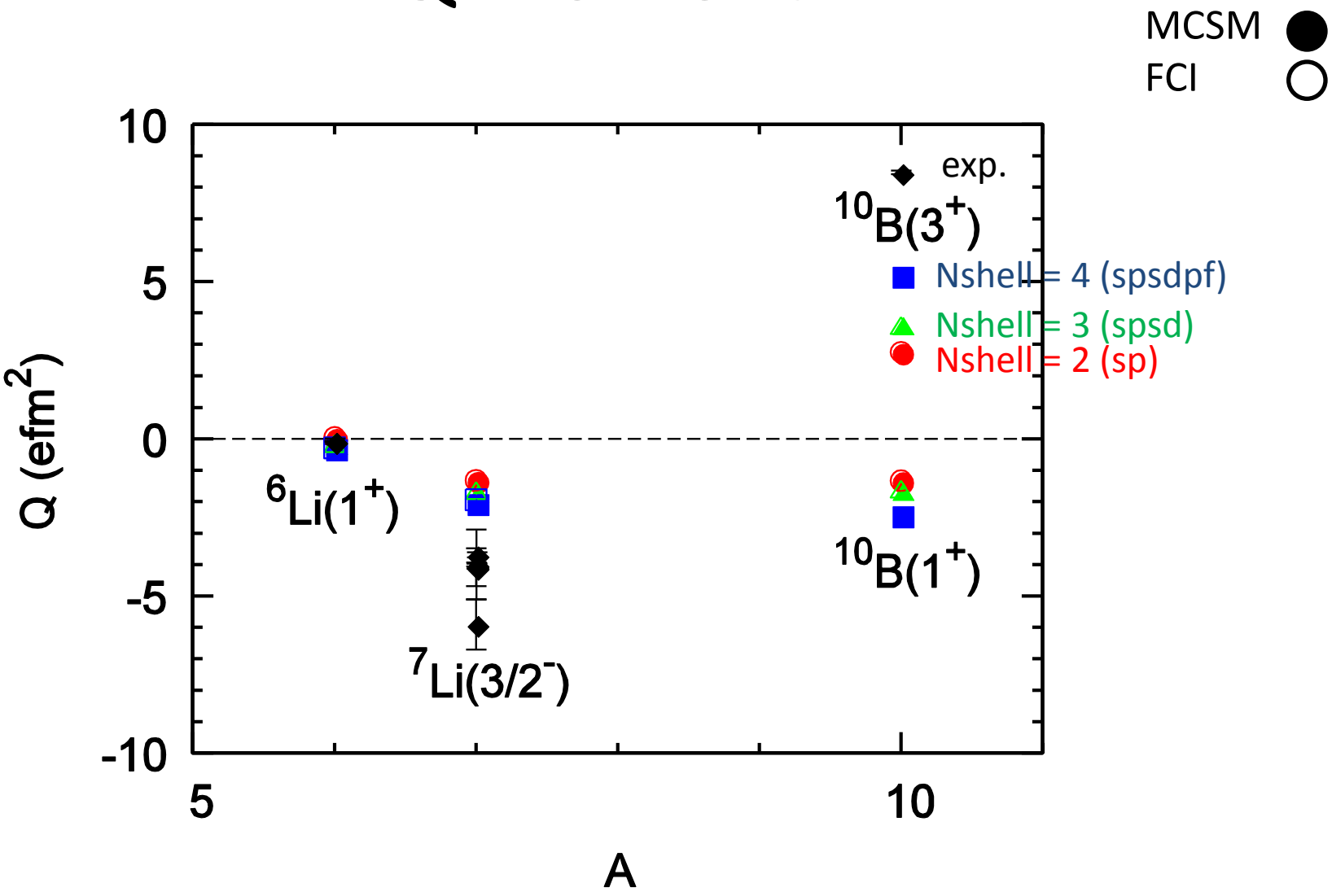
N_{shell} = 2 (s,p)
0.044 efm^2 (MCSM)
0.043 efm^2 (FCI)

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

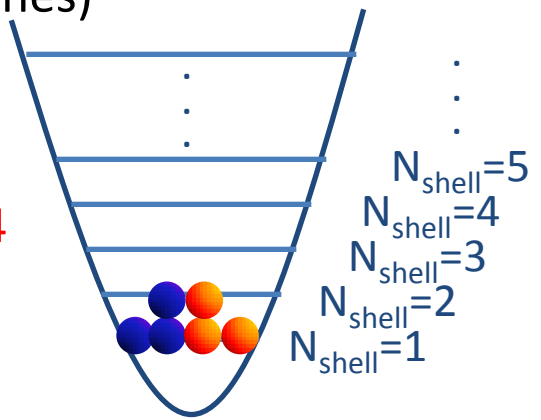


MCSM & FCI results are consistent within the size of symbols

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

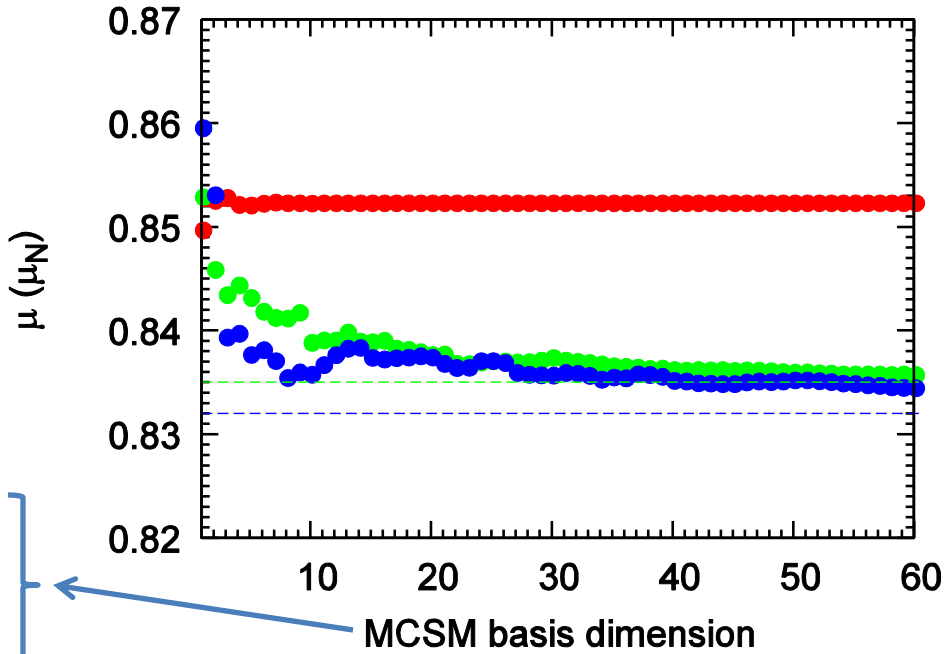
- Comparison of MCSM (solid symbols) w/ FCI (dashed lines)
  @ Nshell = 2 (s,p), 3 (s,p,sd), & 4 (s,p,sd,pf)

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



H = Hint + β Hcm, (β = 0)

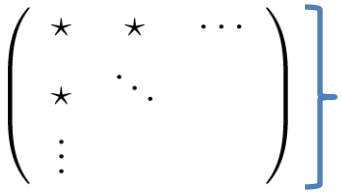
w/o Coulomb force



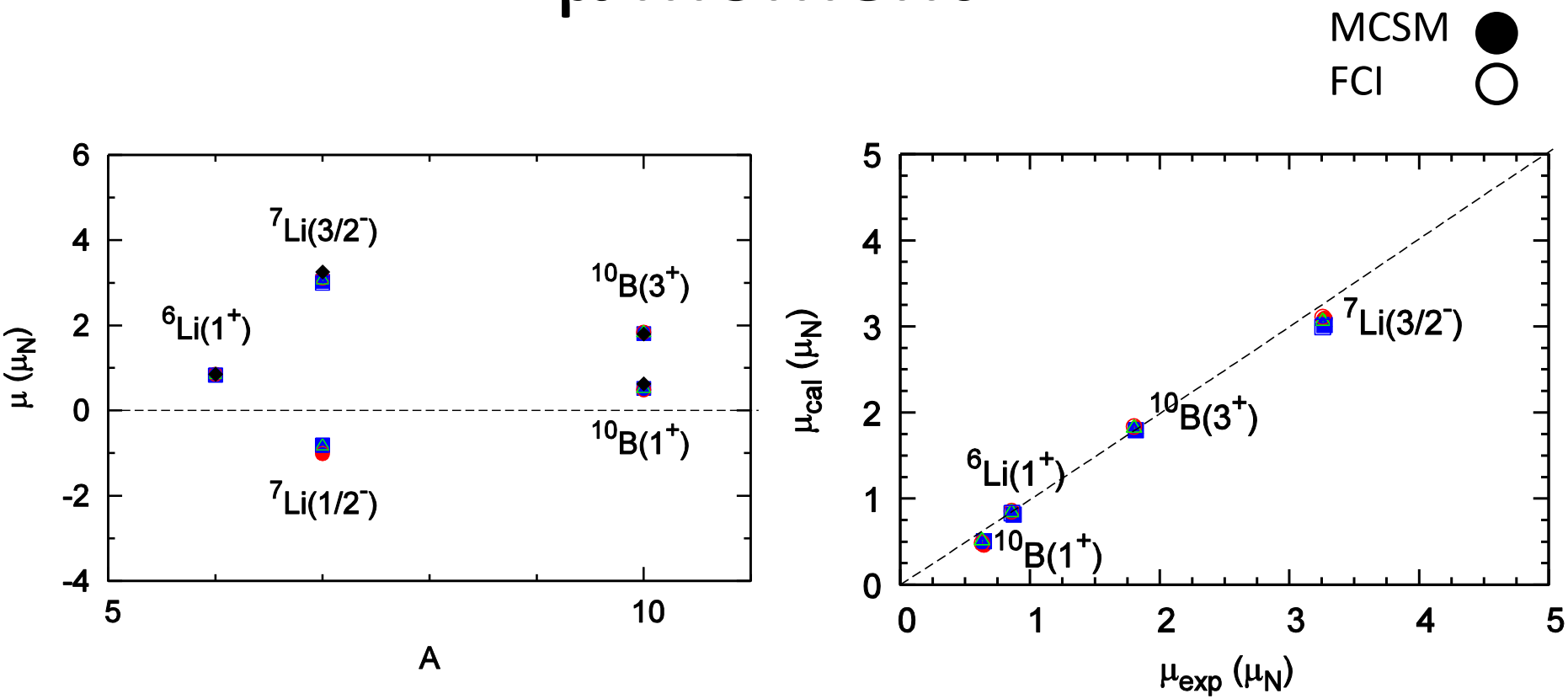
Nshell = 2 (sp)
0.852 μN (MCSM)
0.852 μN (FCI)

Nshell = 3 (spsd)
-0.836 μN (MCSM)
-0.833 μN (FCI)

Nshell = 4 (spsdpf)
-0.835 μN (MCSM)
-0.832 μN (FCI)



μ moment

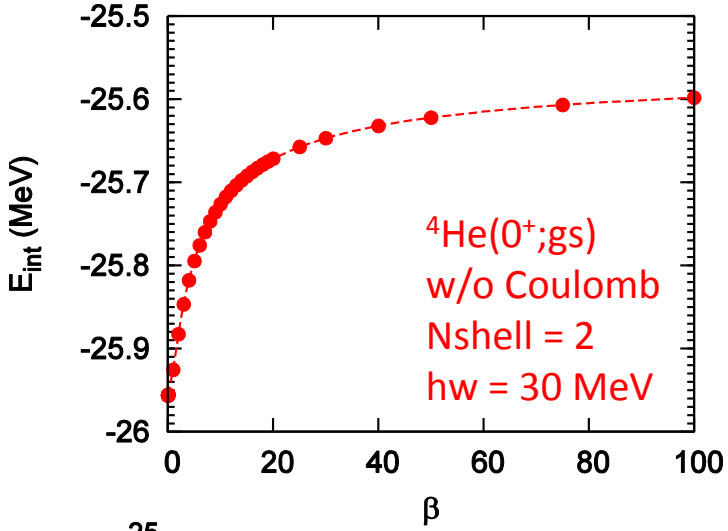


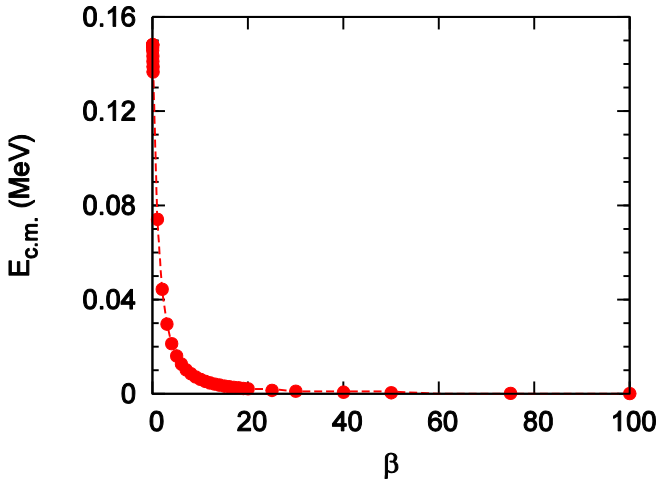
MCSM & FCI results are consistent with each other, and μ moments are well-reproduced even at small Nshell.

Spurious CoM & Coulomb force

Spurious CoM

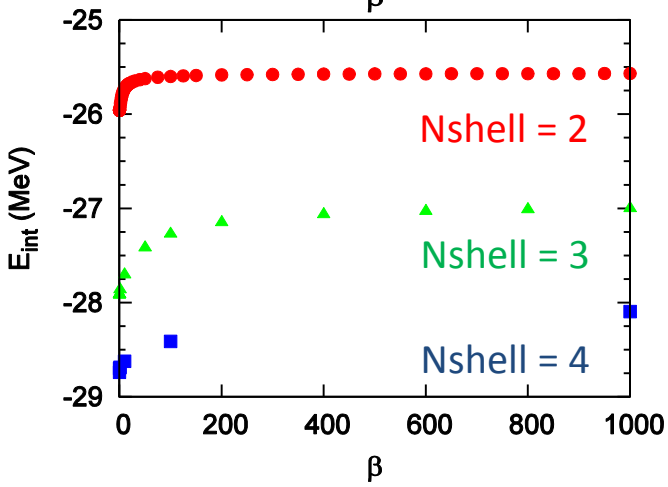
- Gloeckner-Lawson (Energy-shift) method $H_\beta = H_{int} + \beta H_{c.m.}$

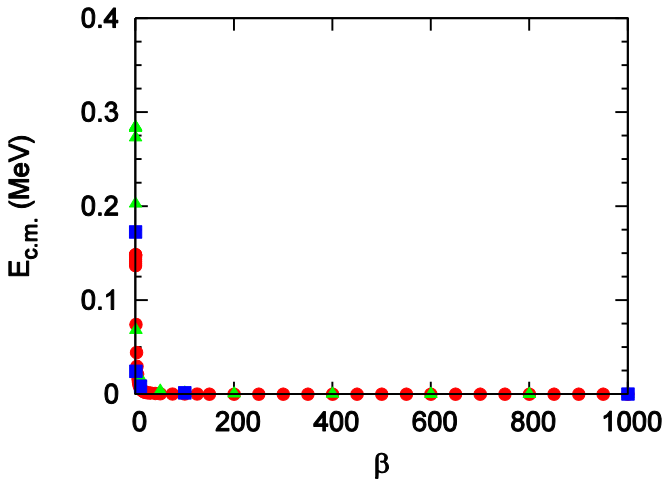




MCSM ●

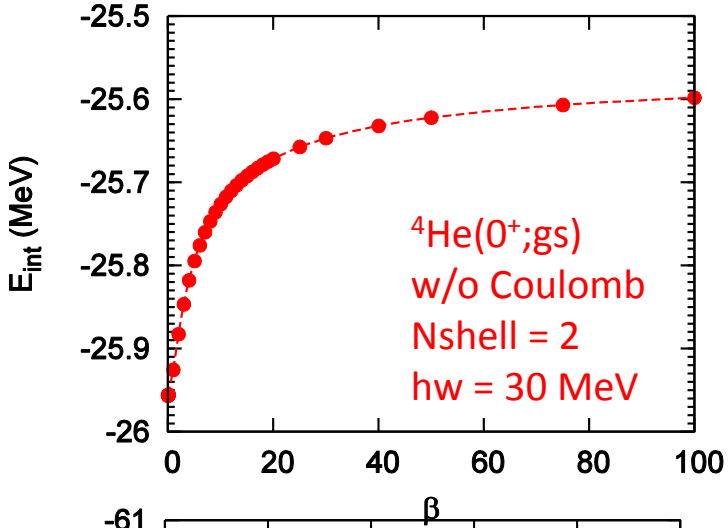
FCI ------

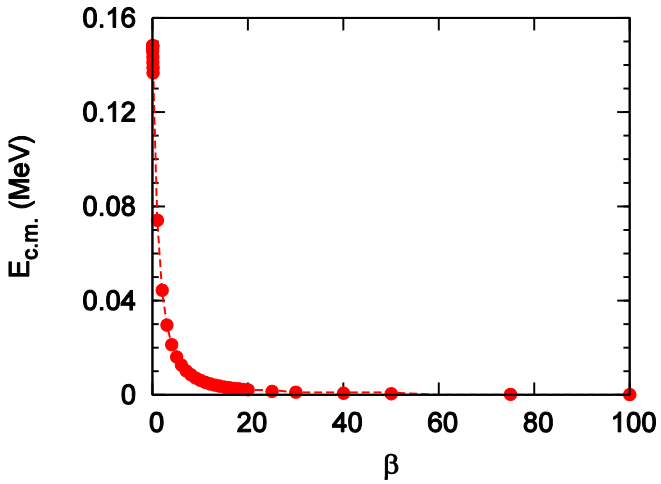




Spurious CoM

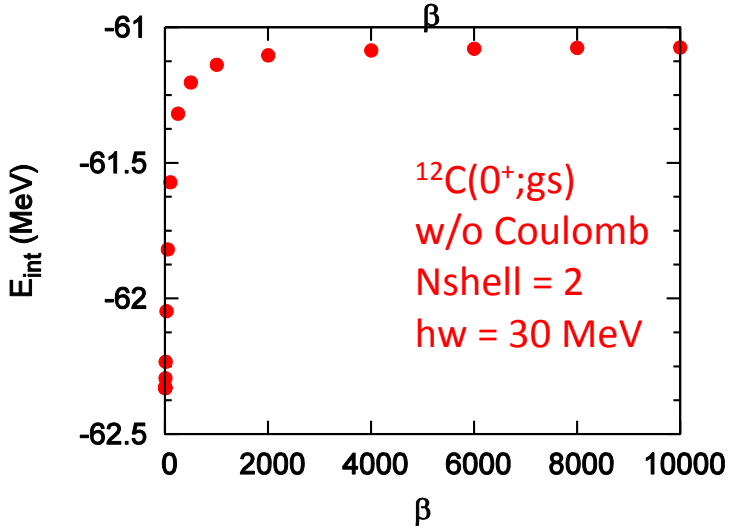
- Gloeckner-Lawson (Energy-shift) method $H_\beta = H_{int} + \beta H_{c.m.}$

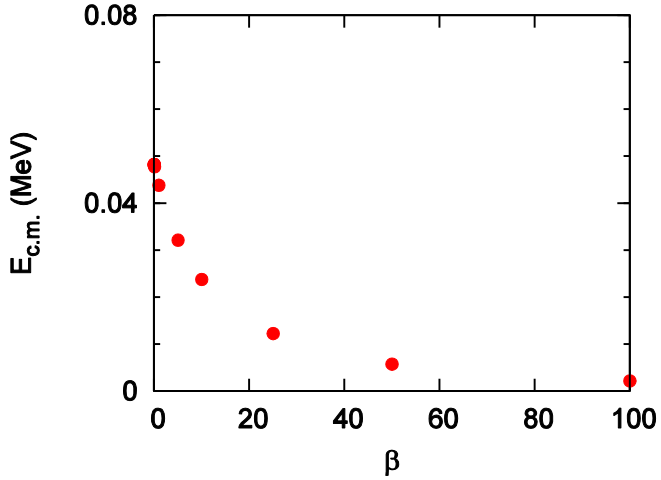




MCSM ●

FCI ------





Coulomb force

- Helium-4 gs energy @ Nshell=2

	E (MeV)		
	w/o Coulomb	w/ perturb. Coulomb	w/ Coulomb
2shl, hw = 10MeV	-13.43387	-12.81455	-12.81455
2shl, hw = 15MeV	-20.44253	-19.69512	-19.69512
2shl, hw = 20MeV	-24.2554	-23.41786	-23.41786
2shl, hw = 25MeV	-25.75932	-24.86775	-24.86775
2shl, hw = 30MeV	-25.95602	-25.02968	-25.02968
2shl, hw = 35MeV	-25.16687	-24.19965	-24.19965
2shl, hw = 40MeV	-23.36445	-22.34998	-22.34998

Coulomb force can be treated perturbatively at least @ Nshell = 2.

Tests in sd shell

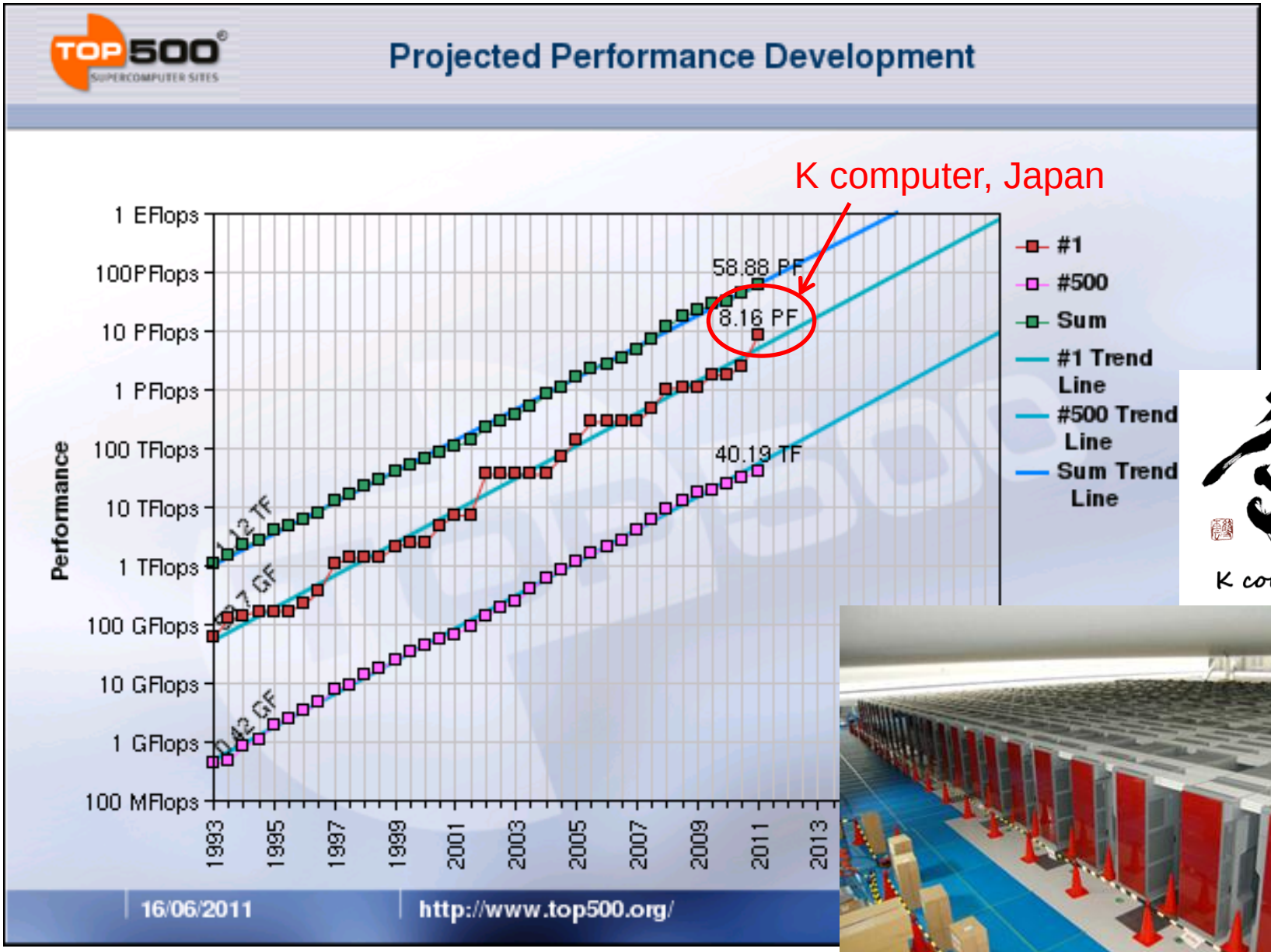
Test calculations in sd-shell nuclei

- Ground-state energies: Hint (MeV)
- For hw = 25 MeV w/ JISP16 w/o Coulomb
- MCSM results @ 100 basis dim. w/o energy-variance extrp.

$$H_\beta = H_{int} + \beta H_{c.m.}$$

	Nshell = 3		Nshell = 4		Nshell = 5	
	β = 0	β = 100	β = 0	β = 100	β = 0	β = 100
16O(0+)	-103.099	-101.409	-122.360	-117.324	-138.655	
20Ne(0+)	-121.741	-117.399	-147.118	-142.967		
24Mg(0+)	-162.293	-157.369	-189.263	-191.723		
32S(0+)	-281.815	-279.978	-328.835	-329.245		
36Ar(0+)	-322.953	-322.157	-374.714	-372.403		
40Ca(0+)	----------	----------	-438.364	-432.321		

Application to K-computer



K computer

Japanese “K computer” got rank 1 in the world.

The construction will be completed at Nov. 2012.

SPARC64 VIIIfx 548352 cores

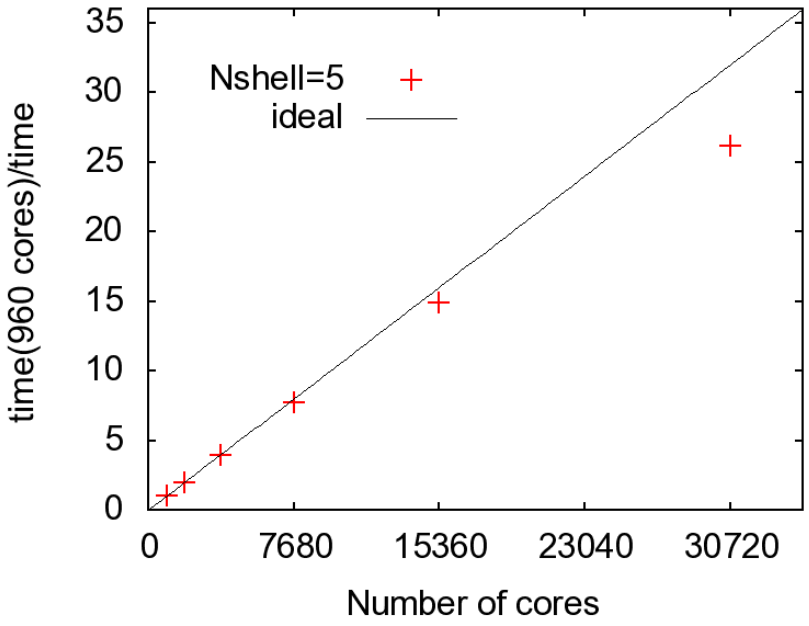
What is the application program to run on it

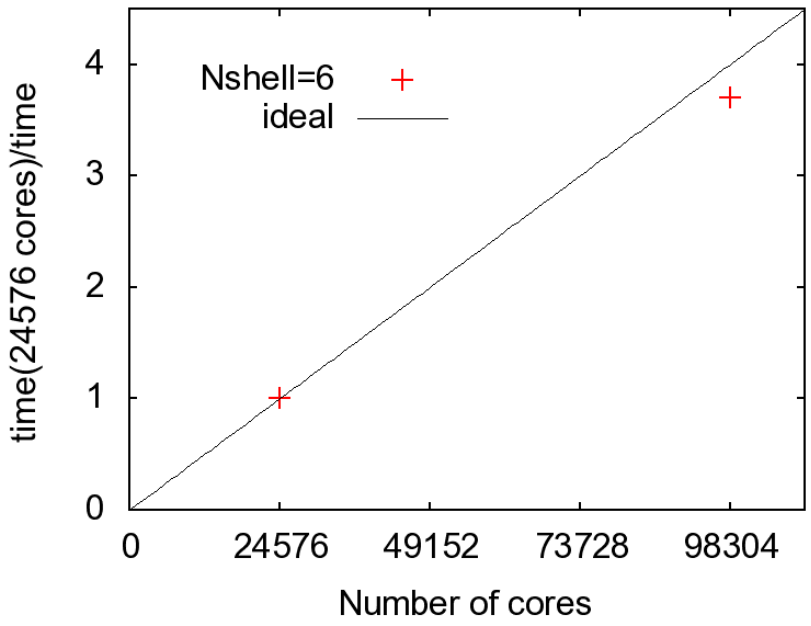
Strategic 5 Field

- Field 1: Computational Life Science and Application in Drug Discovery and Medical Development
- Field 2: Computational Materials Science Initiative (CMMI)
- Field 3: Projection of global change toward the mitigation of natural disasters
- Field 4: Next Generation Manufacturing
- Field 5: The origin of matter and the universe
  - Lattice QCD
  - Nucleus
  - Supernova Explosion
  - Early Star Formation

Parallel efficiency @ K-computer

- Optimization of 15th basis dim. of the 4He (0+) w.f. in Nshell=5 w/ 100 CG iterations
- Optimization of 48th basis dim. of the 4He (0+) w.f. in Nshell=6 w/ 100 CG iterations

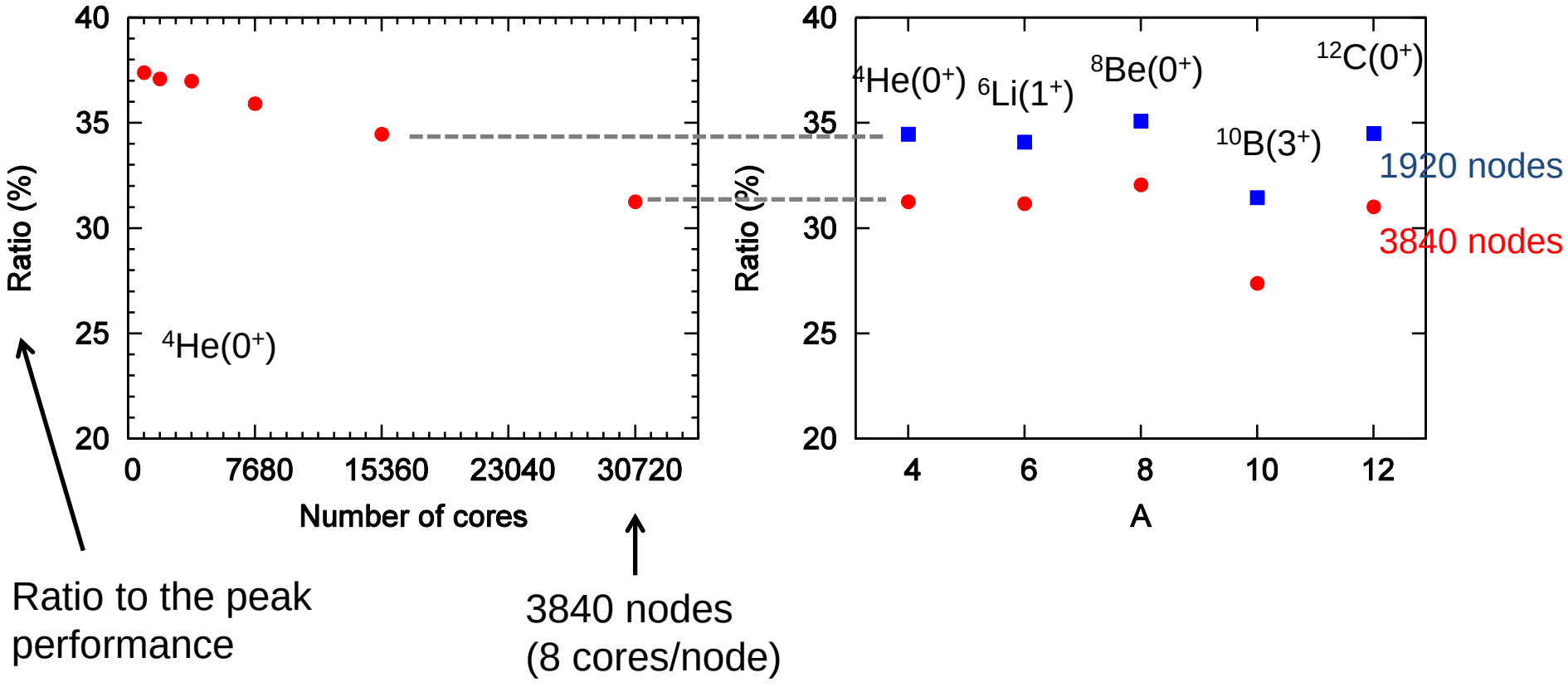




Note: it is a tentative result by early access to the K-computer at AICS, RIKEN.

Ratio to the peak performance @ K computer (phase IV-1)

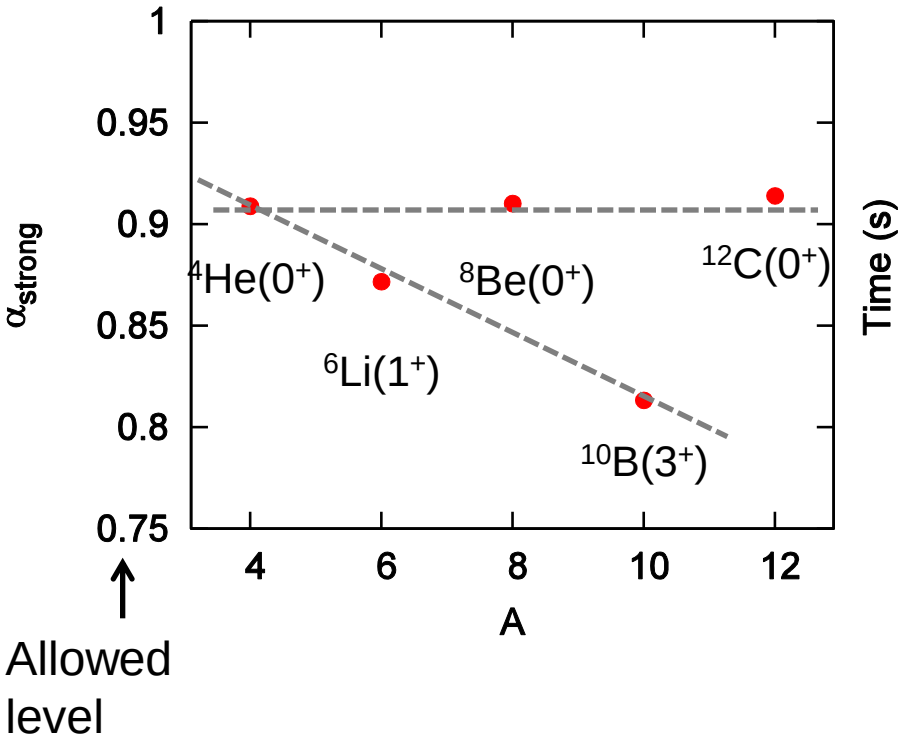
- Test case: Optimization of 15th basis dim. of the w.f. in Nshell=5 w/ 100 CG iterations w/o preprocessing (MPI/OpenMP, 8 threads)

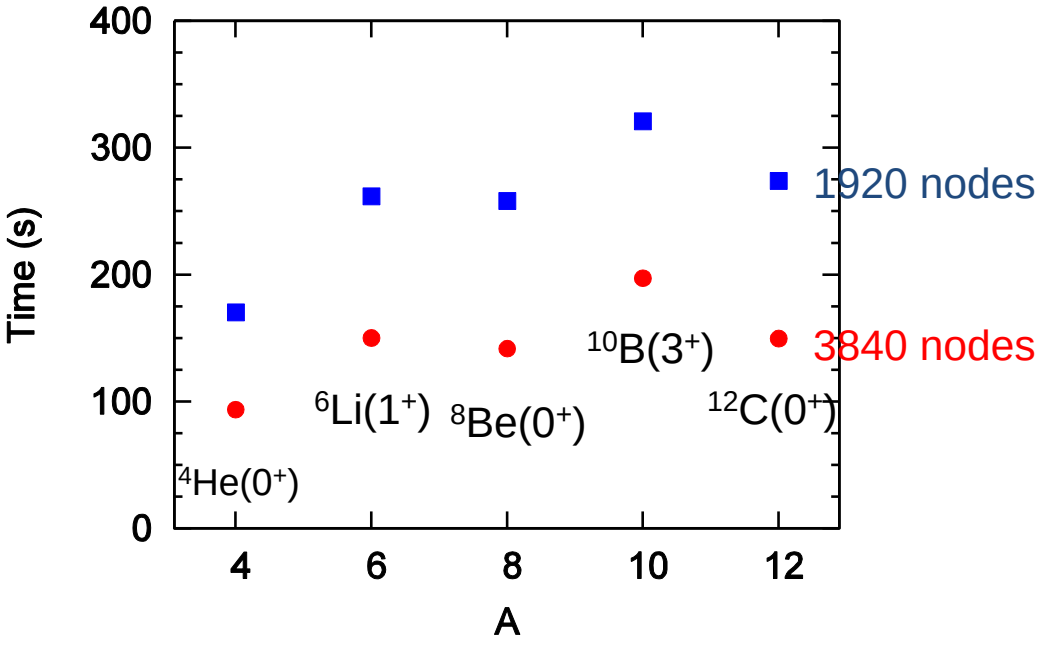


Note: it is a tentative result by early access to the K-computer at AICS, RIKEN.

Strong scaling @ K computer (phase IV-1)

- Test case: Optimization of 15th basis dim. of the w.f. in Nshell=5 w/ 100 CG iterations w/o preprocessing (MPI/OpenMP, 8 threads)





Definition (in this case): $\alpha_{strong} = (T_{1920\ nodes}/T_{3840\ nodes}) / (3840\ nodes/1920\ nodes)$

Note: it is a tentative result by early access to the K-computer at AICS, RIKEN.

Summary

- MCSM can be applied to the no-core calculations.

  Benchmarks for the p-shell & some tests for the sd-shell nuclei have been performed.

  - MCSM & FCI results for the p-shell nuclei are consistent with each other.

Perspective

- MCSM algorithm
  - Larger model spaces (Nshell = 5, 6, …), Nshell vs Nmax?
  - Inclusion of the (effective) 3-body force
  - Coupling to the continuum states
- Physics
  - Cluster(-like) states (12C Hoyle state, …)
  - Unnatural parity states
- Tuning of the MCSM code on the K Computer

END