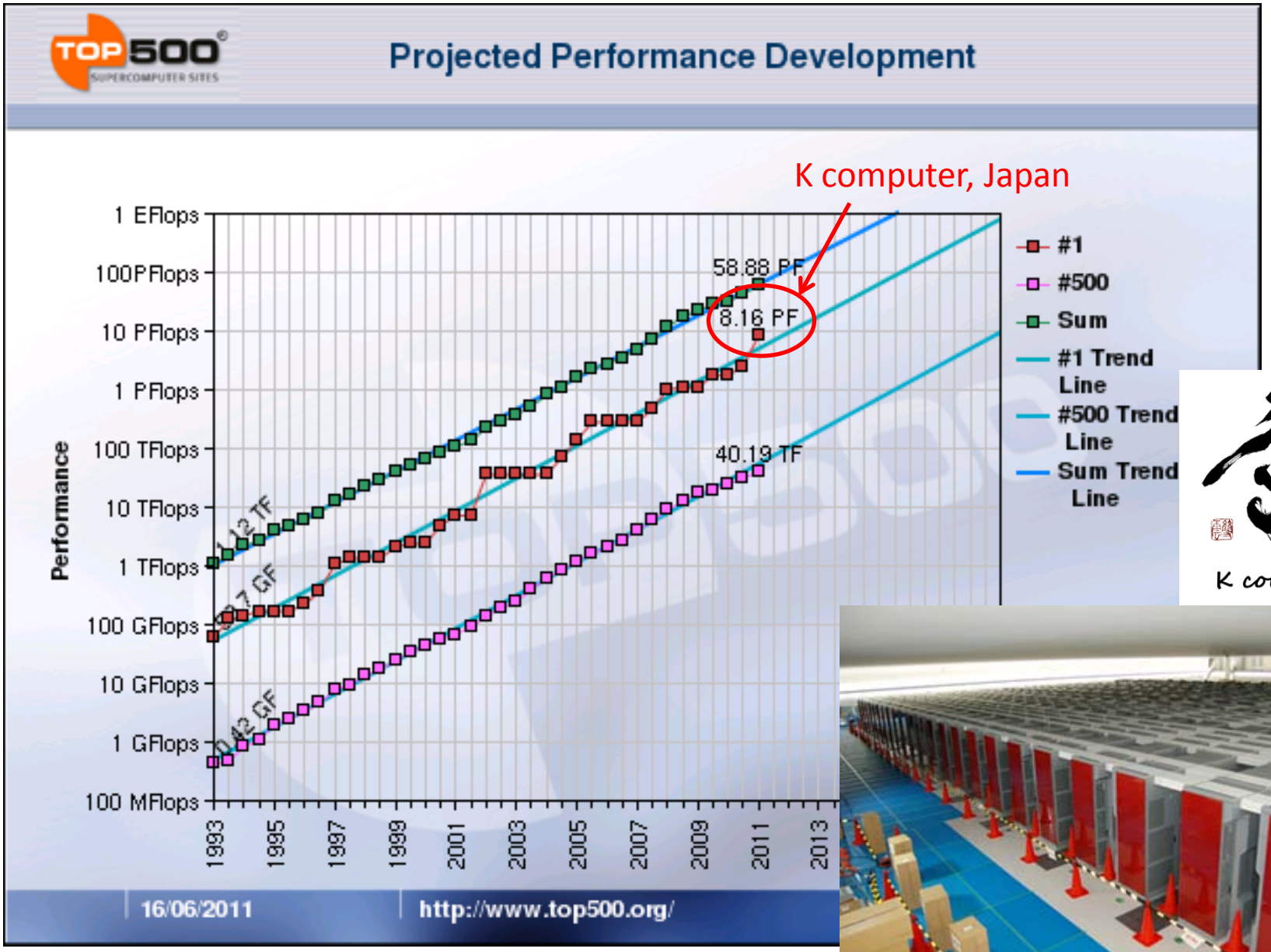
Recent developments toward large-scale shell-model calculations

Noritaka Shimizu
Center for Nuclear Study, University of Tokyo

Y. Utsuno (JAEA), T. Mizusaki (Senshu Univ.),
T. Otsuka (Univ. of Tokyo), M. Honma (Aizu Univ.),
T. Abe (Univ. of Tokyo), Y. Tsunoda (Univ. of Tokyo),



京
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 ?

In view of truncation approaches to full LSSM space

Many efforts have been paid to develop truncation scheme
consisting of form of basis and way of selection.

- *t*-particle *t*-hole truncation + Lanczos method
  spherical Slater determinant
- Generator coordinate method
  (J-projected) deformed Slater determinant or quasi-particle vacua
- Monte Carlo Shell Model
  J-projected deformed Slater determinants
- VAMPIR
  J-projected quasi-particle vacua
- Importance Truncated Shell Model
  spherical Slater determinant
- Projected CI
  J-projected deformed Slater determinants
- Variational Monte Carlo method, DMRG, and so on ...

They are variational approaches, which always provide us with upper limit of exact value.
It is difficult to know how far it is from the exact one.

Energy variance extrapolation

Monte-Carlo Shell Model

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

A tool to go beyond the conventional diagonalization method

The shell-model wave function is described
by a linear combination of parity, angular-momentum
projected Slater determinants

$$\left|\Psi\right\rangle = \sum_{i=k}^{N_{MCSM}} c_k P^{\pi} \sum_{K=-J}^{J} g_K P^{J,\pi}_{MK} \left|\phi(D^{(k)})\right\rangle$$

MCSM basis, deformed Slater det.

$$|\phi\rangle = \prod_{\alpha=1}^{N} \left(\sum_{i=1}^{N_{sp}} c_i^{\dagger} D_{i\alpha} \right) |-\rangle$$

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

$\hat{h}(\sigma)$ one-body Hamiltonian
σ... auxiliary field
random numbers
generated stochastically

Increase the MCSM basis, or number of defomed Slater det. till energy converges

Angular-momentum projection ... 3-dimension integral (discretized)
Small disk I/O

Advantageous for parallel computation, bases and mesh points

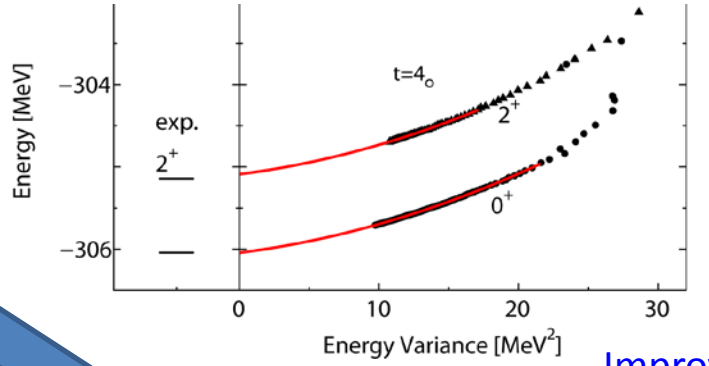
Developments of the Monte Carlo shell Model towards “K computer”

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

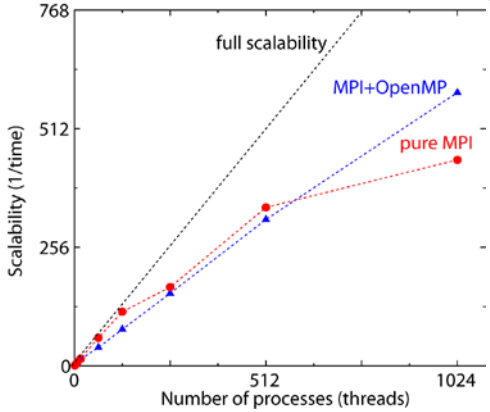
N. Shimizu, Y. Utsuno, T. Mizusaki, T. Otsuka, T. Abe, and M. Honma, Phys. Rev. C **82,** 061305(R) (2010).

PC cluster
100CPU parallel

- Precise estimation of energy eigenvalue by variance extrapolation



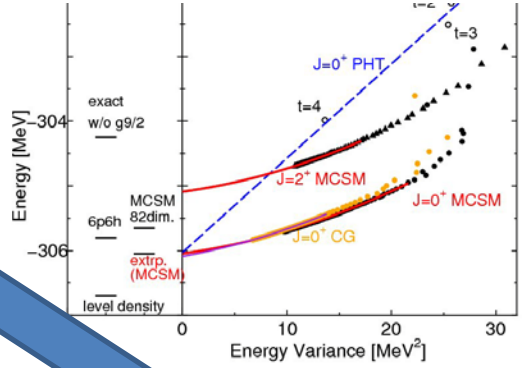
Parallel efficiency



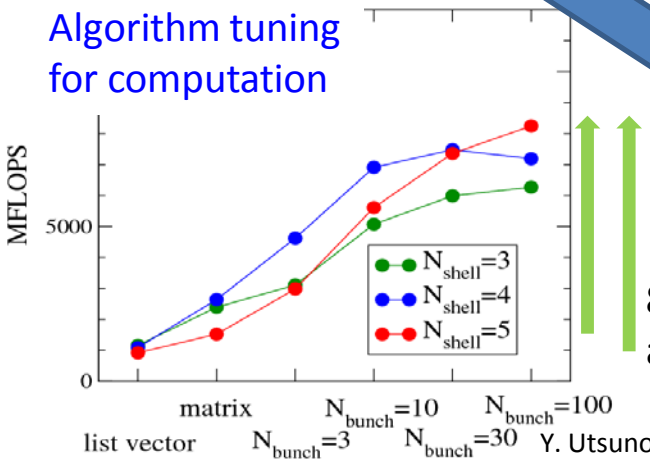
OpenMP+MPI hybrid parallel

1024 cores

Improvement of the MCSM by Conjugate Gradient method



Algorithm tuning for computation



8 times faster at maximum

Y. Utsuno, N. Shimizu, T. Otsuka, and T. Abe, to be submitted.

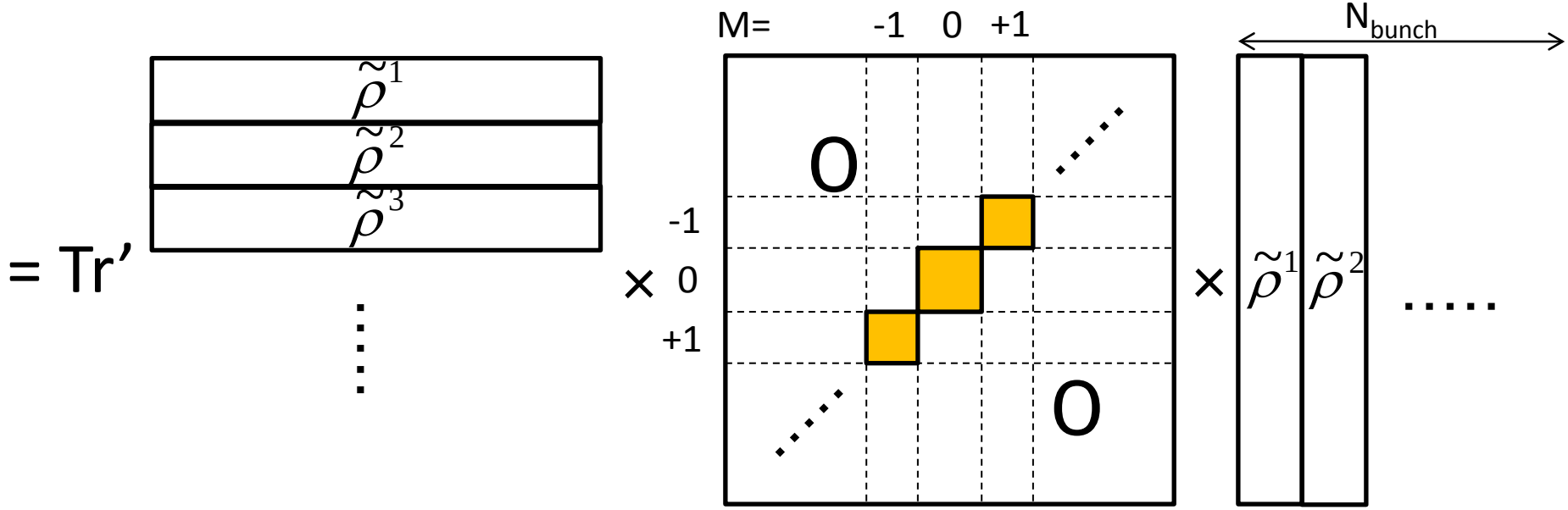
SPARC64 VIIIfx 548352 cores K computer

New algorithm for evaluating Hamiltonian matrix elements in the MCSM

hot spot: calculation of the matrix element of two-body int.

$$\hat{V} = \sum_{i<j,k<l} v_{ijkl} c_i^\dagger c_j^\dagger c_l c_k \qquad \rho_{ij} = \frac{\langle \phi | c_j^\dagger c_i | \phi' \rangle}{\langle \phi | \phi' \rangle} \qquad \langle \phi | \hat{V} | \phi' \rangle = \sum_{i<j,k<l} v_{ijkl} (\rho_{ki}\rho_{lj} - \rho_{kj}\rho_{li})$$

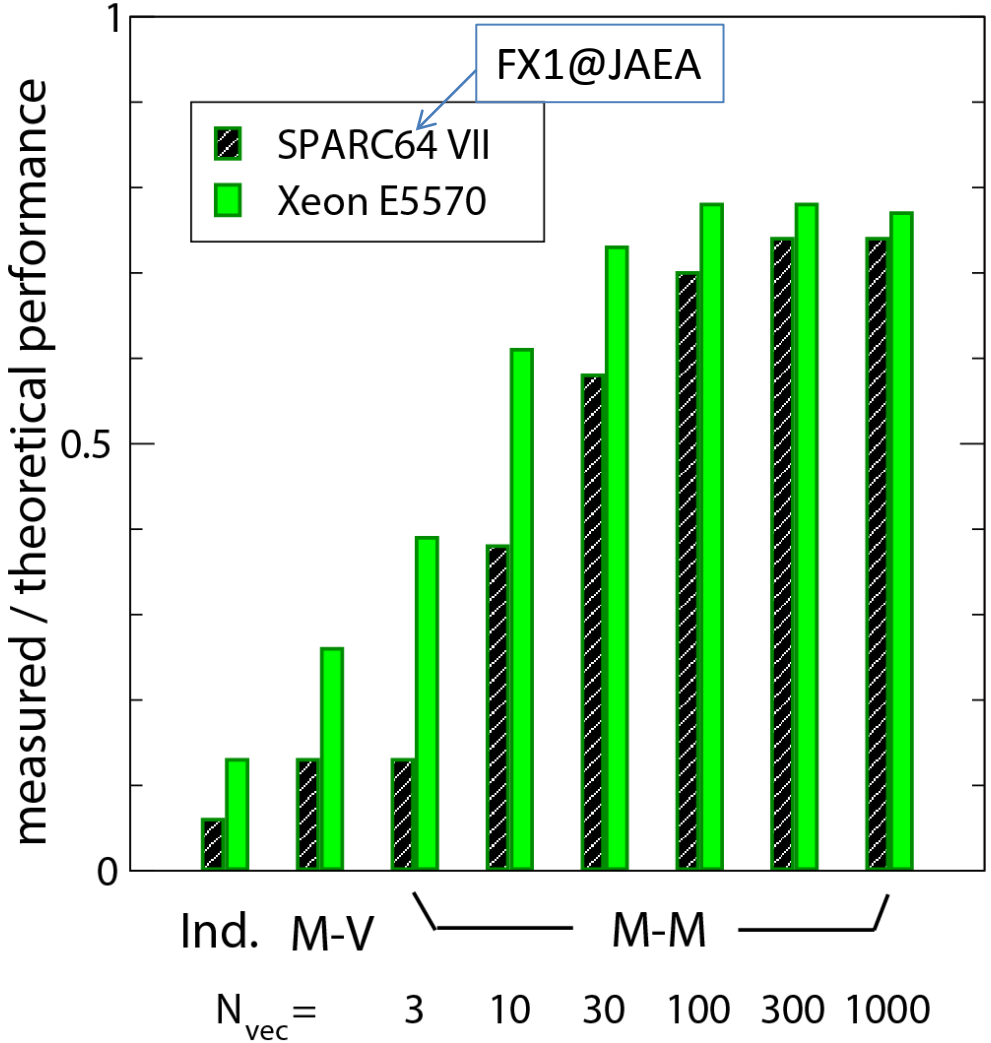
$$\langle \phi | \hat{V} | \phi' \rangle = \frac{1}{2} \sum_{i,k} \rho_{ki} \left(\sum_{j,l} v_{ijkl} \rho_{lj} \right) = \frac{1}{2} \sum_{(ki)} \rho_{(ki)} \left(\sum_{jl} v_{(ki),(lj)} \rho_{(lj)} \right)$$



Product of a sparse matrix and a vector is replaced by the product of dense matrices

Matrix product is performed by DGEMM subroutine in BLAS library, which is highly tuned

Tuning by 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

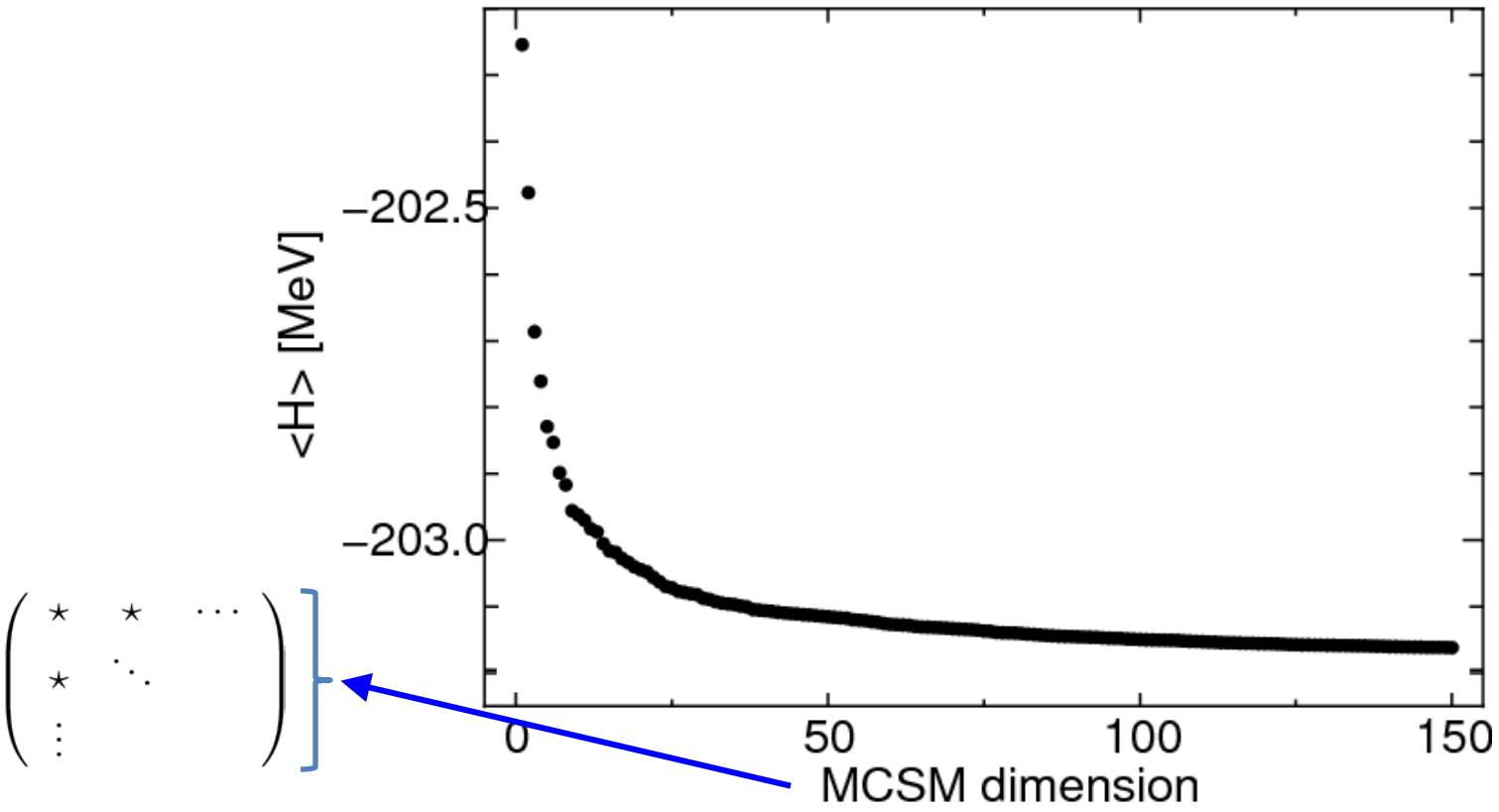
Matrix product e.g.
(390 x 390) x (390 x $2N_{bunch}$)

N_{bunch} controllable tuning parameter
chunk size

Courtesy of Y. Utsuno

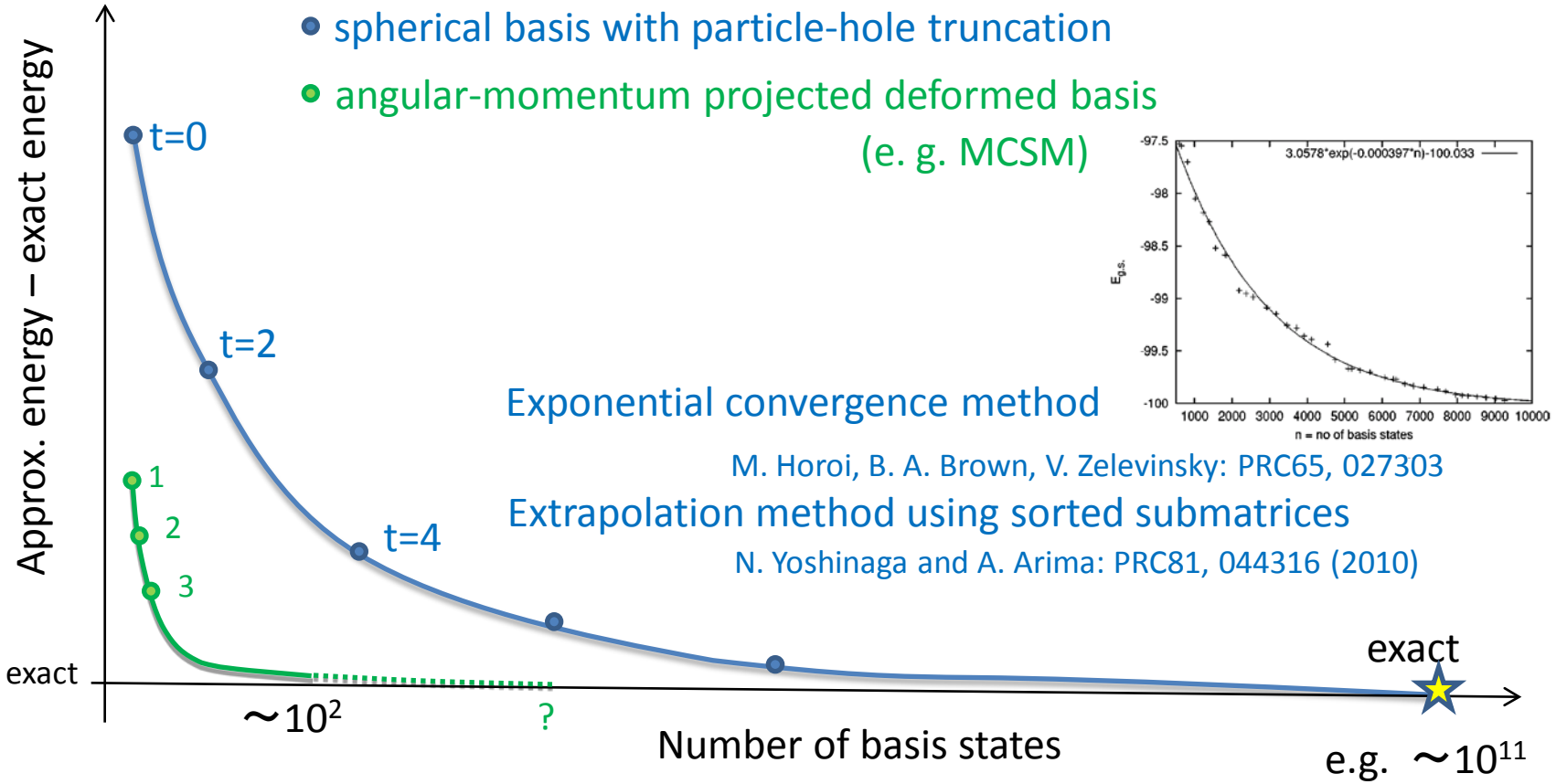
How far from the exact eigenvalue?

^{56}Ni in pf shell, 0^+_1, 10^9 m-scheme dimension



- Very small difference between the MCSM and exact solution
  - About 99% correlation energy (i.e., gain from HF) can be gained typically.
- It is not easy to see where the energy converges.

Extrapolation method: spherical basis vs. projected deformed basis



MCSM, PCI, VAMPIR, HMD, ITSM, ...

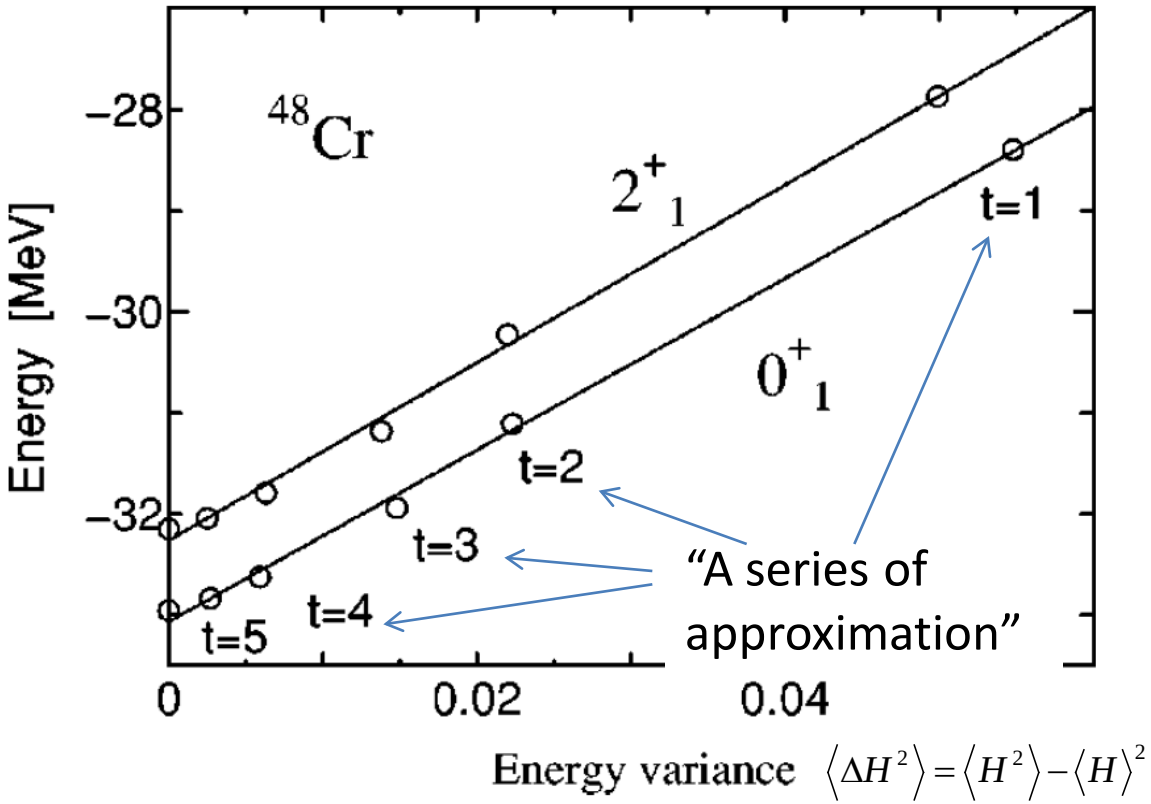
Needs extrapolation method which works independently of the basis representation

Exponential fit causes slow convergence and big uncertainty

→ Extrapolation method using **energy variance**

What is the energy-variance extrapolation?

Demonstrated by Mizusaki in the framework of conventional shell model



"A series of approximation"

Energy variance is defined as

$$\langle \Delta H^2 \rangle = \langle H^2 \rangle - \langle H \rangle^2$$

If the wave function is an exact eigenstate of the Hamiltonian, energy variance is exactly zero

$$\langle \Delta H^2 \rangle = 0$$

A series of approximated wave functions:

$$\langle H \rangle = E_0 + a\langle \Delta H^2 \rangle + b\langle \Delta H^2 \rangle^2 + \ldots$$

With a sequence of approximate energies,

extrapolate $\langle \Delta H^2 \rangle \to 0$ so that $\langle H \rangle$ becomes E_0, true energy.

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

Obstacle of the MCSM+extrapolation: computation time for energy variance, $\langle H^2 \rangle$

The expectation value of general four-body operator in deformed Slater determinants is obtained by Wick's theorem :

2-body int. $\langle \phi | \hat{V} | \phi' \rangle = \sum_{i<j,k<l} v_{ijkl} (\rho_{ki}\rho_{lj} - \rho_{kj}\rho_{li})$ 2-fold loops, 2 terms

4-body int.

$$\frac{\langle \phi | \hat{V}^2 | \phi' \rangle}{\langle \phi | \phi' \rangle} = \frac{1}{16} \sum_{ijkl\alpha\beta\gamma\delta} \overline{v}_{ijkl}\overline{v}_{\alpha\beta\gamma\delta}$$
$$\Big((1-\rho)_{k\alpha}(1-\rho)_{l\beta}\rho_{\gamma i}\rho_{\delta j} - (1-\rho)_{k\alpha}(1-\rho)_{l\beta}\rho_{\gamma j}\rho_{\delta i}$$
$$-(1-\rho)_{l\alpha}(1-\rho)_{k\beta}\rho_{\gamma i}\rho_{\delta j} + (1-\rho)_{l\alpha}(1-\rho)_{k\beta}\rho_{\gamma j}\rho_{\delta i}$$
$$+\rho_{\gamma\alpha}(1-\rho)_{l\beta}\rho_{ki}\rho_{\delta j} - \rho_{\gamma\alpha}(1-\rho)_{k\beta}\rho_{li}\rho_{\delta j}$$
$$-\rho_{\gamma\alpha}(1-\rho)_{l\beta}\rho_{kj}\rho_{\delta i} + \rho_{\gamma\alpha}(1-\rho)_{k\beta}\rho_{lj}\rho_{\delta i}$$
$$-\rho_{\delta\alpha}(1-\rho)_{l\beta}\rho_{ki}\rho_{\gamma j} + \rho_{\delta\alpha}(1-\rho)_{k\beta}\rho_{li}\rho_{\gamma j}$$
$$+\rho_{\delta\alpha}(1-\rho)_{l\beta}\rho_{lj}\rho_{\gamma i} - \rho_{\delta\alpha}(1-\rho)_{k\beta}\rho_{lj}\rho_{\gamma i}$$
$$-\rho_{\gamma\beta}(1-\rho)_{l\alpha}\rho_{ki}\rho_{\delta j} + \rho_{\gamma\beta}(1-\rho)_{k\alpha}\rho_{li}\rho_{\delta j}$$
$$+\rho_{\gamma\beta}(1-\rho)_{l\alpha}\rho_{kj}\rho_{\delta i} - \rho_{\gamma\beta}(1-\rho)_{k\alpha}\rho_{lj}\rho_{\delta i}$$
$$+\rho_{\delta\beta}(1-\rho)_{l\alpha}\rho_{ki}\rho_{\gamma j} - \rho_{\delta\beta}(1-\rho)_{k\alpha}\rho_{li}\rho_{\gamma j}$$
$$-\rho_{\delta\beta}(1-\rho)_{l\alpha}\rho_{lj}\rho_{\gamma i} + \rho_{\delta\beta}(1-\rho)_{k\alpha}\rho_{lj}\rho_{\gamma i}$$
$$+\rho_{ki}\rho_{lj}\rho_{\gamma\alpha}\rho_{\delta\beta} - \rho_{ki}\rho_{lj}\rho_{\delta\alpha}\rho_{\gamma\beta} - \rho_{li}\rho_{kj}\rho_{\gamma\alpha}\rho_{\delta\beta} + \rho_{li}\rho_{kj}\rho_{\delta\alpha}\rho_{\gamma\beta}\Big)$$

8-fold loops, 24 terms

$$\hat{V} = \sum_{i<j,k<l} v_{ijkl} c_i^\dagger c_j^\dagger c_l c_k$$

$$\rho_{ij} = \frac{\langle \phi | c_j^\dagger c_i | \phi' \rangle}{\langle \phi | \phi' \rangle}$$

$$\Gamma_{ik} = \sum_{jl} v_{ijkl}\rho_{lj}$$

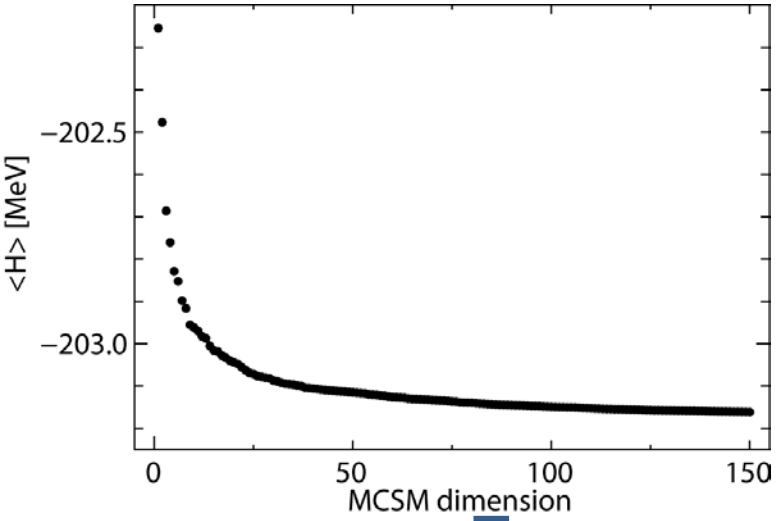
$$\frac{\langle \phi | \hat{H}^2 | \psi \rangle}{\langle \phi | \psi \rangle} = \sum_{i<j,\alpha<\beta} \left(\sum_{k<l} v_{ijkl}((1-\rho)_{k\alpha}(1-\rho)_{l\beta} - (1-\rho)_{l\alpha}(1-\rho)_{k\beta}) \right) \left(\sum_{\gamma<\delta} v_{\alpha\beta\gamma\delta}(\rho_{\gamma i}\rho_{\delta j} -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

Separability of H^2

two independent inside loops

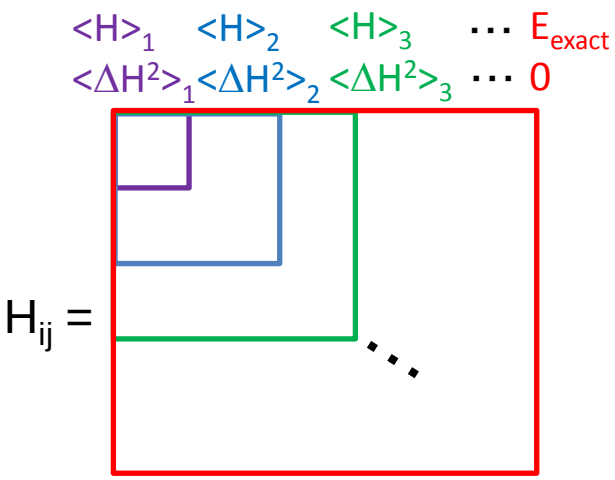
6-fold loops, matrix-product form

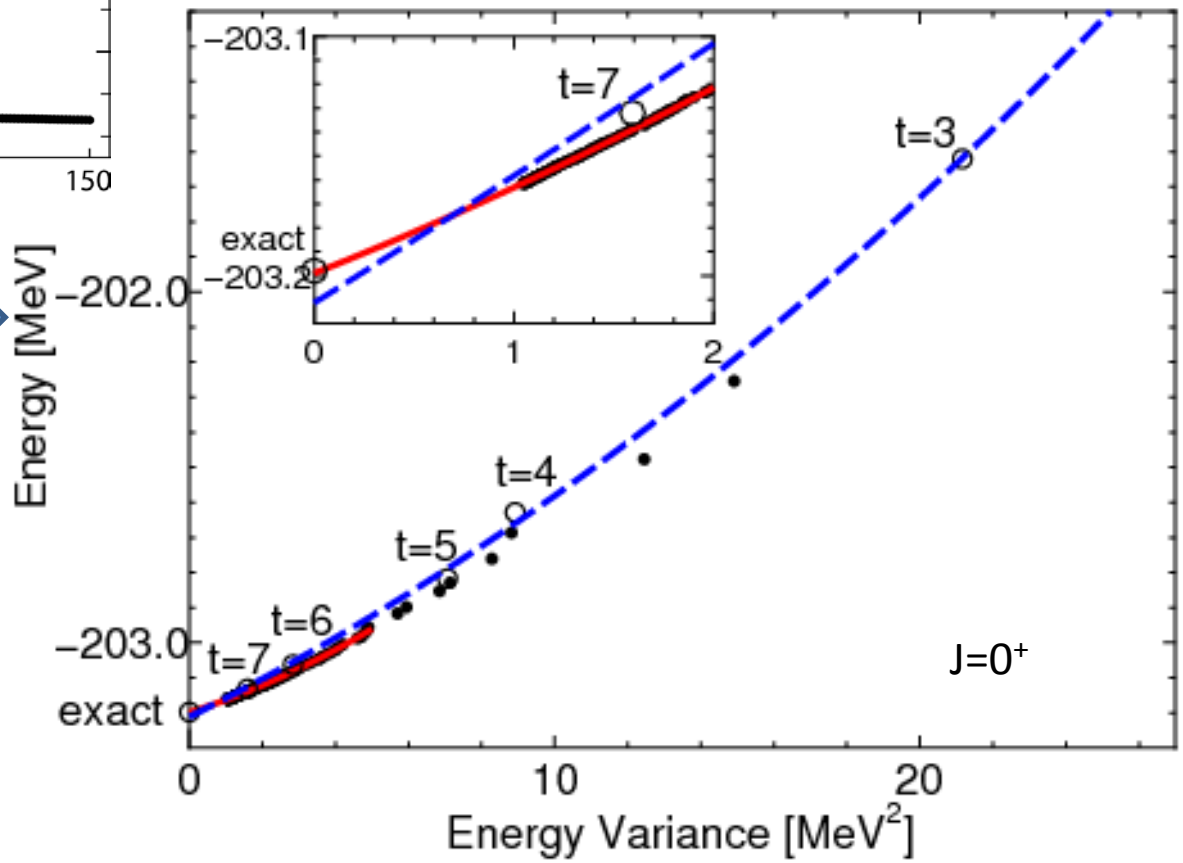
Result of energy variance extrapolation in the MCSM: ^{56}Ni in *pf*-shell



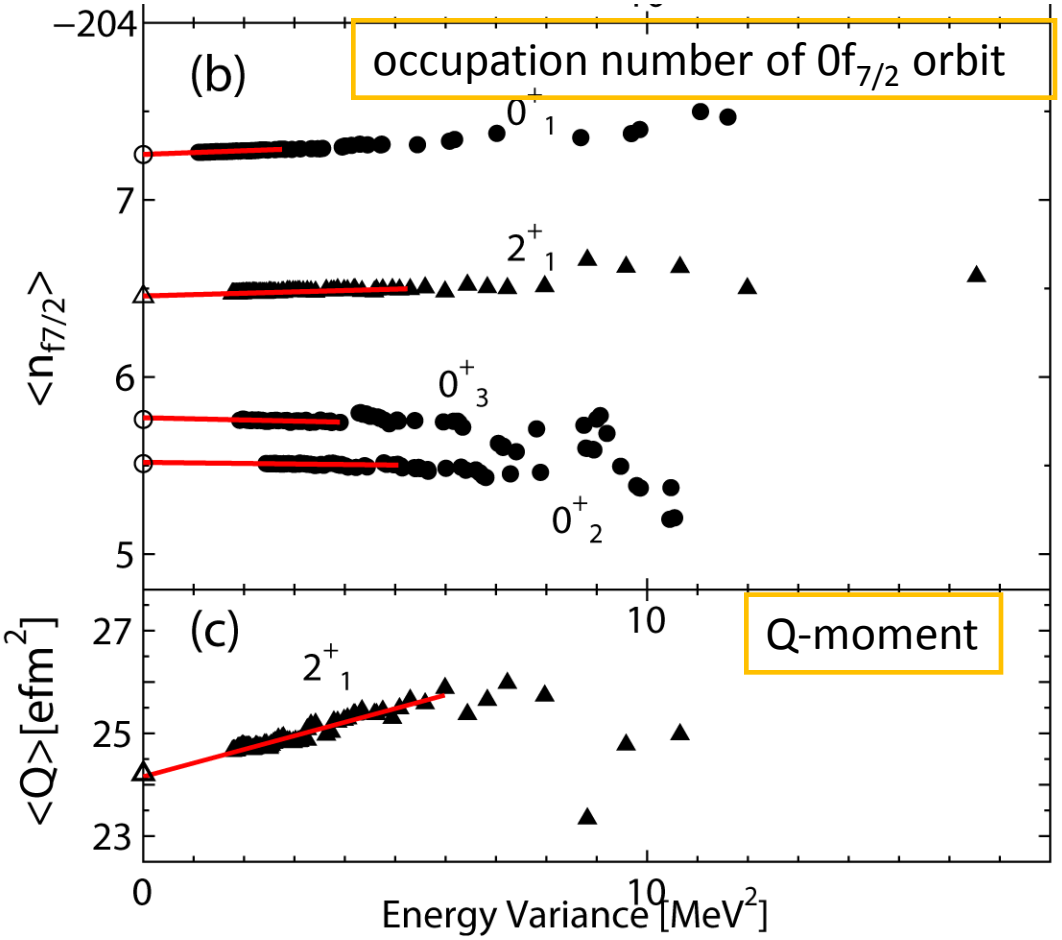
Red solid line : 2nd order extrapolation for the MCSM

Blue dashed line : 2nd order extrapolation of *t*-particle *t*-hole truncation in spherical basis





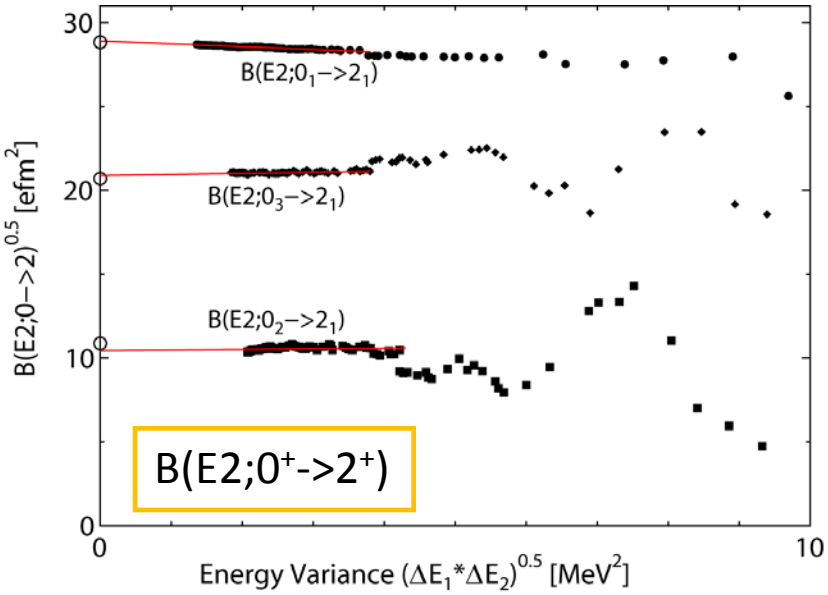
Extrapolation method in observables : ^{56}Ni in pf-shell



solid symbol : MCSM

red line: 1st order extrapolation of the MCSM

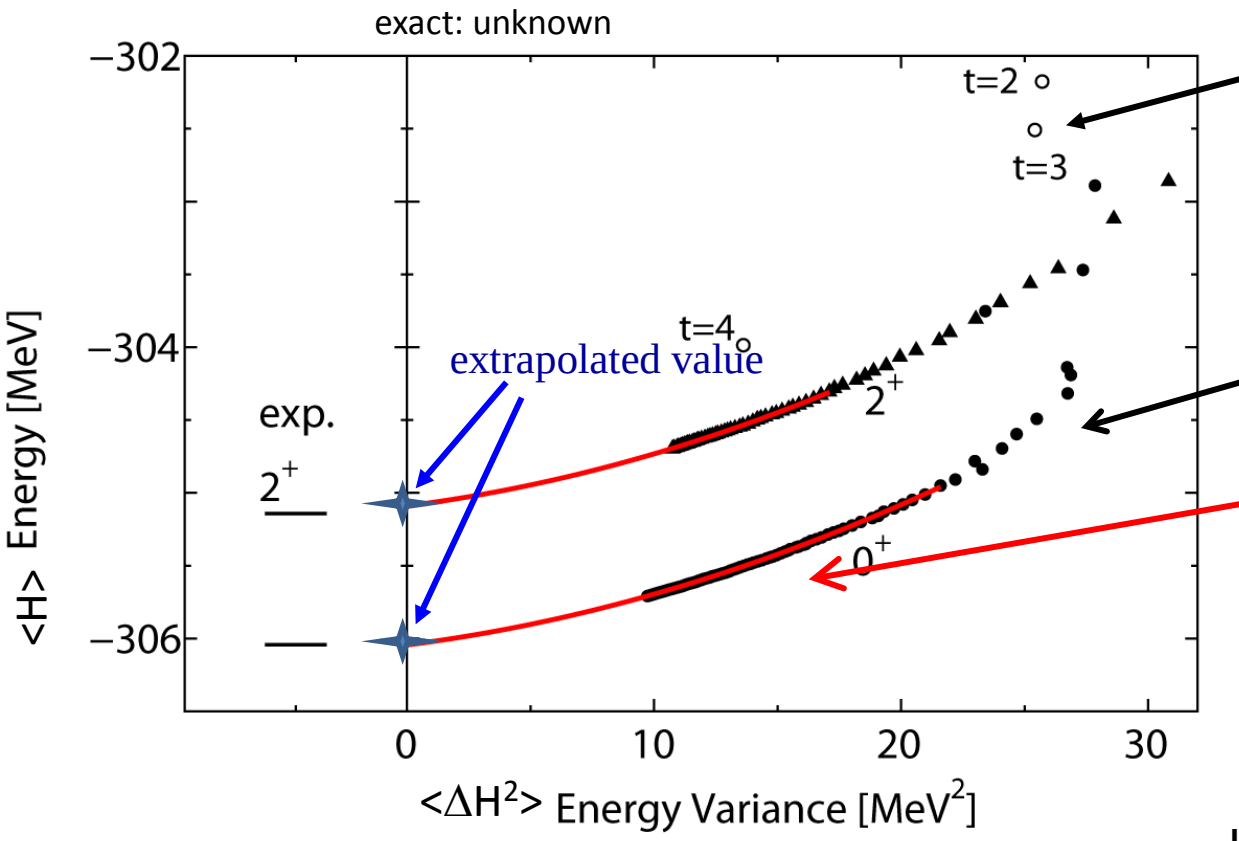
open symbol : exact



MCSM+1st order extrapolation shows good predictive power in various physical quantities in addition to energy eigenvalues

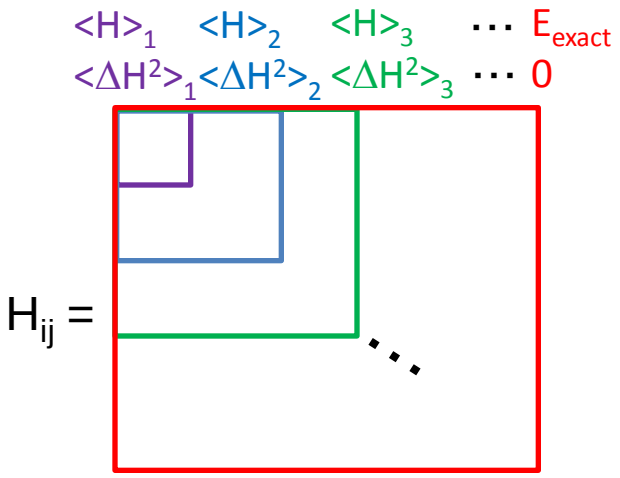
MCSM + energy-variance extrapolation ^{64}Ge with ^{40}Ca core

(24 valence particles in pf+g9/2 space, corresponding the diagonalization of 1.7 x10^{14} *m*-scheme dimension)



diagonalization with
t-particle *t*-hole truncation

Monte Carlo Shell Model
+ extrapolation



N. Shimizu, Y. Utsuno, T. Mizusaki, T. Otsuka,
T. Abe, and M. Honma, Phys. Rev. C **82,** 061305(R) (2010).

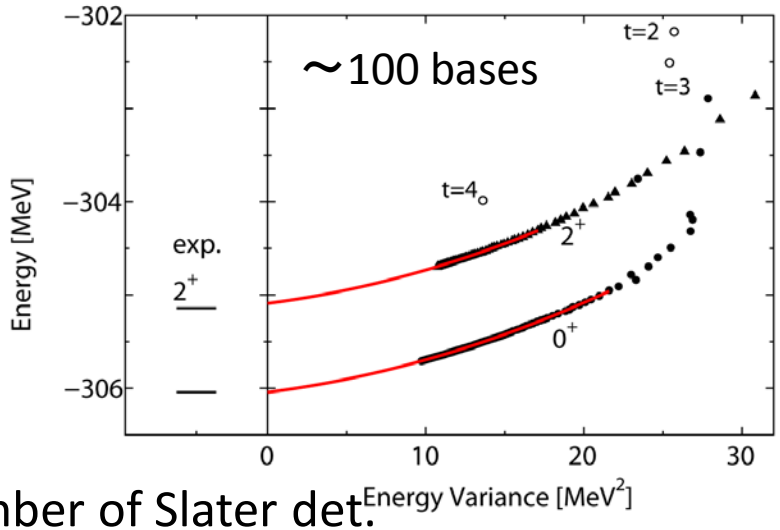
For more efficient computation

Monte-Carlo Shell Model method: Wave function of the nuclear shell model is described by a linear combination of angular-momentum (and parity) projected Slater determinants

$$|\Psi\rangle = \sum_{i=k}^{N_{MCSM}} c_k P^{\pi} \sum_{K=-J}^{J} g_K P^{J,\pi}_{MK} |\phi(D^{(k)})\rangle \qquad |\phi\rangle = \prod_{\alpha=1}^{N} \left(\sum_{i=1}^{N_{sp}} c_i^{\dagger} D_{i\alpha} \right) |-\rangle$$

MCSM basis, deformed Slater det.

By using the energy variance of the approximated wave functions, we estimate the exact eigenvalue precisely.
The computation of the energy variance needs a lot of computer resources, which is proportional to the number of bases squared.



➡ Efficient computation with a small number of Slater det.

Energy minimization by Conjugate Gradient method

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

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

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

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

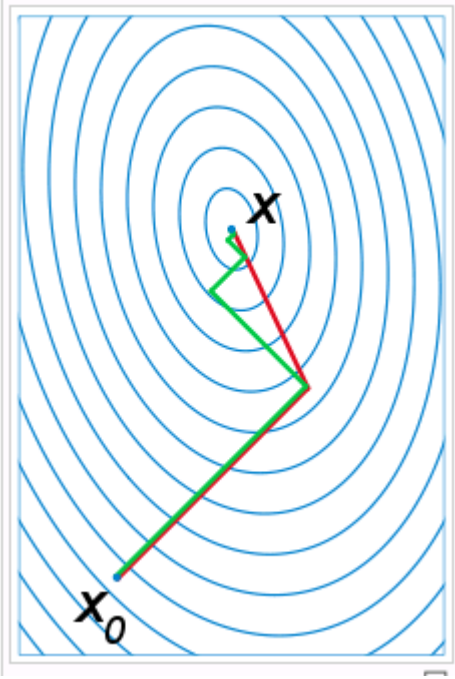
Step1 : Generate basis candidate by auxiliary field technique stochastically

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

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



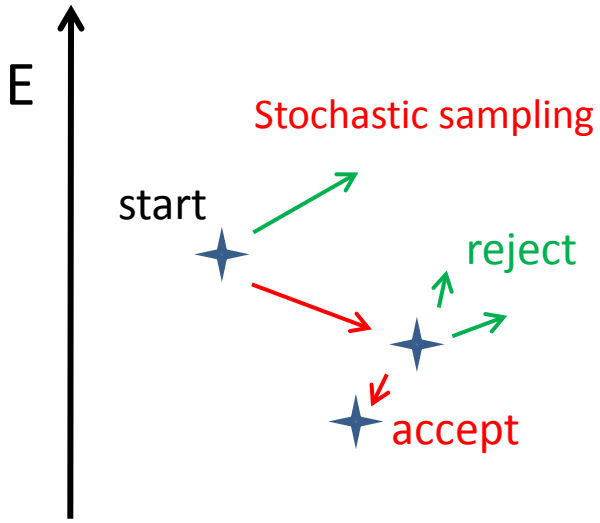
Conjugate gradient taken from wikipedia

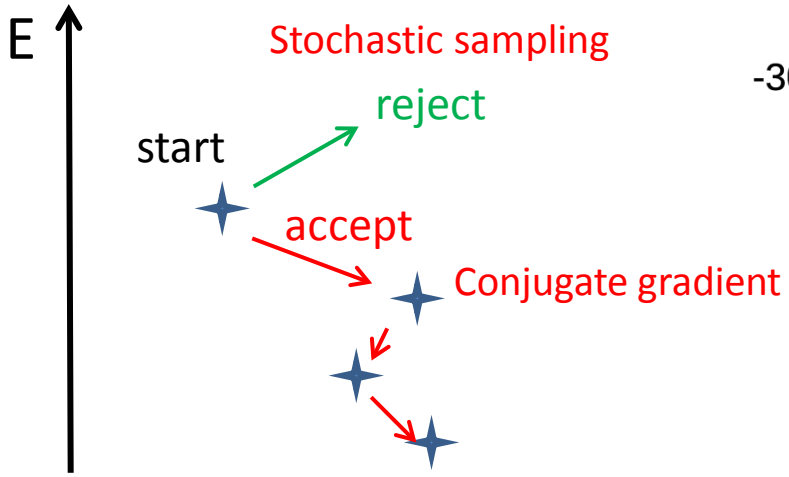
Few Determinant Approximation
M. Honma, B.A.Brown, T. Mizusaki, and T. Otsuka
Nucl. Phys. A 704, 134c (2002)

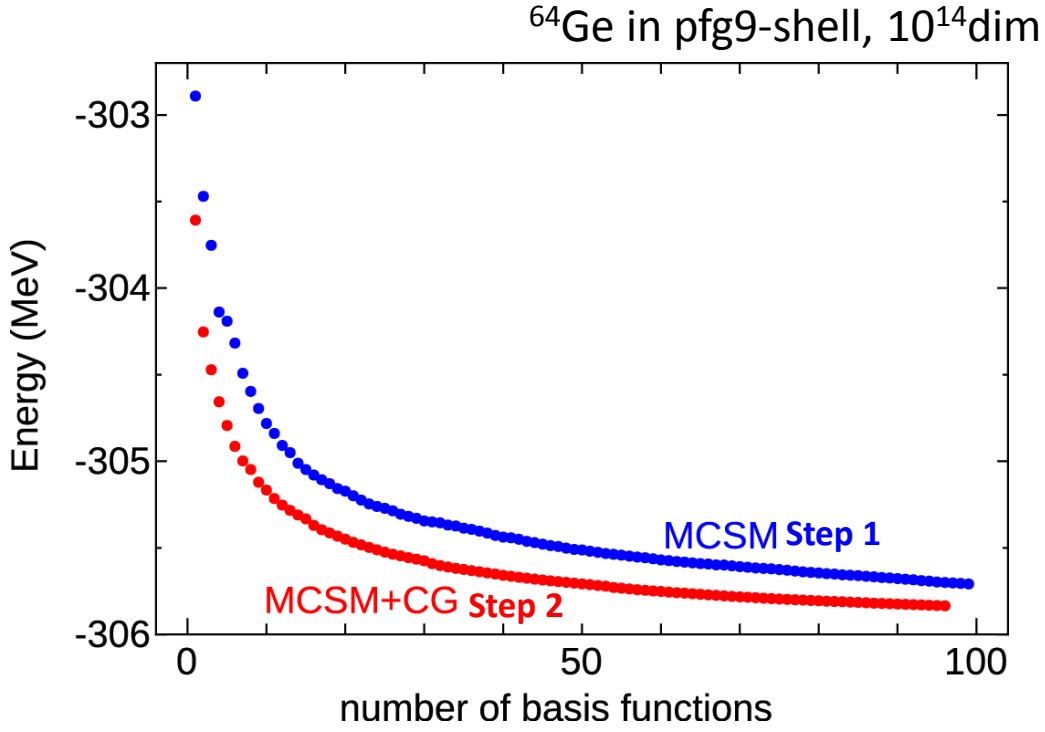
Hybrid Multi-Determinant
G. Puddu, Acta Phys. Polon. B42, 1287 (2011)

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

Energy minimization by Conjugate Gradient method



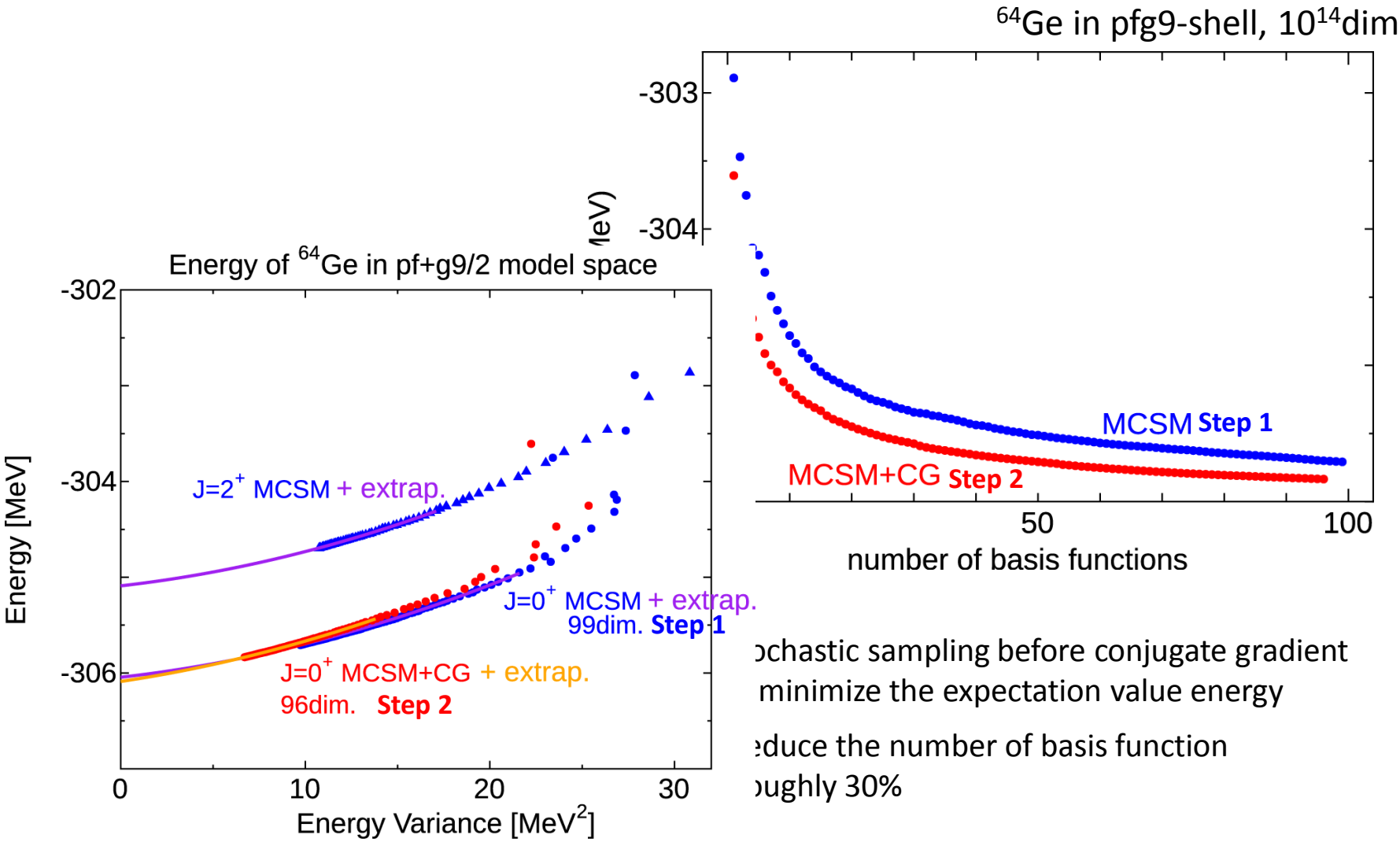




Stochastic sampling before conjugate gradient to minimize the expectation value energy

reduce the number of basis function roughly 30%

Energy minimization by Conjugate Gradient method

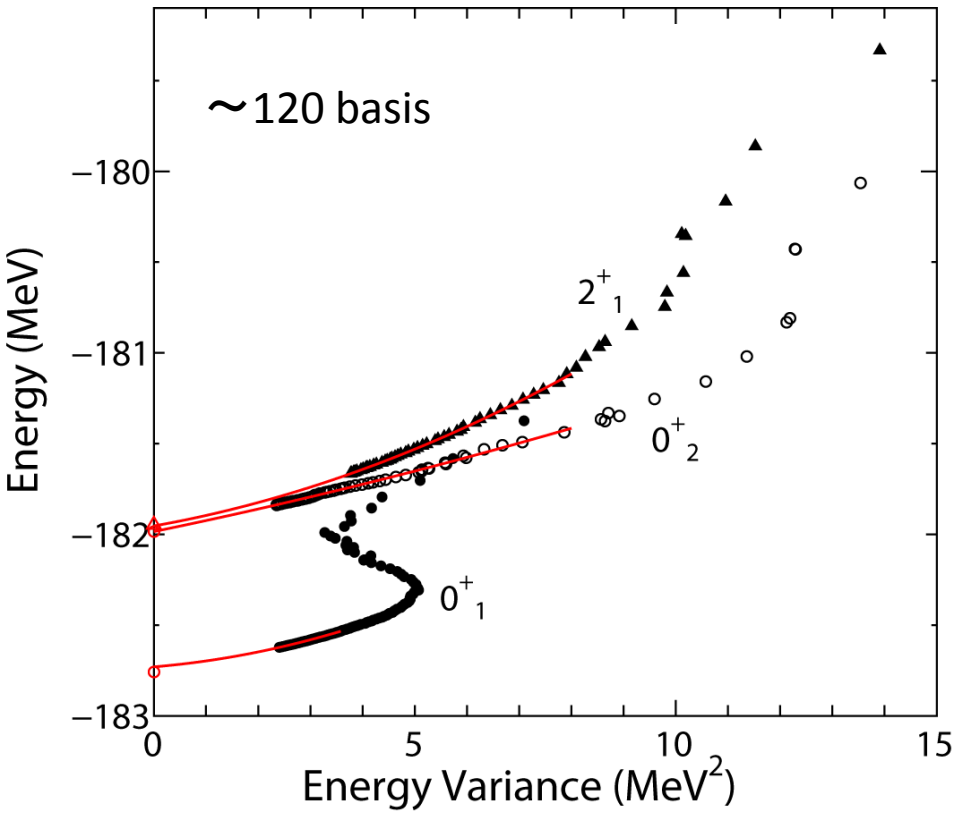


ochastic sampling before conjugate gradient
minimize the expectation value energy

educe the number of basis function
oughly 30%

A possible problem: trapped by another excited state

^{72}Ge, f5pg9, JUN45 int. 1.4x10^{8} m-scheme dim.



The 0^+_1 MCSM wave function up to 20 bases is trapped by the 0^+_2 state.

This situation is rear, the structure of 0^+_2 state is close to the projected Slater det. the ground state includes much many-body correlations.

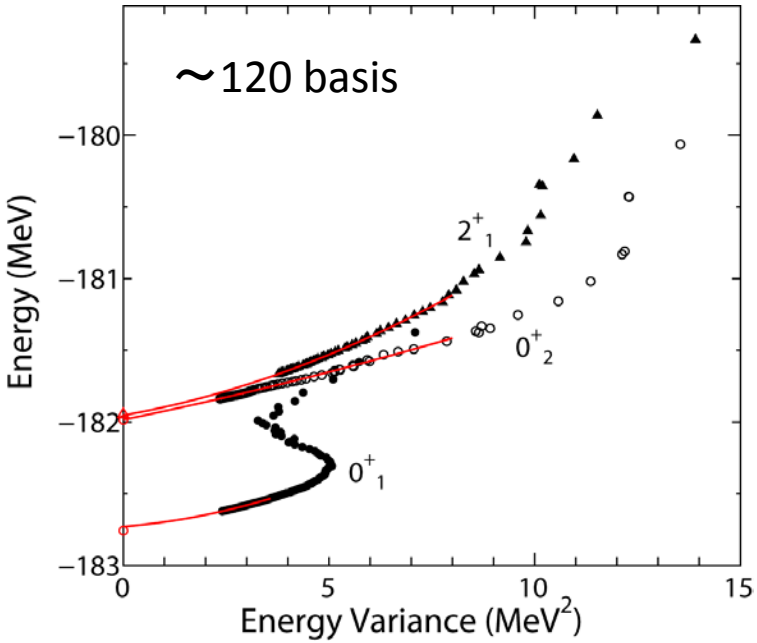
Step 3 : simultaneous optimization of many bases

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

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

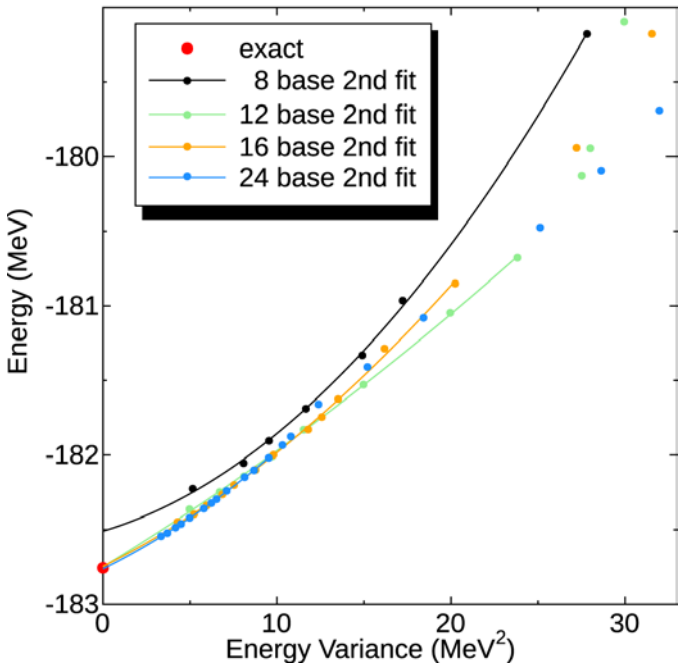
minimization of all $D^{(n)}$, not sequential opt.

^{72}Ge, JUN45 int. 1.4x10^8 m-scheme dim.



sequential optimization of each base, 704 parameters resulting in 120 bases

^{72}Ge, JUN45, ground state



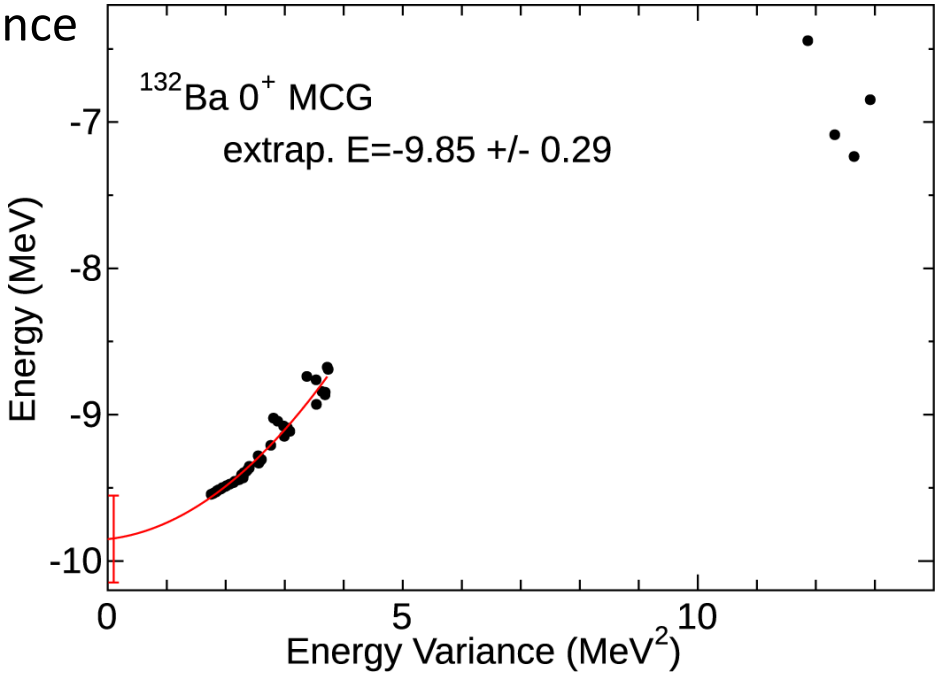
optimization of 24 bases, 16896 parameters with simultaneous variation
many-basis correlation is included from beginning

A possible problem: narrow region for fit

N,Z=50~82, P+QQ int.
triaxial deformed Xe, Ba isotopes

In some cases, the range of the variance is too small to make stable fit

2^{nd} order polynomial fit causes large uncertainty of the extrapolation



Re-ordering of the basis functions

Ansatz: Energy-variance extrapolation method always works and the extrapolated value is independent of the ordering of basis functions ...

A sequence of the approximated wave functions

$$\left|\Psi_1\right\rangle = c_1^{(1)}\left|\phi_1\right\rangle$$

$$\left|\Psi_2\right\rangle = c_1^{(2)}\left|\phi_1\right\rangle + c_2^{(2)}\left|\phi_2\right\rangle$$

$$\left|\Psi_3\right\rangle = c_1^{(3)}\left|\phi_1\right\rangle + c_2^{(3)}\left|\phi_2\right\rangle + c_3^{(3)}\left|\phi_3\right\rangle$$

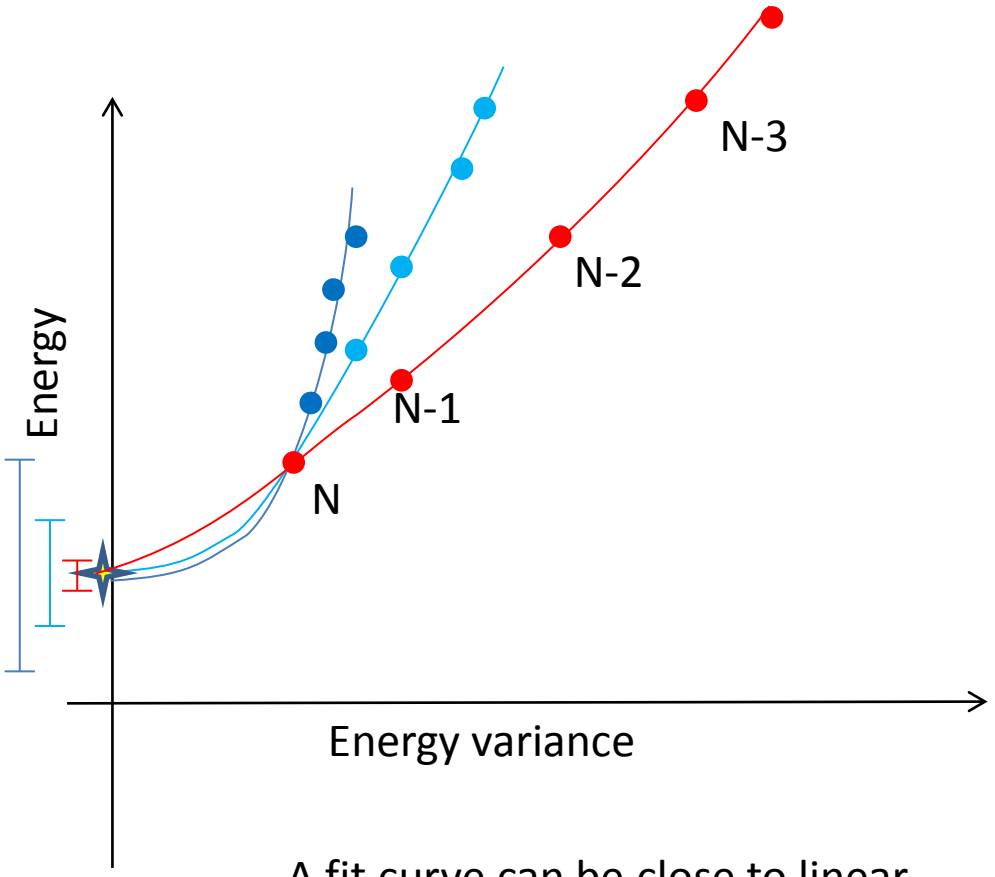
...

$$\left|\Psi_N\right\rangle = \sum_{i=1}^{N} c_i^{(N)}\left|\phi_i\right\rangle$$

Re-ordering

$$\left|\phi_1\right\rangle, \left|\phi_2\right\rangle, \left|\phi_2\right\rangle, \ldots, \left|\phi_N\right\rangle$$

to obtain another sequence and fit



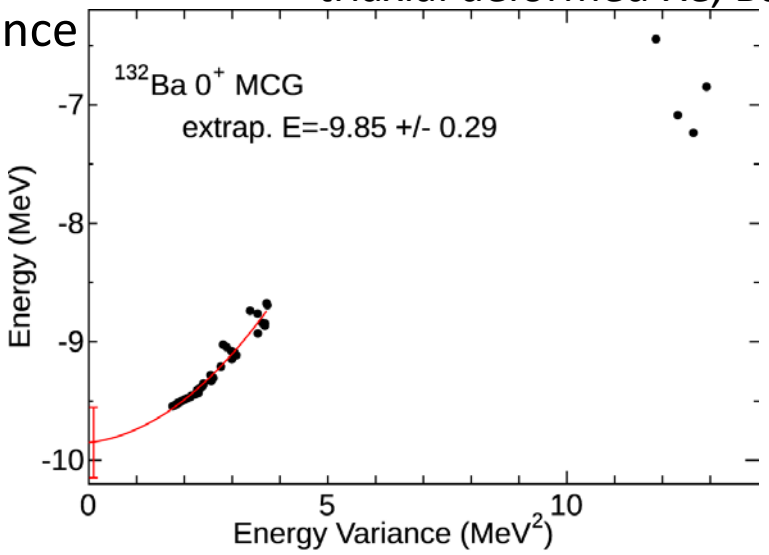
A fit curve can be close to linear

A possible problem: narrow region for fit

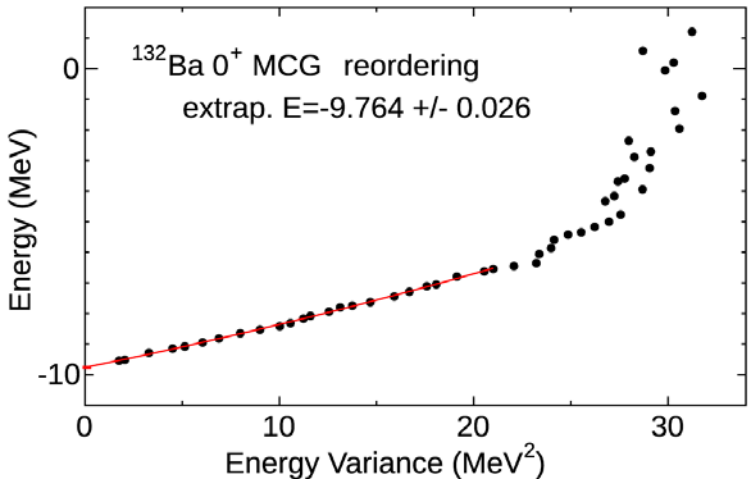
N,Z=50~82, P+QQ int.
triaxial deformed Xe, Ba isotopes

In some cases, the range of the variance is too small to make stable fit

2^{nd} order polynomial fit causes large uncertainty of the extrapolation

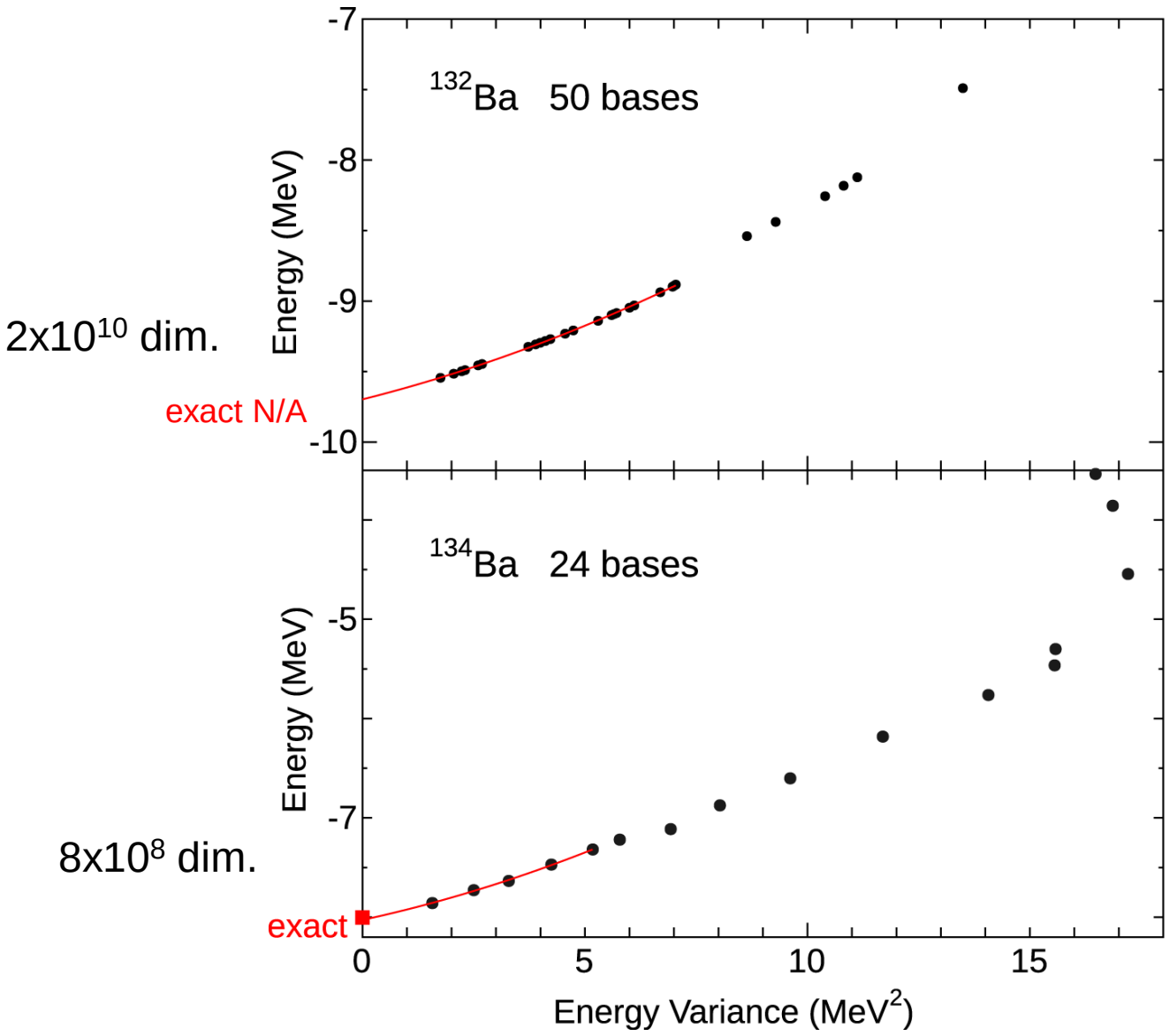


Reordering of the bases decreases the uncertainty of the extrapolated value



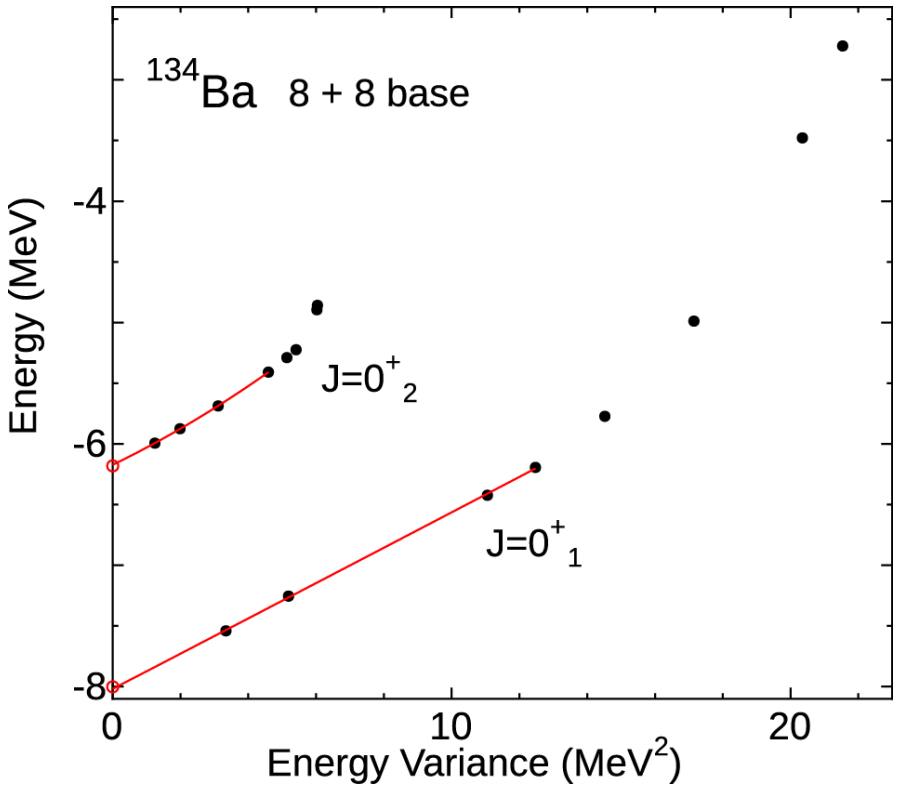
fit curve is close to linear

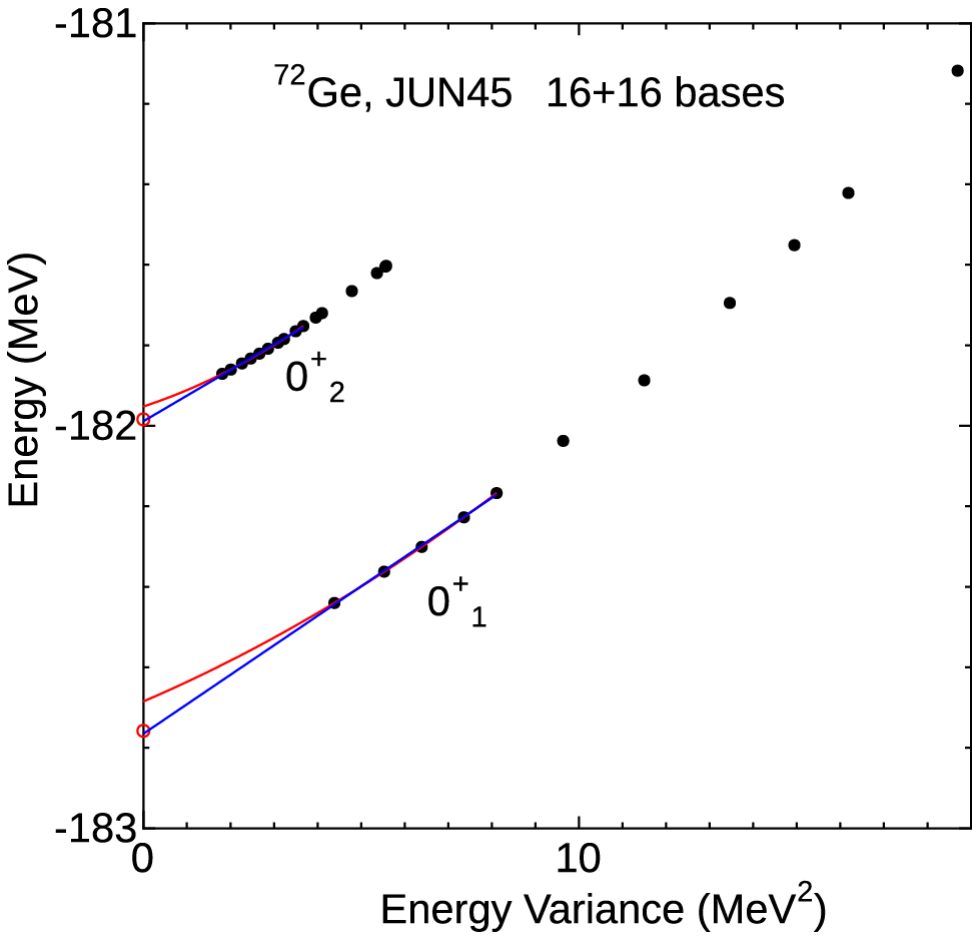
Energy-variance extrapolation for ground state energy



non-yrast states

8 bases are optimized for 0^+_1
additional 8 bases for 0^+_2

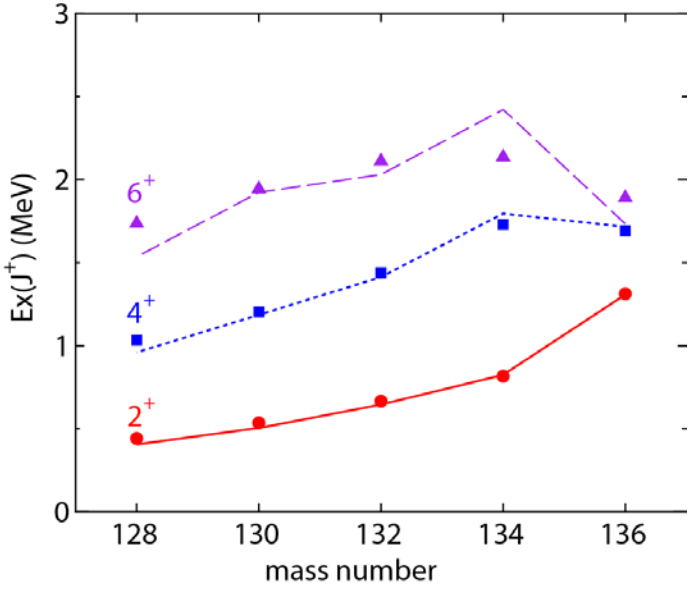


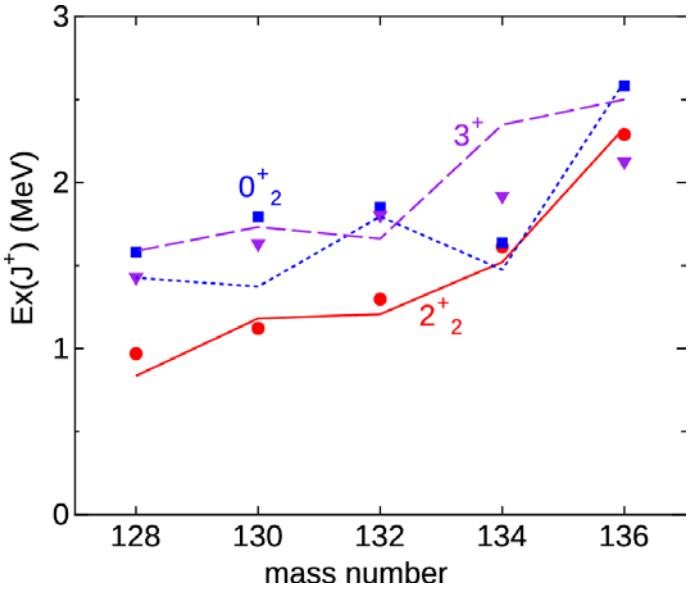


1st order extrapolation

2nd order extrapolation

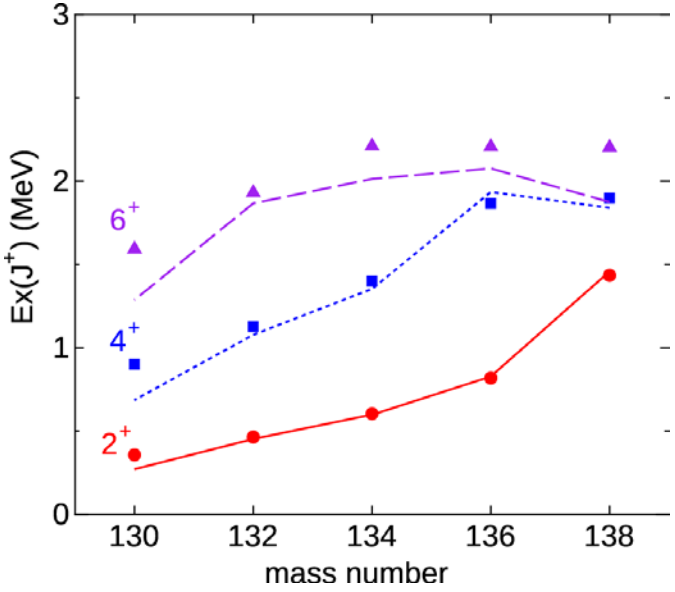
Excitation energies of Xe isotopes

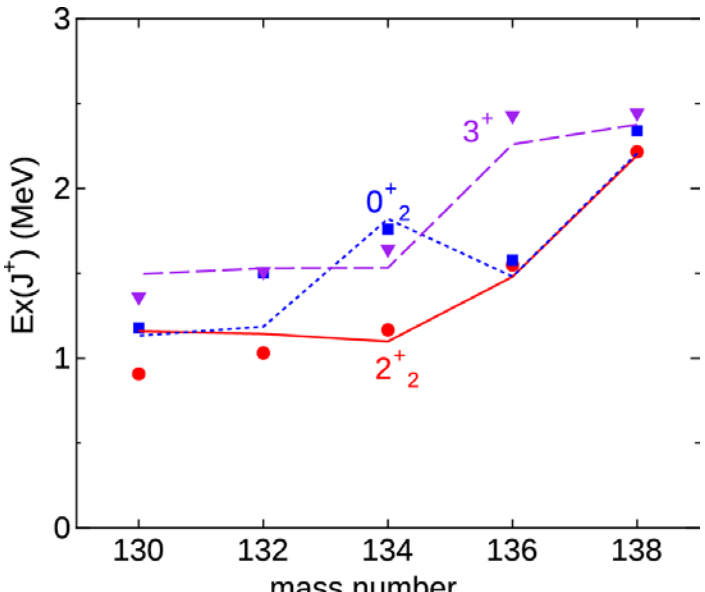




symbol: exp.
line : theory

Excitation energies Ba isotopes





The application of the MCSM+extrapolation method to no-core shell model calculations

T. Abe (Univ. of Tokyo), T. Otsuka (Univ. of Tokyo),
N. Shimizu (Univ. of Tokyo), Y. Utsuno (JAEA),
J. Vary (Iowa), P. Maris (Iowa)

JISP16 NN interaction

- JISP16: J-matrix Inverse Scattering Potential tuned B.E.s up to 16O with phase-shift-equivalent unitary transformation

$$V = \sum_{\Gamma,\Gamma'} \sum_{n=0}^{N_\Gamma} \sum_{n'=0}^{N_{\Gamma'}} |n,\Gamma\rangle V_{n,n'}^{\Gamma,\Gamma'} \langle n',\Gamma'|$$

  - Small matrix of the NN int. in the oscillator basis
  - High quality description of NN potential thru. p-shell nuclei
    -> Reproduce the phase shift, deuteron properties, & B.E.s of some light nuclei
    -> In this sense, JISP16 is the "bare" interaction
  - JISP16 NN int. seems to minimize 3N (many-body) int.

→ feasible for the large-scale computation of nuclear structure

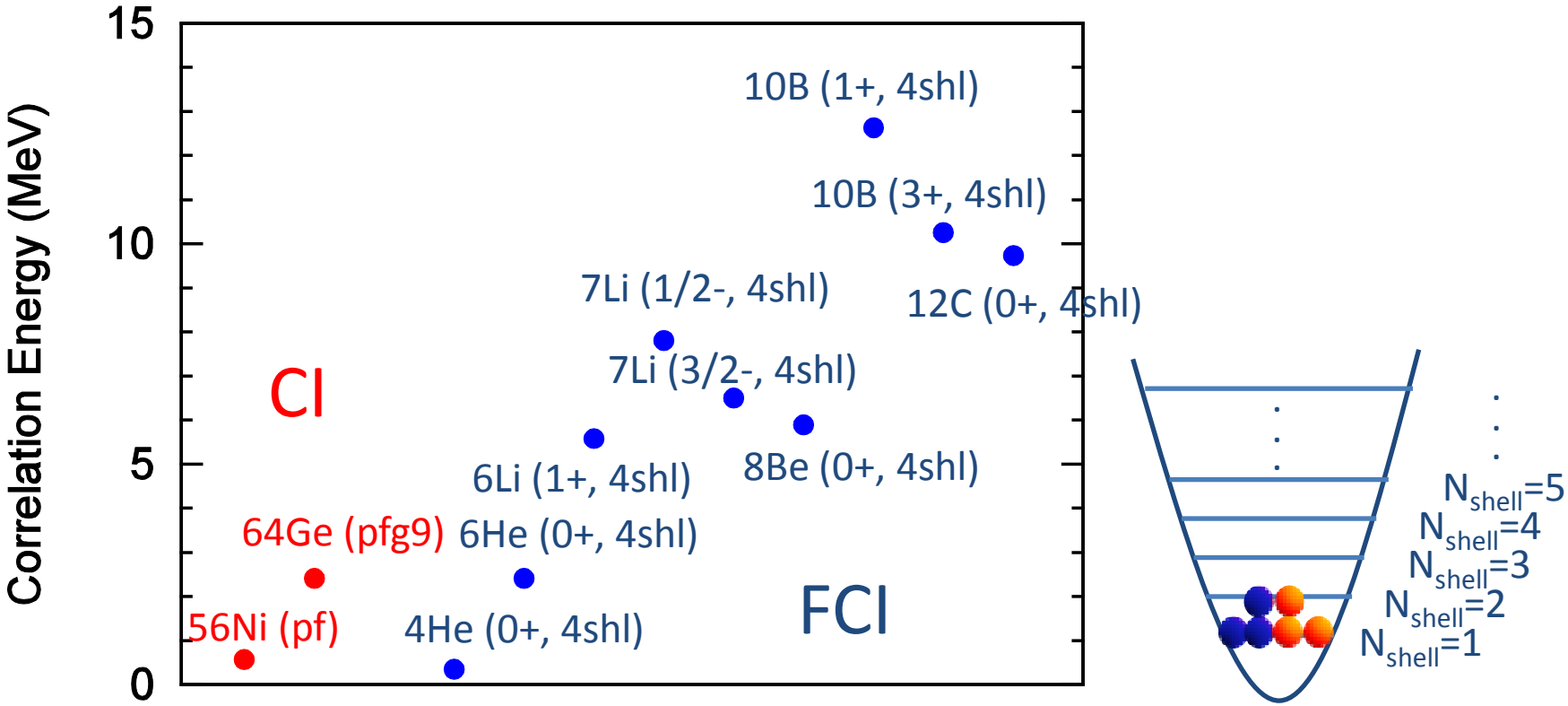
References

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)

Why we need to extrapolate the energies

The first basis of the MCSM

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

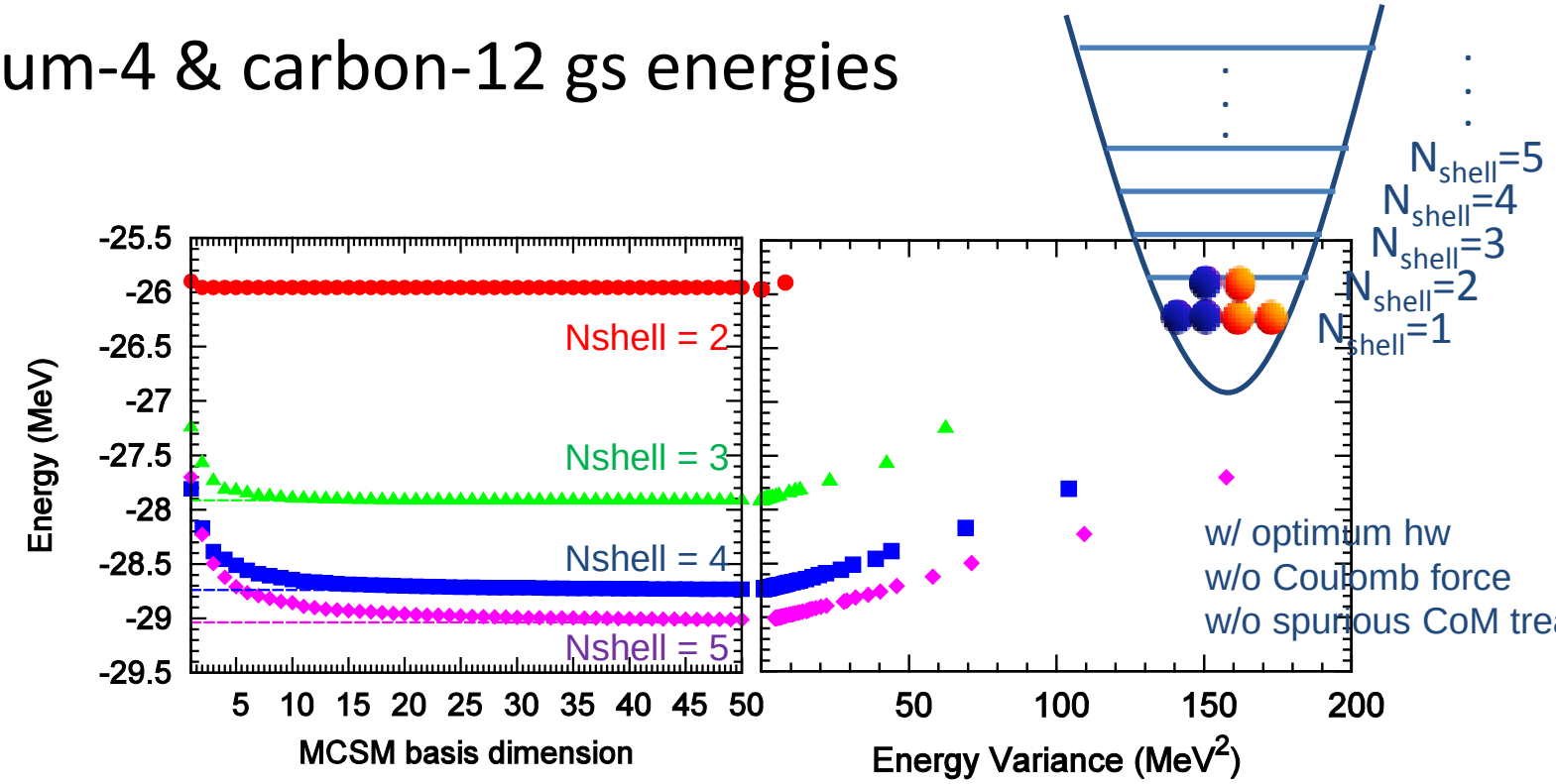


NCSM wf w/ realistic NN int is more correlated (complicated) than SSM wf w/ effective int

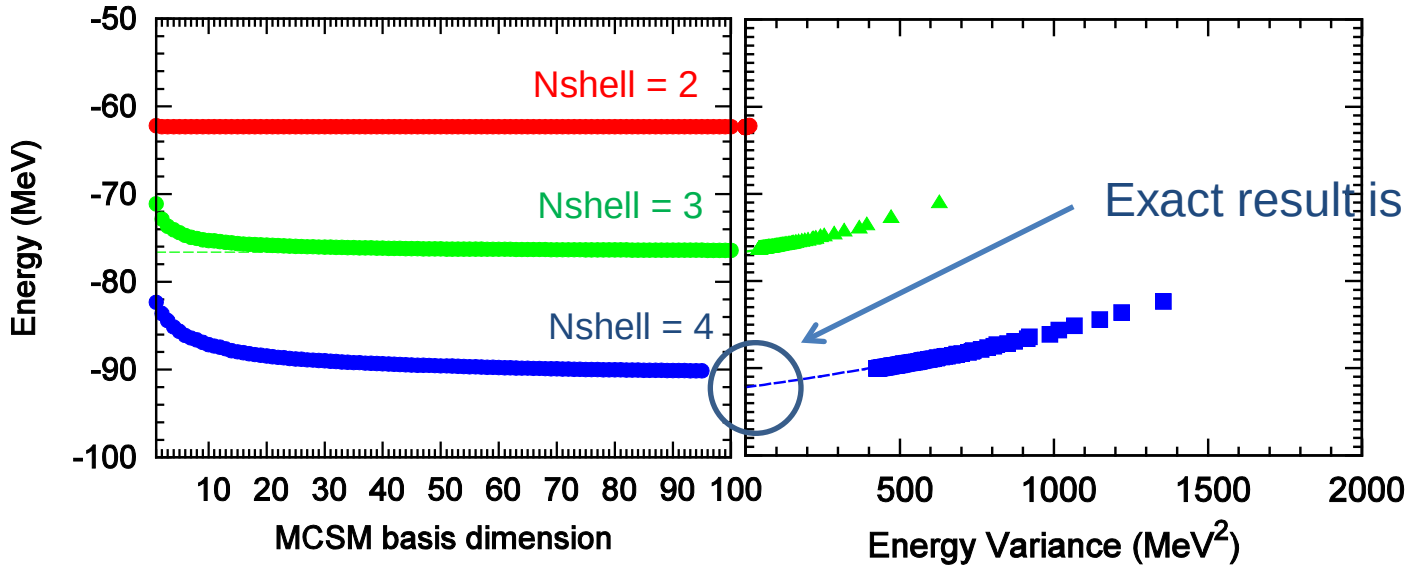
Need energy-variance extrapolation for No-Core MCSM calc

Helium-4 & carbon-12 gs energies

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



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



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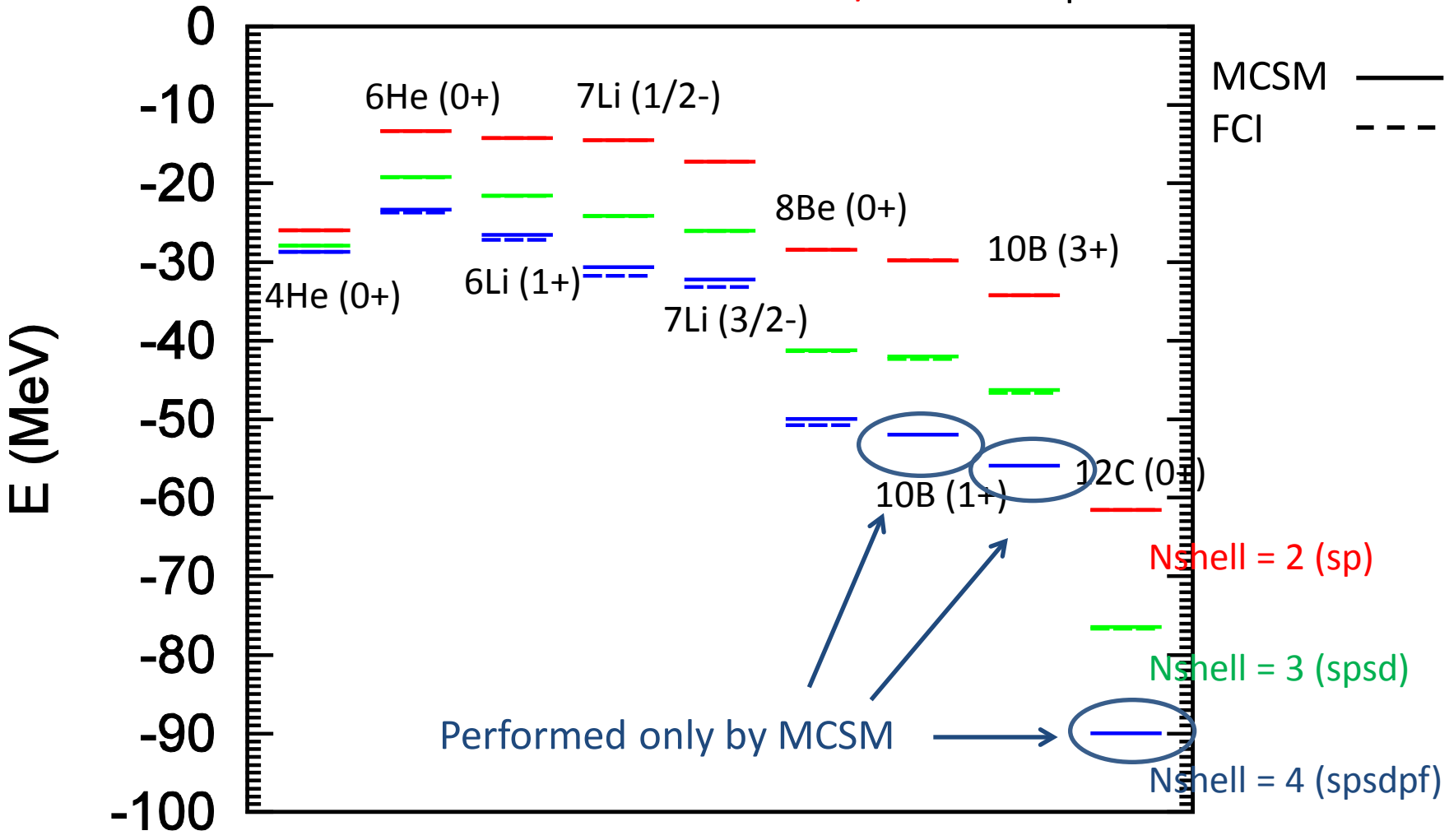
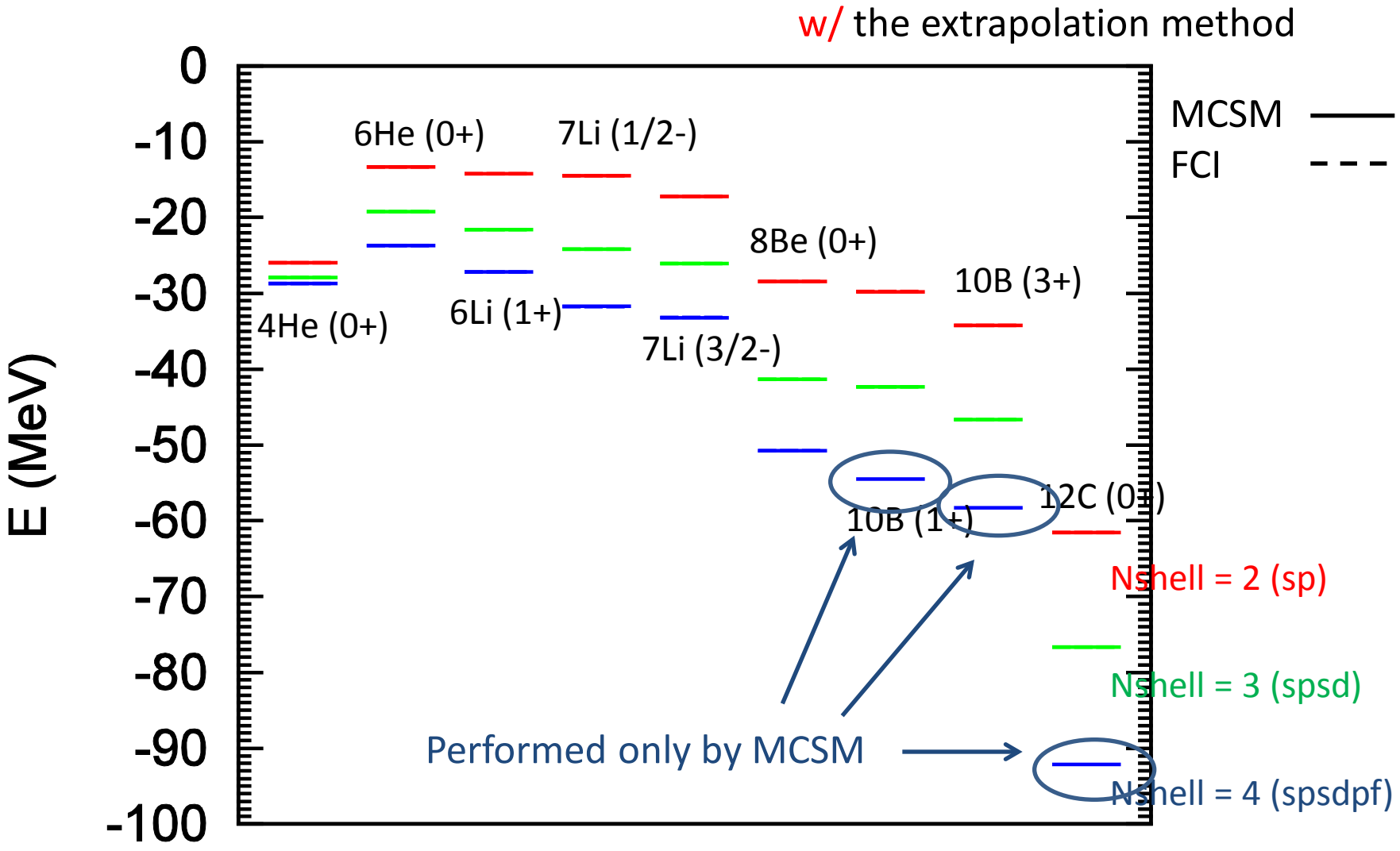
Energies of Light Nuclei

w/o the extrapolation method



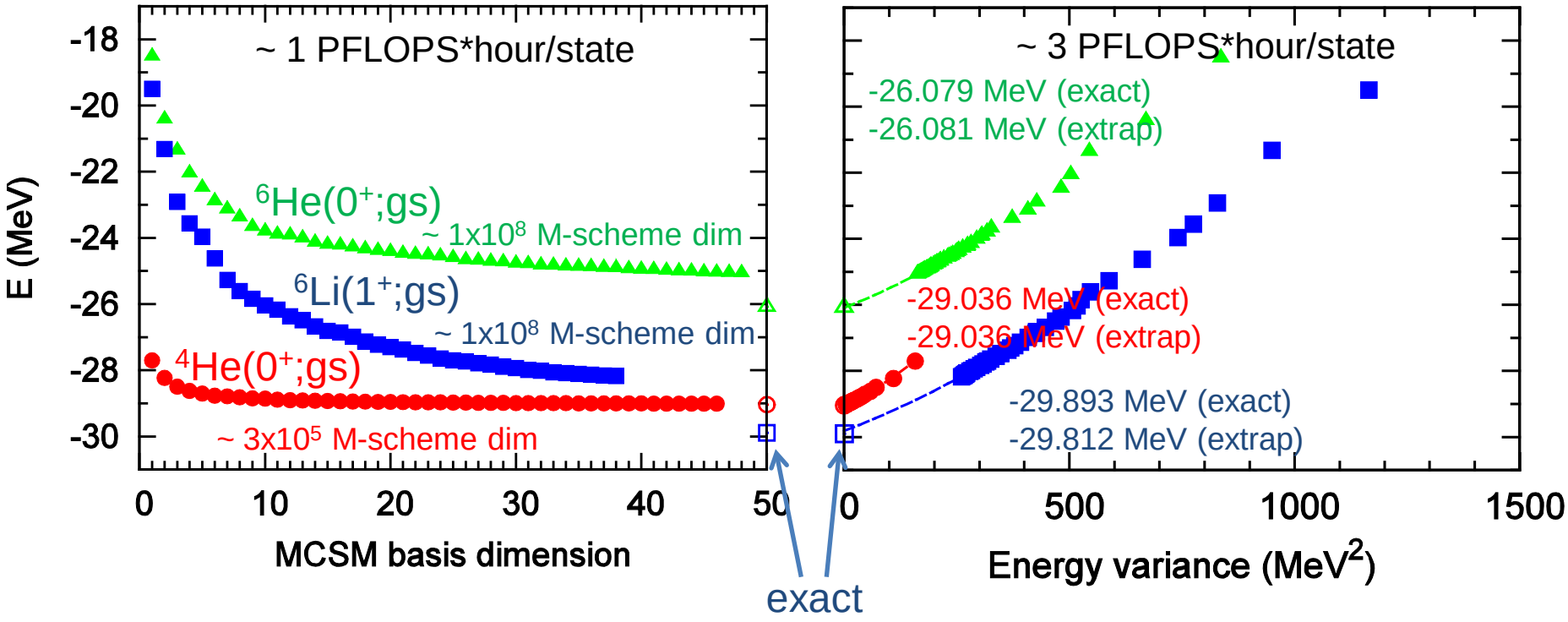
T. Abe, P. Maris, T. Otsuka, N. Shimizu, Y. Utsuno, J. P. Vary

Energies of Light Nuclei



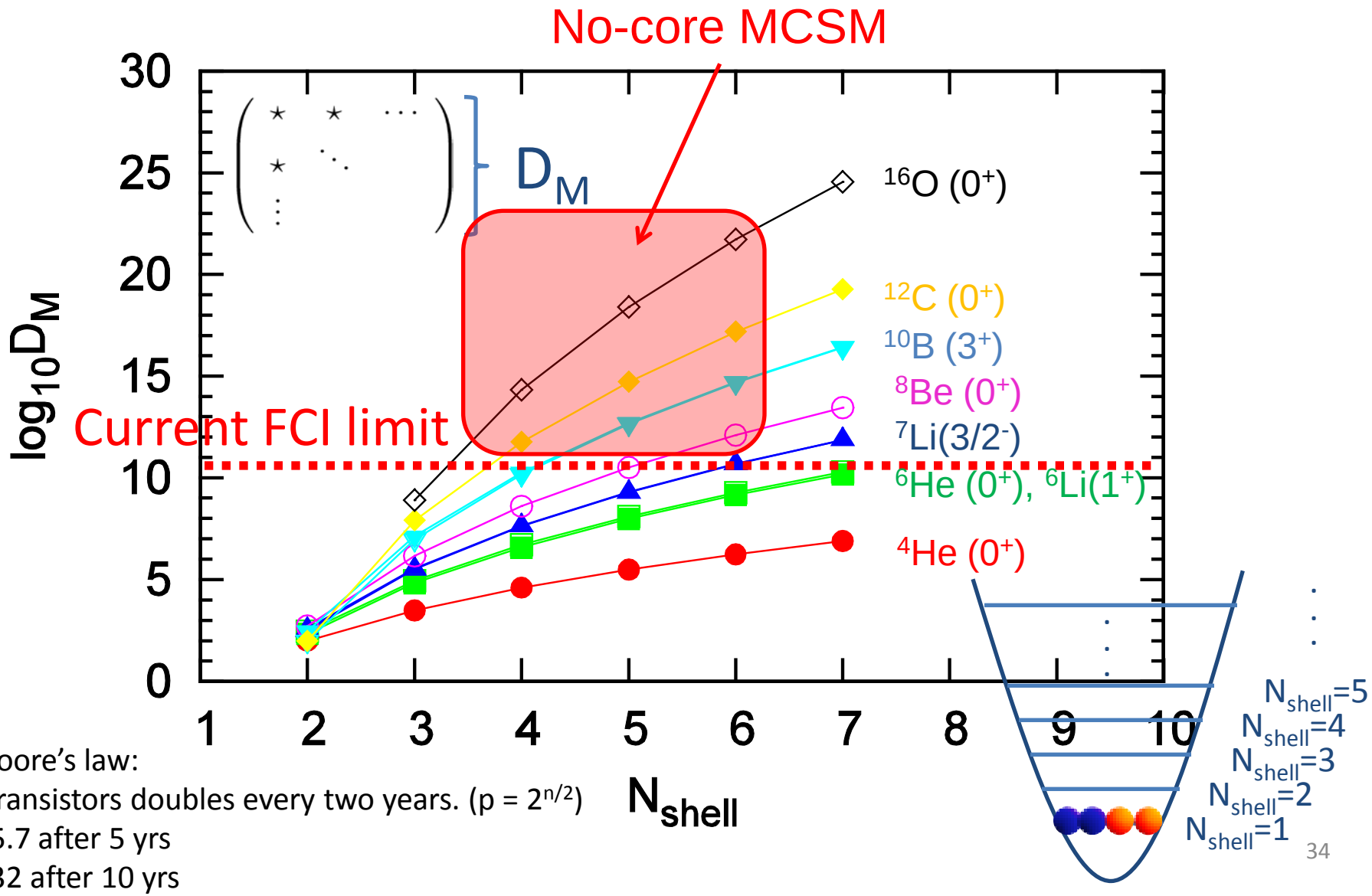
Nshell=5 Calculations

- Benchmark calculation of light nuclei with Nshell=5



- The extrapolated values are obtained within a few 10 keVs uncertainty.

M-scheme dimension



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

aim at many-particle many-hole excited state

Summary

- Energy-variance extrapolation works well in the frameworks of the MCSM, conventional Lanczos method with truncation, and the Variational Monte Carlo. It demonstrates up to 10^{14} dimension system.
- Conjugate Gradient optimization method makes the MCSM calculation more efficiently.
- Many basis optimization enables us to avoid the trapping problem of higher excited state.
- No-core MCSM shows its feasibility in light nuclei.
- The MCSM code is under intensive developments for massive parallel computation and “K computer”.