Shell model calculation
— from basics to the latest methods —

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What we will learn?

- Basics
  - What is Shell Model?
  - Shell model basis states
  - M-scheme
  - Lanczos method
  - Famous shell model codes
- The Latest methods
  - Extrapolation methods

Understanding of nuclear structure

- **To solve many-body problem, we need following:**

  - **Interaction**

  - **Model Space**

  - **Method to solve**

$$H\,|\phi> = E\,|\phi>$$

Interaction

How to solve

Model Space

> In most cases, we have **incomplete** information and we can solve it **incompletely**.

⟶ Two approaches in nuclear structure physics.
One is a mean-field approach.
The other is a SM approach.

Mean field and its extended approach

- **First, Method & Model space are fixed as HF or HFB.**

- **Second, interaction parameters are determined under this condition to reproduce experimental data.**

➡️ **GCM, Projection, Multi-Slater Determinants are introduced.**

⬇️

Interaction parameters must be changed.

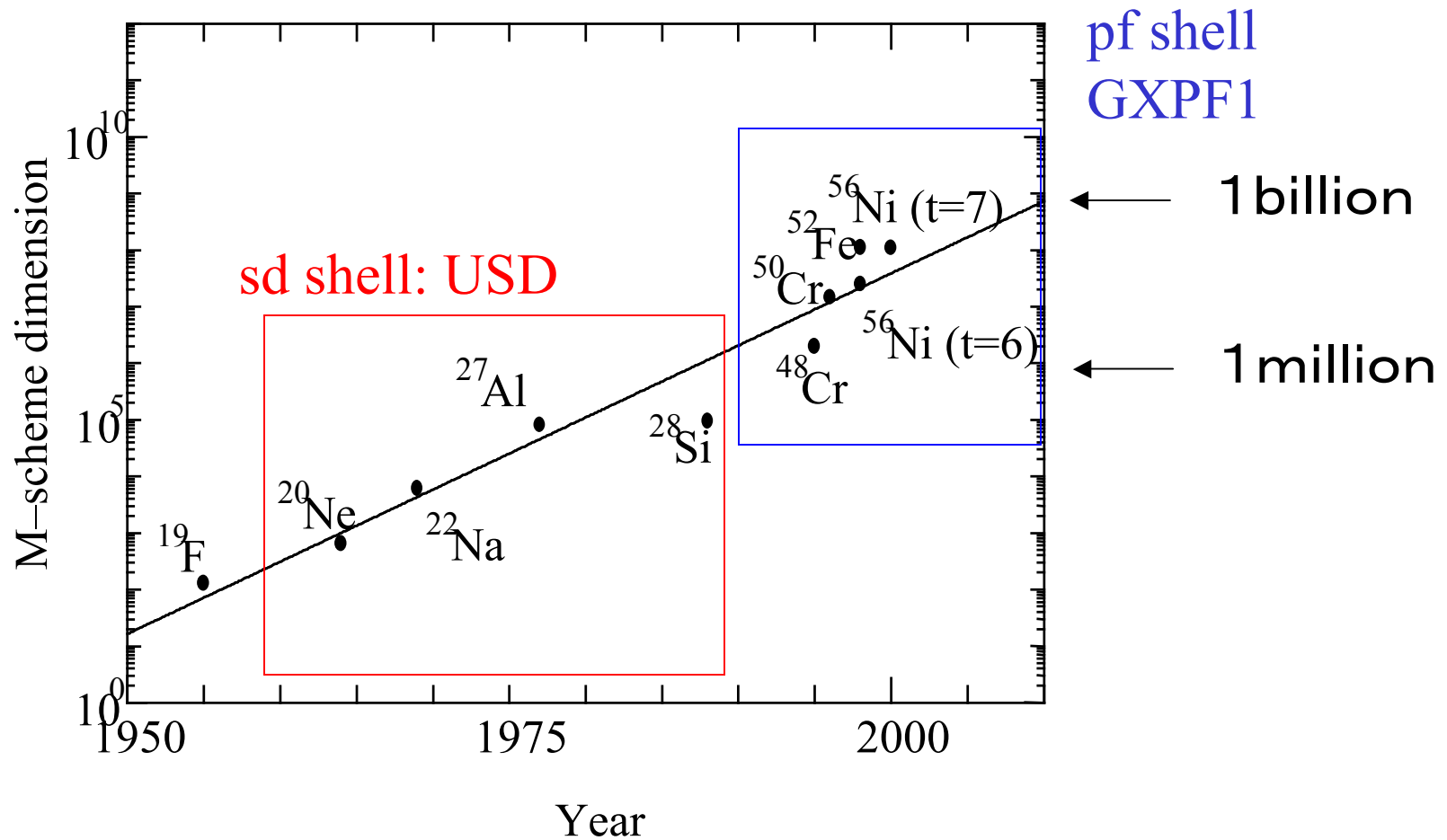# Microscopic shell model approach

- **First, model space & interaction are fixed.**

- **Second, we consider how to solve many-body problem then we solve it (in a approximate way).**

- **Interaction is given microscopically.**

- **Various methods to solve many-body problem**

- **Exact solution exists.**

What is Shell Model?

- Two phases
  - Derivation of interaction
  - Method for large-scale shell model calculations

- We focus the latter issue today.

QCD
↓

Nuclear Force

↓

Effective Interaction for SM

↓

Shell Model Interaction

↓

How to solve Shell Model?

Microscopic shell model
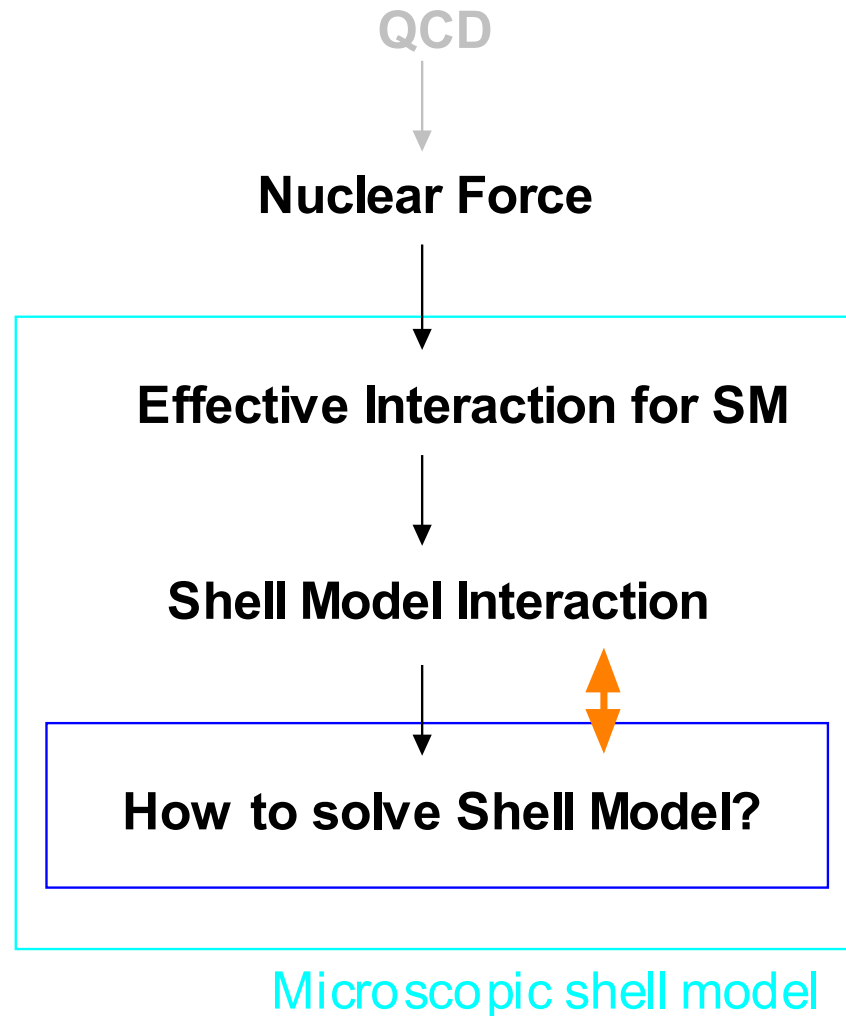
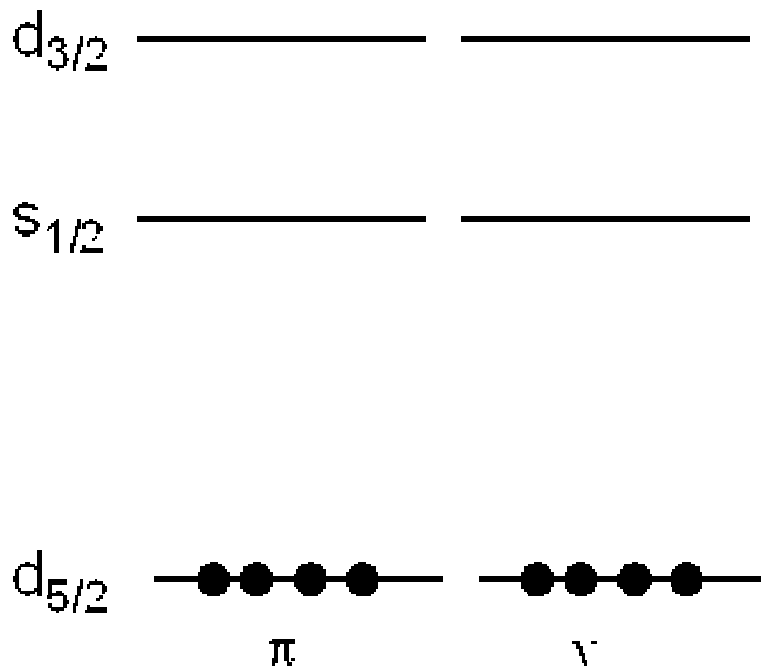Long history of shell model calculations

Shell model space

- Inert core is assumed.
- Shell model space is determined by considering shell gap.
- Shell model space is not so large compared to that of mean-field calculations but we deal with all degrees of freedom within this space.

large shell gap

$d_{3/2}$

$s_{1/2}$

shell model space

$d_{5/2}$

π ν

large shell gap

Inert Core

....
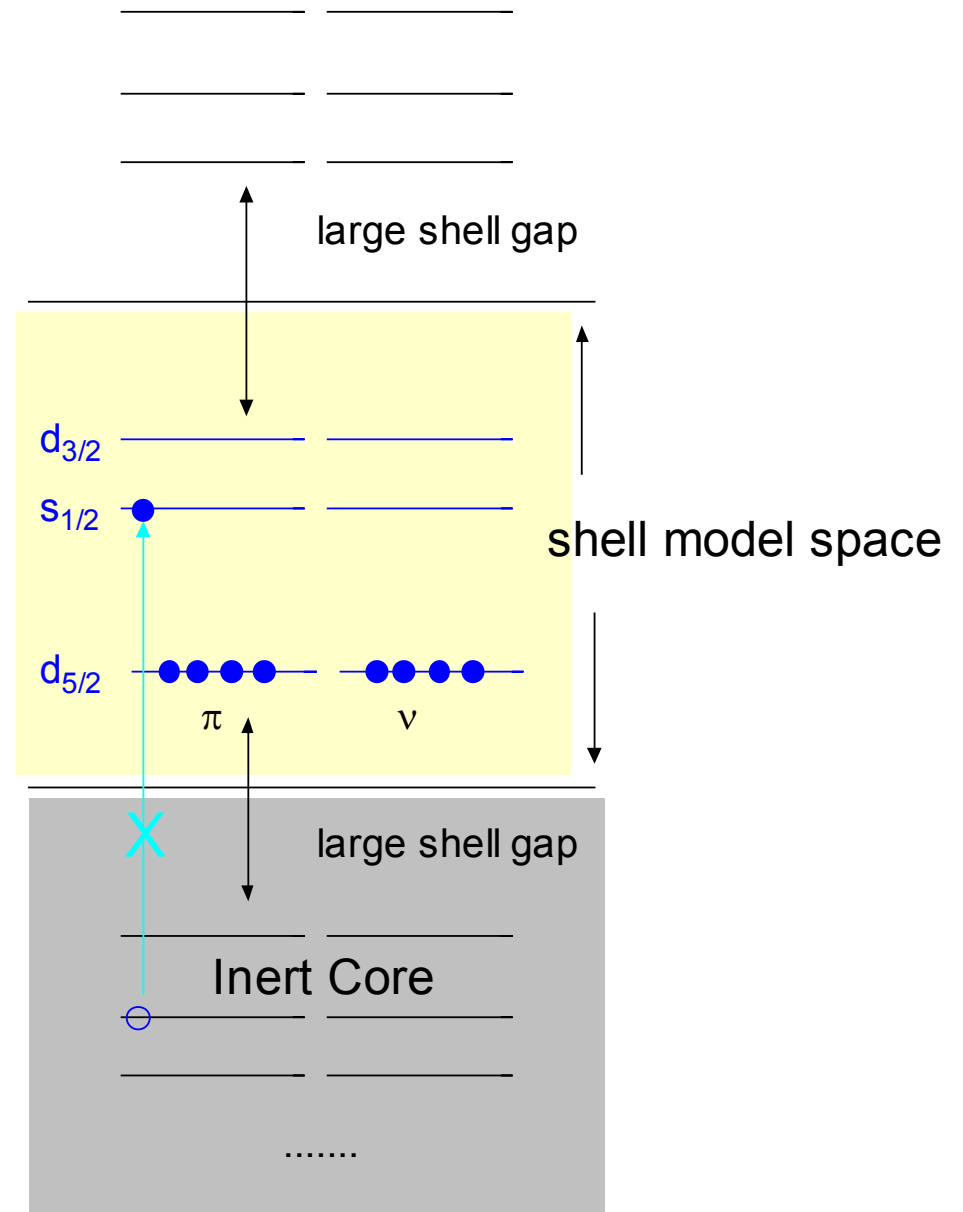
Shell model configurations

$d_{3/2}$ —————— ——————

$s_{1/2}$ —————— ——————

$d_{5/2}$ ●●●● ——— ●●●● ———

π   ν

- Protons and neutrons move all active single particle orbits with following restrictions.
  - Isospin conservation
  - Angular momentum conservation
  - Parity conservation
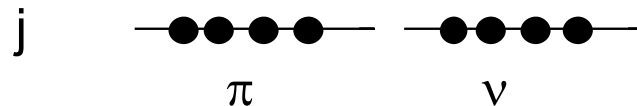- We consider such all many-body configurations.

- Combinatorial problem

Many-body basis

- J orbit has (2J+1) degeneracy for Jz.
- If we put N_π protons and N_ν neutrons on such orbits, number of possible configurations are

$$_{2J+1}C_{N_\pi} \times _{2J+1}C_{N_\nu}$$

- unless relevant conservations are taken into account.
- Number of basis increases in a combinatorial way.

M-scheme basis states

- Sample of M-scheme basis
- Bit-wise representation in computer code
- Mz for proton is 3/2+1/2+1/2-3/2=2/2
- Mz for neutron is -1/2+1/2+1/2-3/2=-2/2
- Total Mz=2/2-2/2=0

$$c_{p1}^{\dagger} c_{p2}^{\dagger} c_{p3}^{\dagger} c_{p4}^{\dagger} c_{n1}^{\dagger} c_{n2}^{\dagger} c_{n3}^{\dagger} c_{n4}^{\dagger} \left| 0 \right\rangle$$
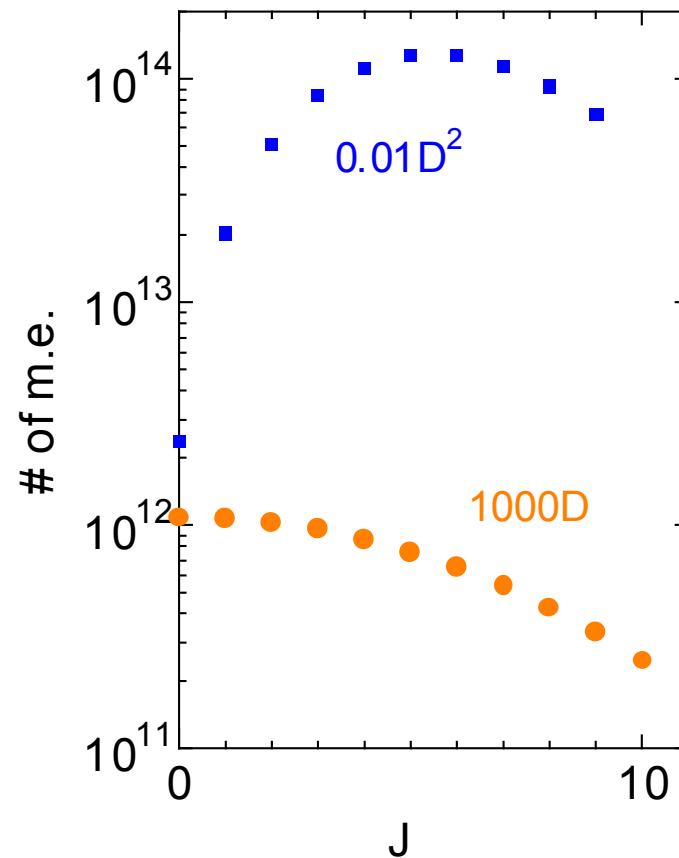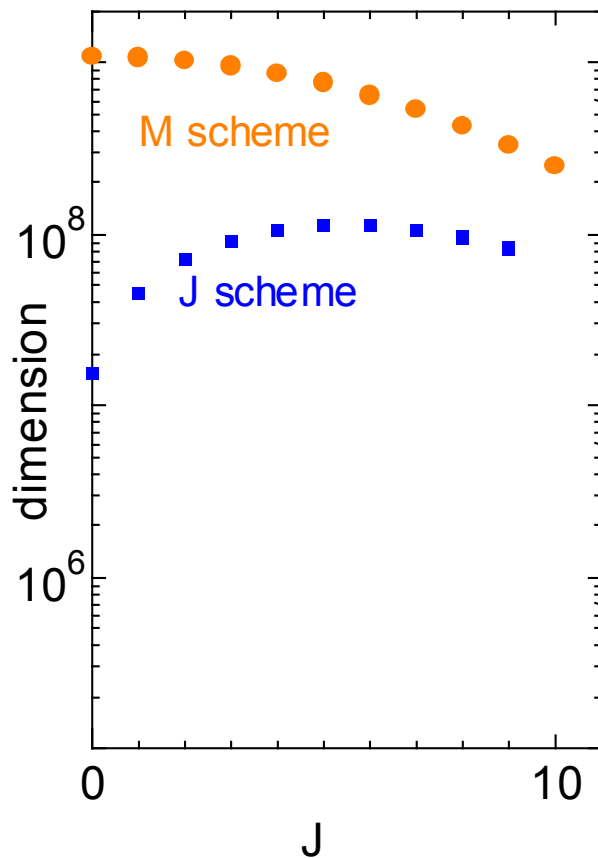
proton

$d_{5/2,3/2,1/2,-1/2,-3/2,-5/2}$						$s_{1/2,-1/2}$		$d_{3/2,1/2,-1/2,-3/2}$			
0	1	1	0	0	0	1	0	0	0	0	1

neutron

$d_{5/2,3/2,1/2,-1/2,-3/2,-5/2}$						$s_{1/2,-1/2}$		$d_{3/2,1/2,-1/2,-3/2}$			
0	0	0	1	0	0	1	0	0	1	0	1

M scheme vs. J scheme

- M scheme has an advantage for large-scale shell model calculations.

- It requires less computer resource (memory).

M scheme for large-scale shell model calculations

- **M-scheme: Evaluation of matrix elements are easy and very fast. Then matrix elements are always calculated when they needed. Two vectors are in memory.**

- **J-scheme: Evaluation of matrix elements needs 6J and CFP and need a lot of CPU power Then matrix elements are in FILE, which is too big. Two vectors are in memory.**

- **M-scheme is better than J-scheme for large-scale shell model calculations.**

$$\begin{pmatrix} \text{SM MATRIX} \end{pmatrix} \begin{pmatrix} \ \end{pmatrix} = E \begin{pmatrix} \ \end{pmatrix}$$

Lanczos method

- For low-lying spectra for quantum many-body systems ie, Shell model, Hubbard model, FQHE, and so on, Lanczos method is convenient.

- H operation enhances low-lying components.

$$\left|\psi_0\right\rangle, H\left|\psi_0\right\rangle, H^2\left|\psi_0\right\rangle, H^3\left|\psi_0\right\rangle, \cdots$$

$$\left|\psi_k\right\rangle \equiv \frac{1}{N_k} H^k\left|\psi_0\right\rangle$$

$$\left|\psi_0\right\rangle, \left|\psi_1\right\rangle, \left|\psi_2\right\rangle, \left|\psi_3\right\rangle, \cdots$$

- We diagonalize the hamiltonian by these basis vectors.

- As these vectors are non-orthgonal, we orthogonalize them.

- These vectors are called Lanczos vectors.

Lanczos method cont'd.

- Lanczos method can covert original matrix to tridiagonal one, which is easily diagonalized.

$$H \longrightarrow \begin{pmatrix} \alpha_1 \beta_1 & & & & \\ \beta_1 \alpha_2 \beta_2 & & & & \\ & \beta_2 \alpha_3 \beta_3 & & & \\ & & \beta_3 \alpha_4 \beta_4 & & \\ & & & \beta_4 \alpha_5 \beta_5 & \\ & & & & \beta_5 \alpha_6 \end{pmatrix}$$

$$|\phi_{L+1}\rangle = H|\phi_L\rangle - \alpha_L|\phi_L\rangle - \beta_L|\phi_{L-1}\rangle$$

$$\alpha_L = \langle\phi_L|H|\phi_L\rangle$$

$$\beta_L = \langle\phi_{L-1}|H|\phi_L\rangle$$

$$E_1 > E_2 > E_3 > E_4 > E_5 > E_6$$

- Ground state energy can be obtained by L Lanczos vectors. We consider convergence of ground state energy as a function of L.

Typical convergence patterns

- Ground state energy is obtained by fewer L, which is general feature even for huge problem.

- Excited energies are also obtained by Lanczos method.

- As H operation can keep symmetries, we can carry out Lanczos method for definite symmetries (spin and parity) even in M-scheme, by choosing symmetry preserving initial wave function.
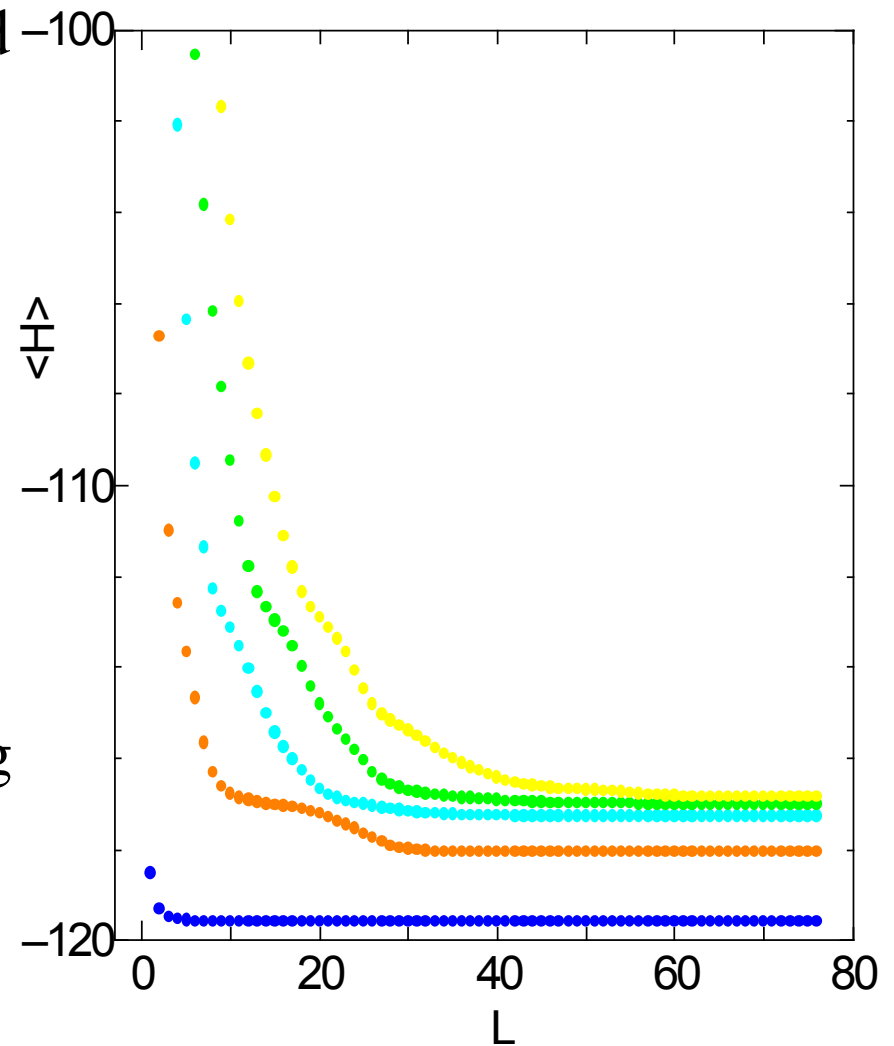
Lanczos shell model codes

- Large-scale shell model codes
  - SM^2(Strasbourg/Madrid)
  - MSHELL (Tokyo, Mizusaki)
  - VECSSE (Tokyo, Sebe)
  - MSU code (MSU, Horoi)

- MSHELL (My shell model code)
  - Code is well fitted for pentium personal computer.
  - Pentium 4 3GHz with 1 gigabyte memory
  - ^{48}Cr (2 million): 5 min for ground state
  - 100 million problem is possible.
  - At next domestic CNS workshop, we may offer a course for this code.

Truncation scheme

- For low-lying states, important subspace is selected in various ways.

- For example, one of natural truncation for fp shell is to use shell gap for N=Z=28. In various papers, the number of excited nucleons across this shell gap is called t. The truncated space is specified by t.

- There are more elaborate truncation schemes.
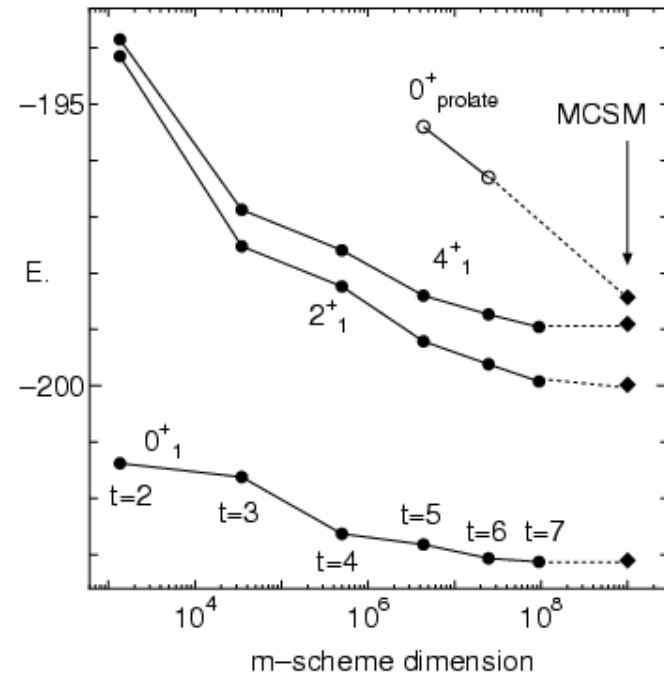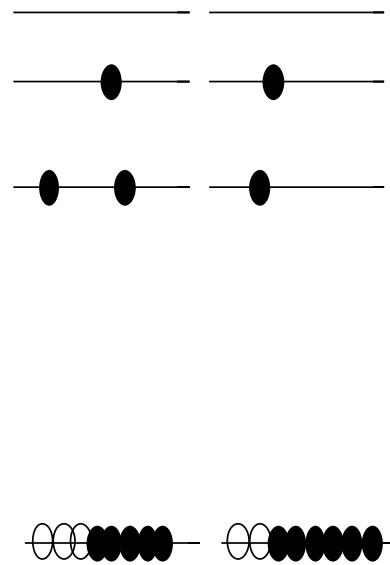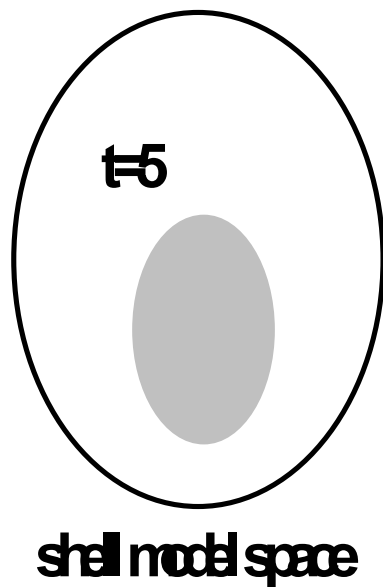
Go beyond Lanczos method

- The method to know the exact energy beyond truncation results
  - Extrapolation method
- The method to solve extremely huge shell model problem
  - MCSM / QMCD (Quantum Monte Carlo Diagonalization method)
  - SMMC (Shell Model Monte Carlo)
  - DMRG (Density Matrix Renormalization Group method, Pittel et al.)
  - VAMPIR

Funny short story!

Folk tale concerning shell model

Once upon a time, at a certain room of a certain university, there is a student.

A student: "I got a result of **2p2h** shell model calculation!"
A professor: "Great! But **3p3h** space may be important?"

The student revised his shell model code and worked hard…
The student: "I got a result of **3p3h** shell model calculation!"
The Professor: "Great! But **4p4h** space might change spectra?"

The student improved his shell model code and worked hard…
The student: "I got a result of **4p4h** shell model calculation!"
The professor: "Great! But **5p5h** space could bring about a considerable change ?"

The student was terribly distressed by this endless game.

Extrapolation is useful to finish such an endless game.

A mathematical method how to evaluate the energies of the whole shell model space by the quantities of truncated shell model spaces

PRC65(2002) 064319, T. Mizusaki and M. Imada

PRC67(2003) 041301R T. Mizusaki and M. Imada

PRC70 (2004) 044316 T. Mizusaki
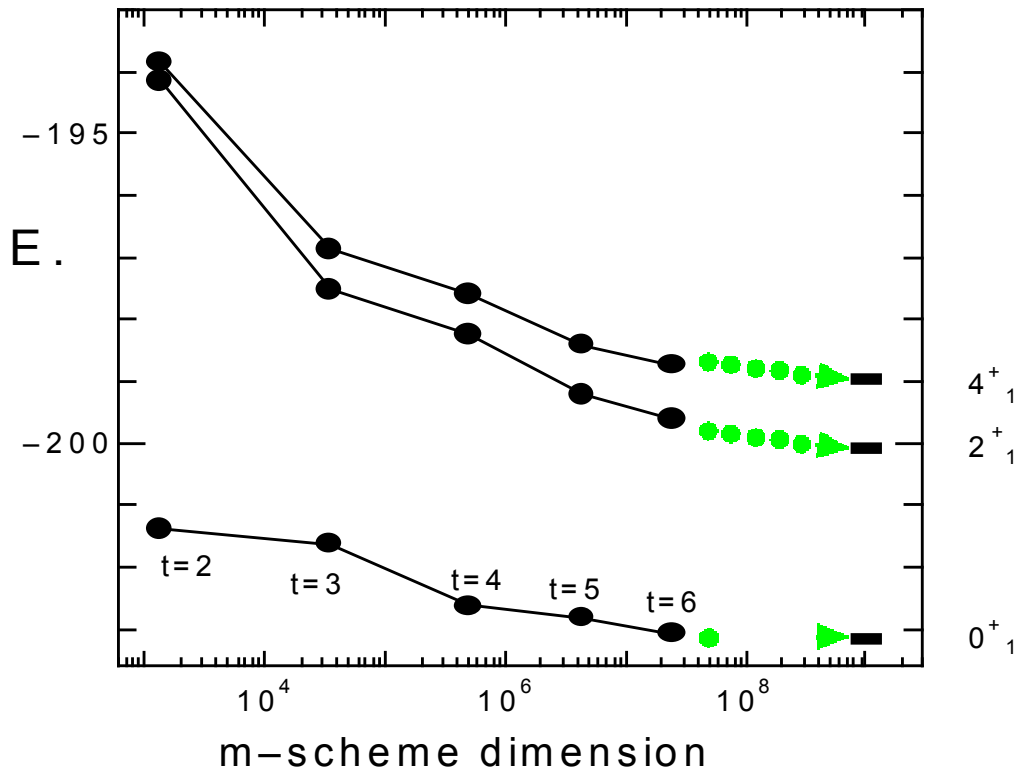
Energy Variance Extrapolation

proportionality

$$\delta E = \langle H \rangle - \langle H \rangle_0$$

$$|\psi\rangle = c|\psi_0\rangle + d|\psi_r\rangle$$

$$\delta E \propto \Delta E$$

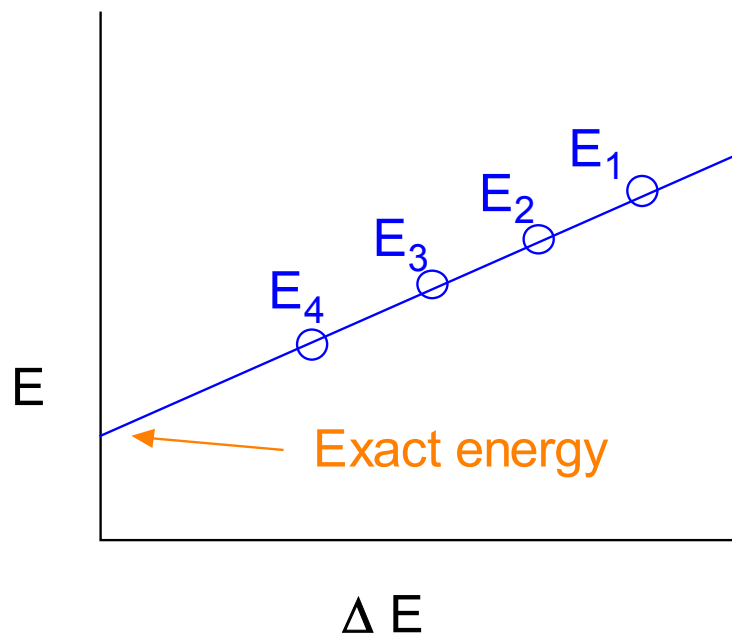$$\Delta E = \frac{\langle H^2 \rangle - \langle H \rangle^2}{\langle H \rangle^2}$$

Proof : expansion by this small d

For a series of systematically approximated wave functions

$$|\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle, \cdots$$

$$E_1 > E_2 > E_3 > \cdots$$
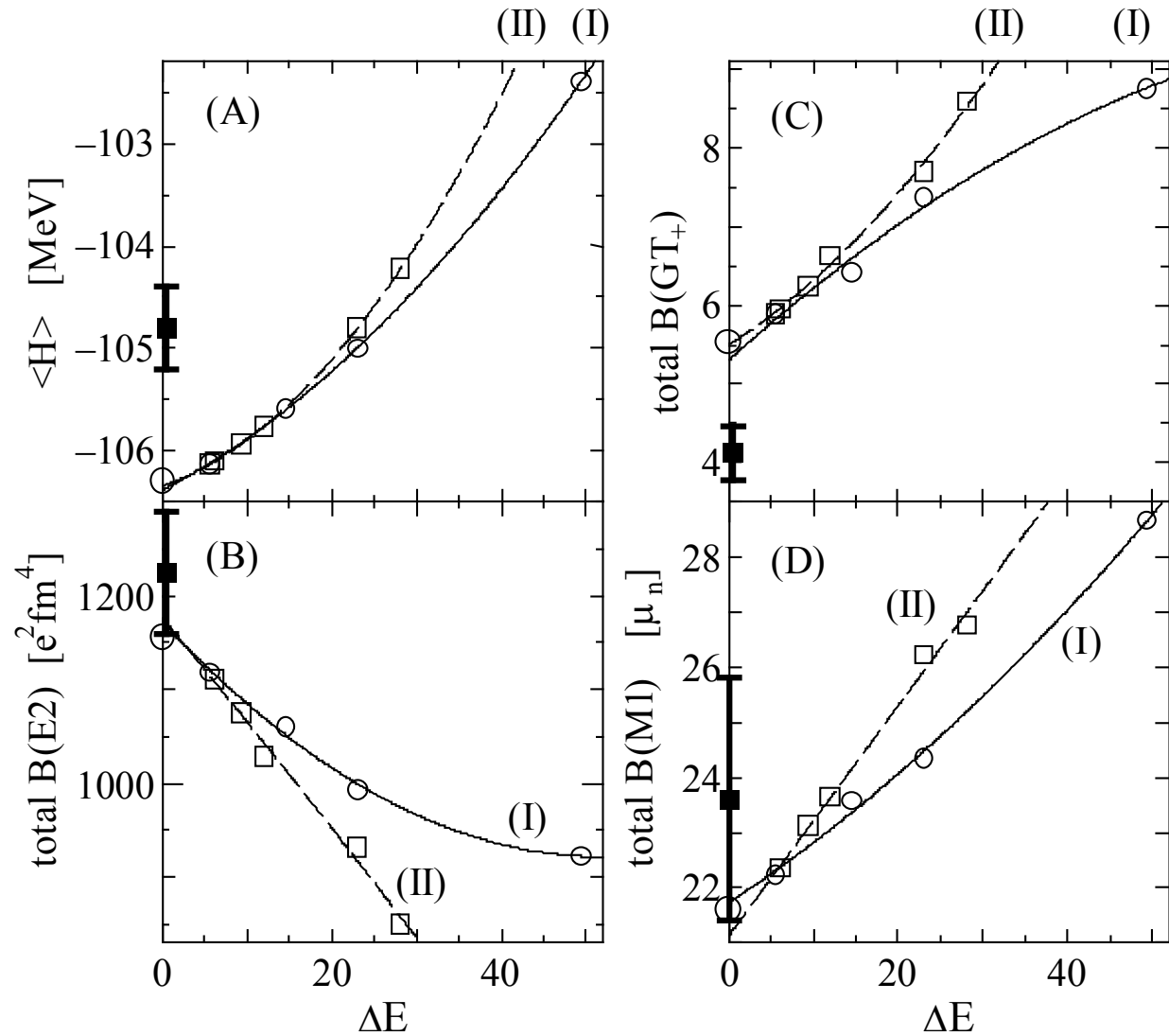
$$\Delta E_1 > \Delta E_2 > \Delta E_3 > \cdots$$

Example of energy variance extrapolation

H³ energy variance extrapolation

- R is a appropriate lowest energy projector, which improves wave function.

- We take R as $\hat{R} = \sqrt{\hat{H}}$

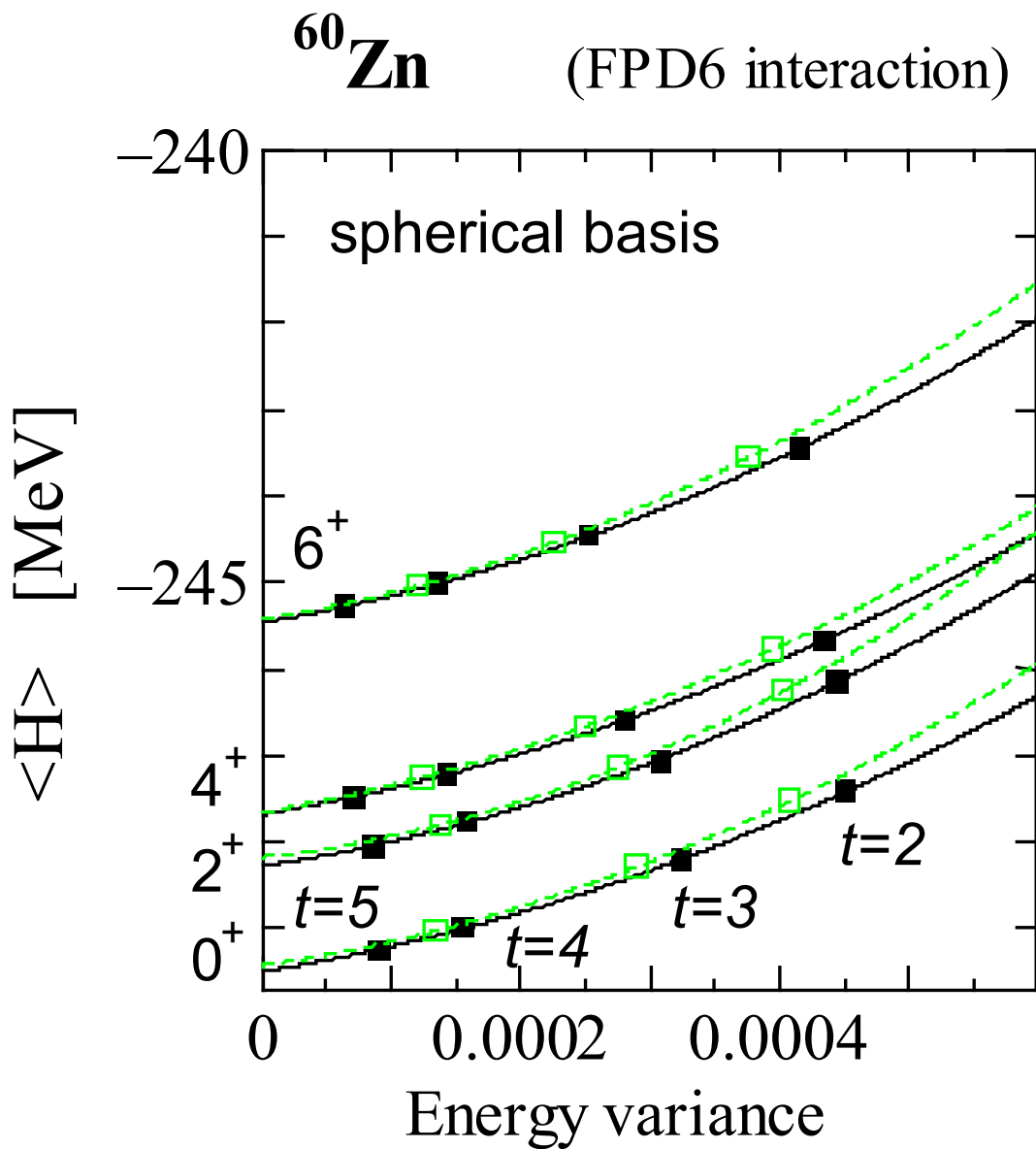- New energy variance extrapolation formula is derived.

$$\left\langle \hat{A} \right\rangle = \frac{\left\langle \phi \middle| \hat{R}^{\dagger} \hat{A} \hat{R} \middle| \phi \right\rangle}{\left\langle \phi \middle| \hat{R}^{\dagger} \hat{R} \middle| \phi \right\rangle}$$

$$\delta E \rightarrow \delta E_{sqrt} = \frac{\left\langle \hat{H}^2 \right\rangle}{\left\langle \hat{H} \right\rangle} - \left\langle \hat{H} \right\rangle_0$$

$$\Delta E \rightarrow \Delta E_{sqrt} = \frac{\left\langle \hat{H}^3 \right\rangle \left\langle \hat{H} \right\rangle - \left\langle \hat{H}^2 \right\rangle^2}{\left\langle \hat{H}^2 \right\rangle^2}$$

$$\Delta E_{sqrt} \propto \delta E_{sqrt}$$

Example of H^3 energy variance extrapolation for ^{60}Zn

^{60}Zn (FPD6 interaction)

spherical basis

6$^+$

4$^+$

2$^+$

0$^+$

t=5

t=4

t=3

t=2

<H> [MeV]

−240

−245

0

0.0002

0.0004

Energy variance

Energy variance extrapolation with deformed basis

- Projected deformed basis

$$P_{MK}^J \left| \psi \right\rangle \qquad \left| \psi \right\rangle = \prod_\alpha a_\alpha^\dagger \left| 0 \right\rangle \qquad a_\alpha^\dagger = \sum_i D_{\alpha,i} c_i^\dagger$$

- Variation after projection is a good approximation.

$$\delta \left\{ \frac{\left\langle \psi \left| HP^J \right| \psi \right\rangle}{\left\langle \psi \left| P^J \right| \psi \right\rangle} \right\} = 0$$

How to generate a series of wave functions

- Structure of VAP wave function can be varied in a following way.

$$\left| \psi(x) \right\rangle = \prod_\alpha a_\alpha^\dagger(x) \left| 0 \right\rangle \qquad a_\alpha^\dagger(x) = \sum_i D_{\alpha,i}^{(min)} x_i c_i^\dagger$$

For instance,
$x_i = 1$ for lower orbits
$x_i = x$ for upper orbits

$$\left| \psi(x=1) \right\rangle = \left| \psi_{min} \right\rangle$$

Test for 2 billion problem

- ^{60}Zn

- fp shell

- fpd6 interaction

- 2×10^9 dimension for M=0 state

- Two extrapolations based on the spherical basis and deformed basis
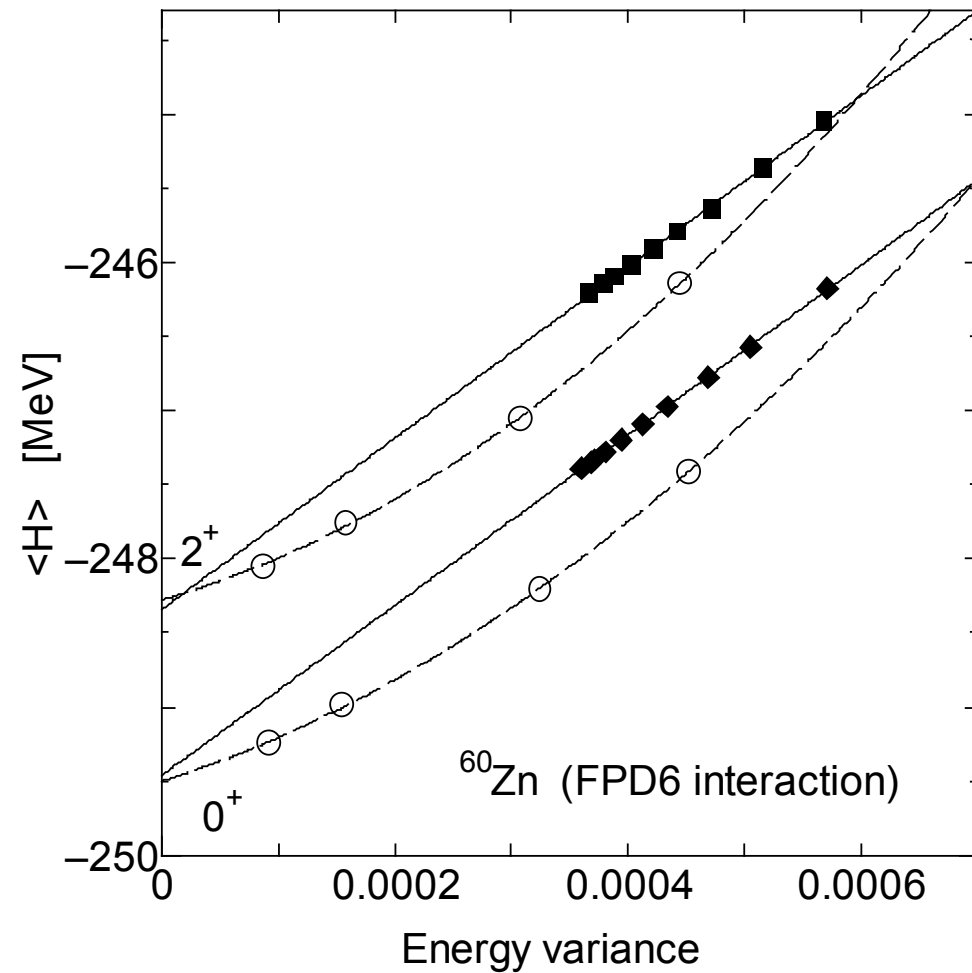
Summary

- You learned following items.

    - Basics of shell model calculations
        - M-scheme & J-scheme
        - Lanczos algorithm
        - Truncation scheme
    - The latest methods
        - Energy variance extrapolation
        - Other methods