

Shell model approach to exotic
nuclei—description by monopole-
based universal interaction and
development of a new MCSM code

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Outline

- Shell model: Very quantitative description of nuclei is possible
 - (1) when a good interaction is provided and
 - (2) when the Hamiltonian is diagonalized numerically.
- My talk is:
 1. How to construct a good effective interaction?
 - Focusing on “shell evolution” around $N=28$ and beyond with “monopole-based universal interaction”
 2. How to solve a large-scale problem?
 - Recent development of a new Monte Carlo shell model code

Collaborators

- Monopole-based universal interaction

Takaharu Otsuka (Univ. Tokyo/MSU), Alex Brown (MSU), Michio Honma (Aizu Univ.), Takahiro Mizusaki (Senshu Univ.), Toshio Suzuki (Nihon Univ.), Naofumi Tsunoda (Univ. Tokyo), Koshiroh Tsukiyama (Univ. Tokyo), Morten Hjorth-Jensen (Univ. Oslo)

- Development of a new MCSM code

Noritaka Shimizu (Univ. Tokyo), Takaharu Otsuka (Univ. Tokyo), Takashi Abe (Univ. Tokyo)

– For *ab initio* calculation with JISP16

P. Maris (Iowa St. Univ.), J.P. Vary (Iowa St. Univ.)

Conventional picture about shell evolution

- Woods-Saxon potential
 - One-body picture
 - gives overall agreement with experiment near stable nuclei.
 - Slow and monotonic evolution

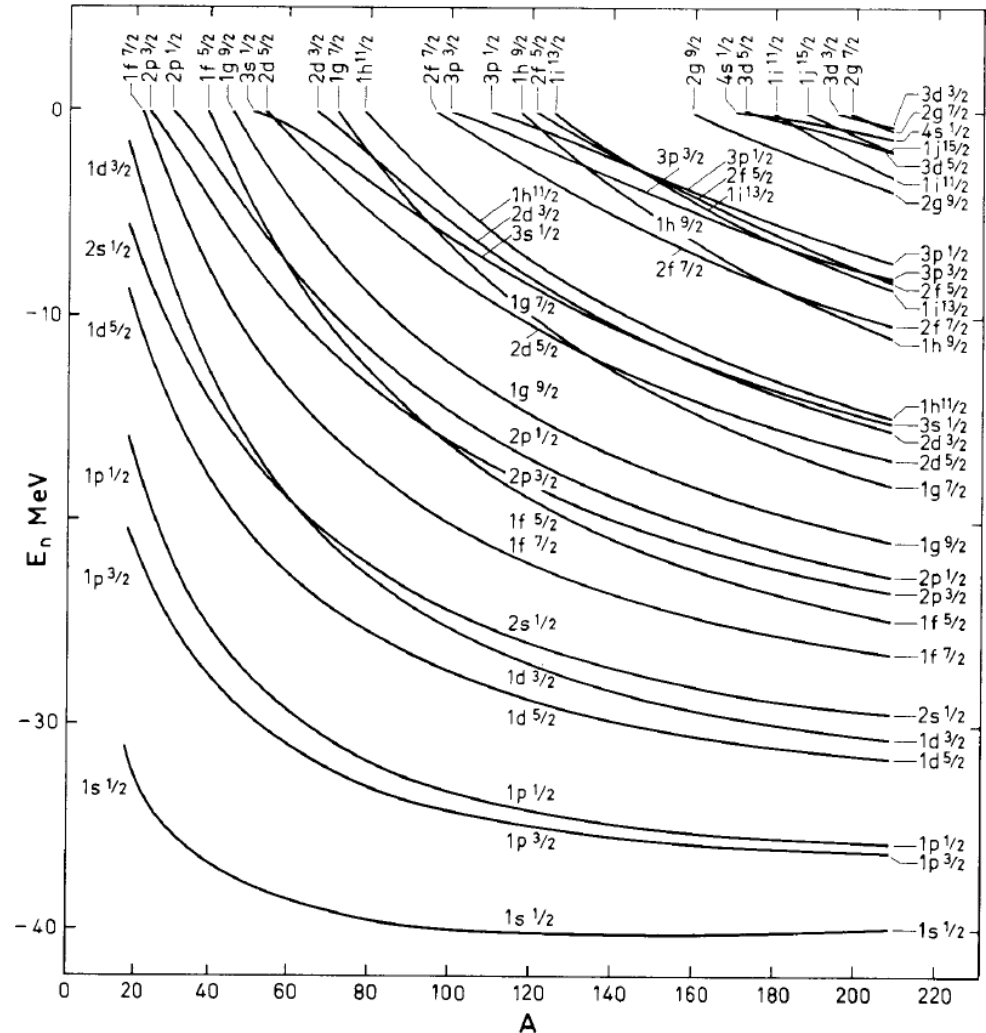
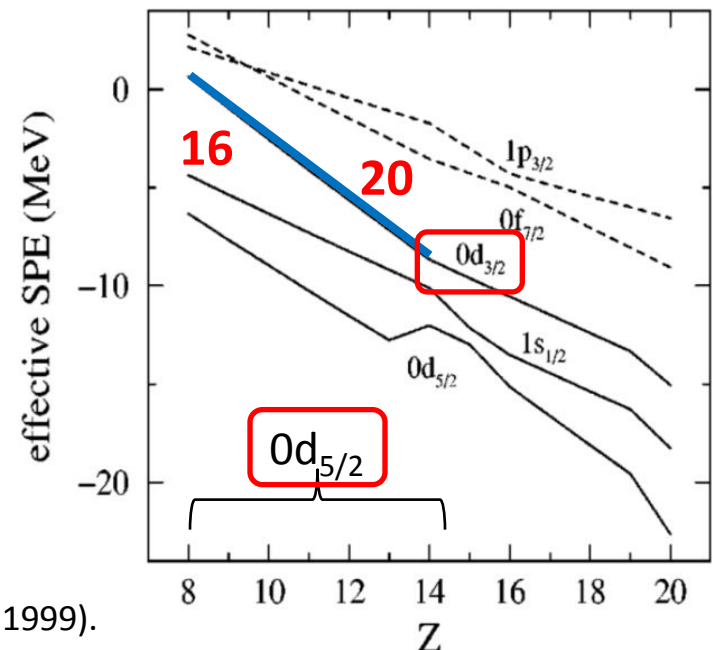
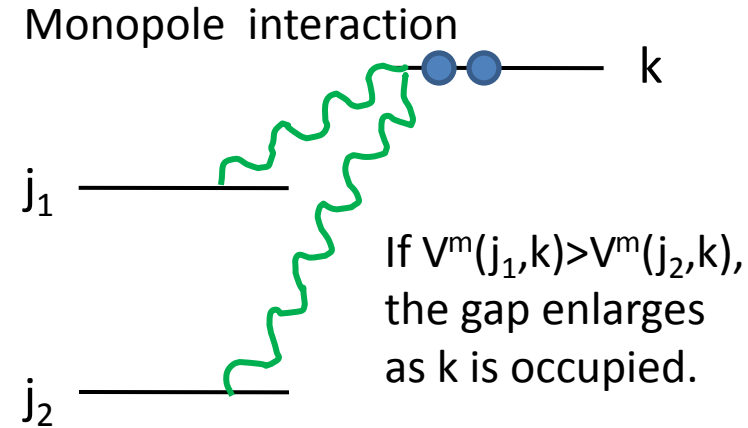


Figure 2-30 Energies of neutron orbits calculated by C. J. Veje (private communication).

Two-body picture about shell evolution

- What causes the change of shell gap: difference in mean force between orbits
 - Sometimes gives a **sharp** evolution
 - **Sensitive to the Fermi surface** and can be **non-monotonic**.
- What we want:
 - To detect those features
 - To account for and predict the shell evolution from more basic point of view



Spin dependence and the tensor force

- Origin of the drastic change
 - Spin dependence (T. Otsuka et al., Phys. Rev. Lett. 87, 082502 (2001).)

- Tensor force

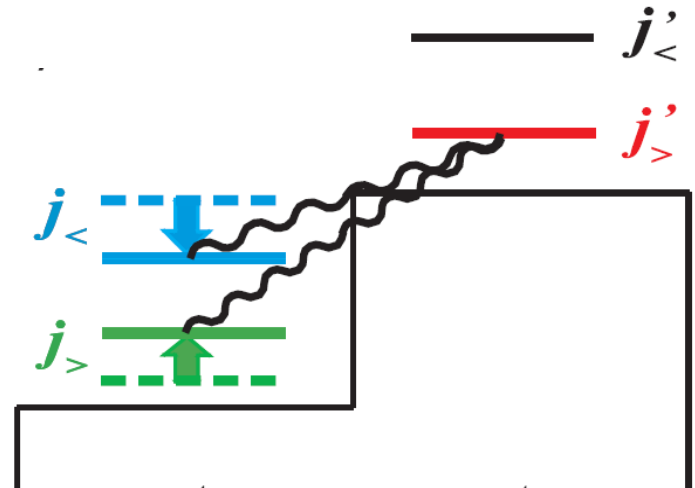
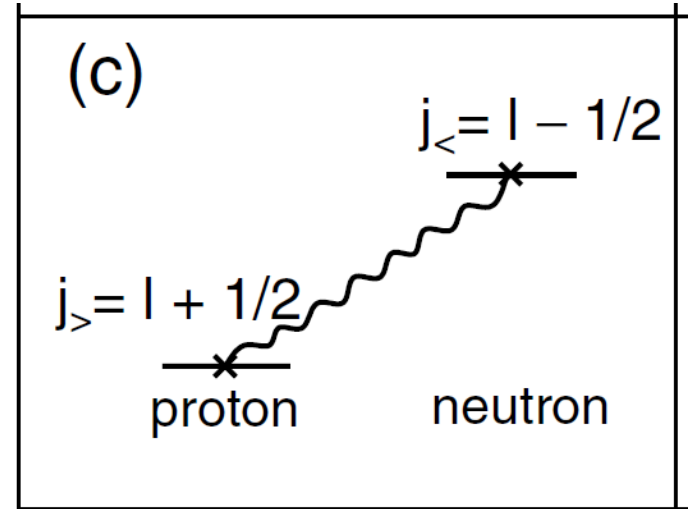
$$(2j_{>} + 1)V_{j_{>},j'}^T + (2j_{<} + 1)V_{j_{<},j'}^T = 0;$$



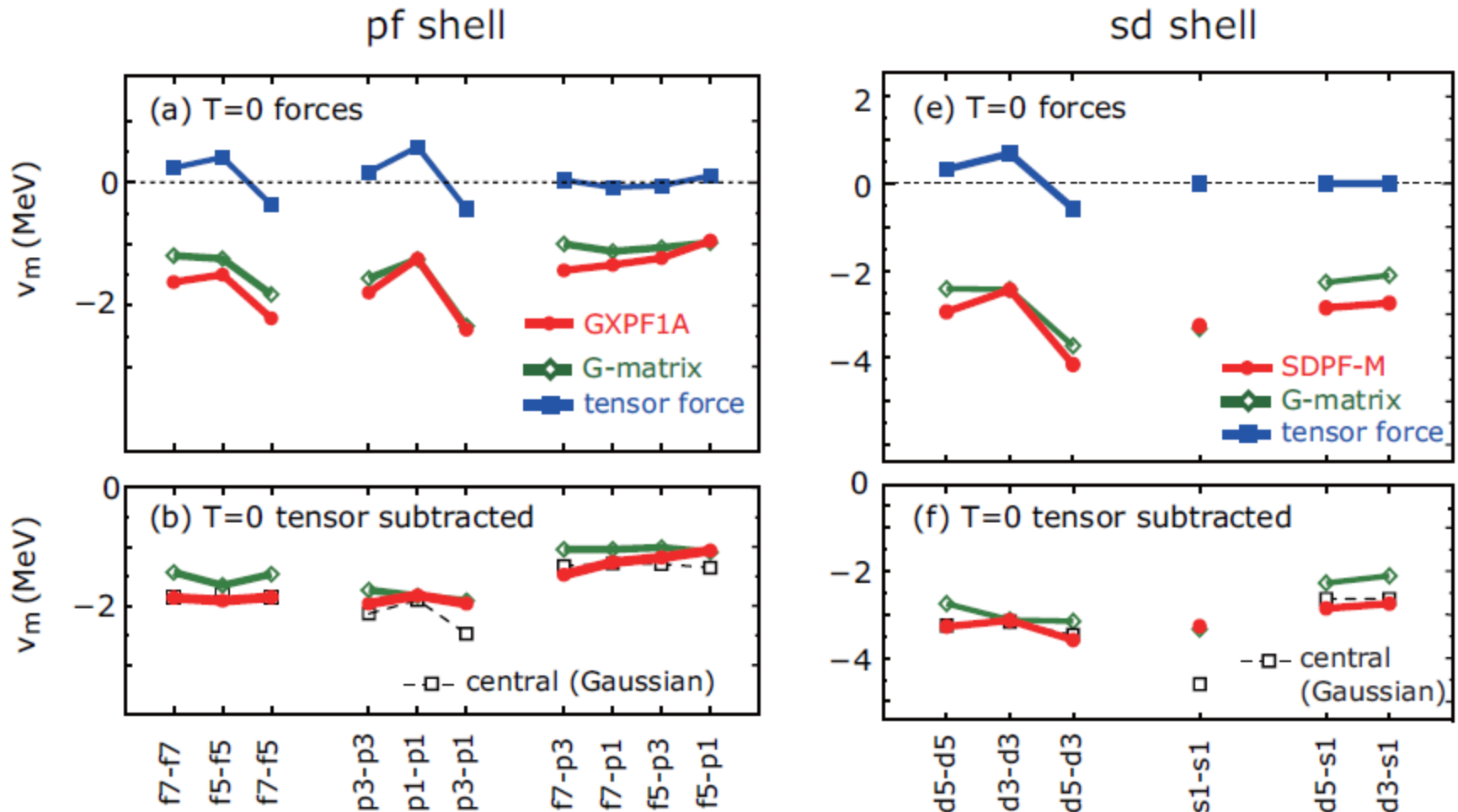
Attraction between $j_{>}$ and $j'_{<}$
 Repulsion between $j_{>}$ and $j'_{>}$



Large effect on the LS splitting



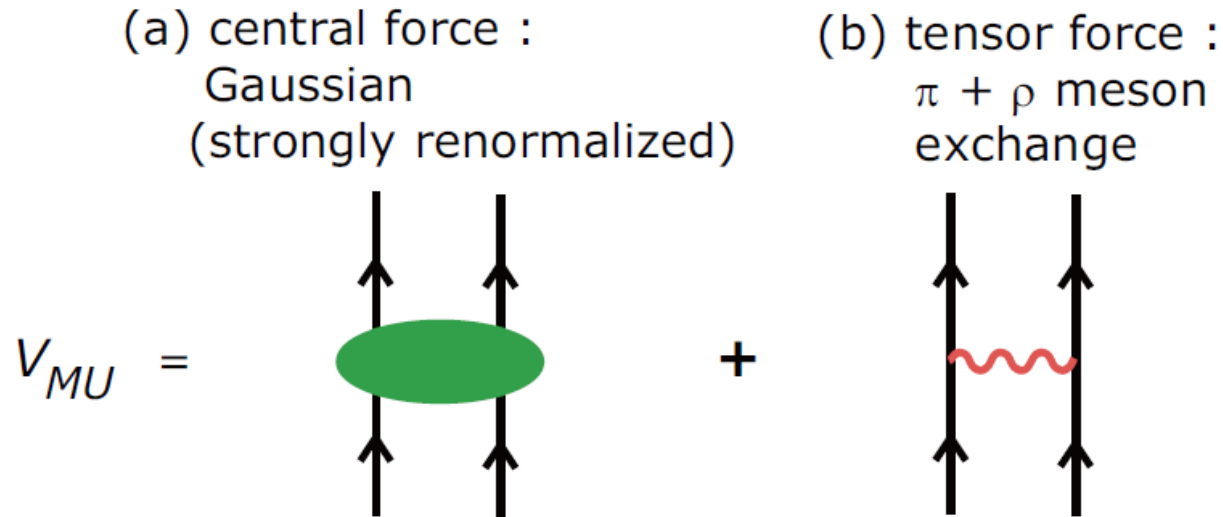
Simplicity of tensor-subtracted monopole



T. Otsuka, T. Suzuki, M. Honma, Y. Utsuno, N. Tsunoda, K. Tsukiyama, M. Hjorth-Jensen.,
 Phys. Rev. Lett. 104, 012501 (2010).

- A simple Gaussian force fits excellently.

Monopole-based universal interaction



- Tensor force

- Spin and node dependence

- Spin dependence : direction of j and j' (different sign)
 - Node dependence: strength is larger between orbits with the same node

- Central force

- Node dependence only

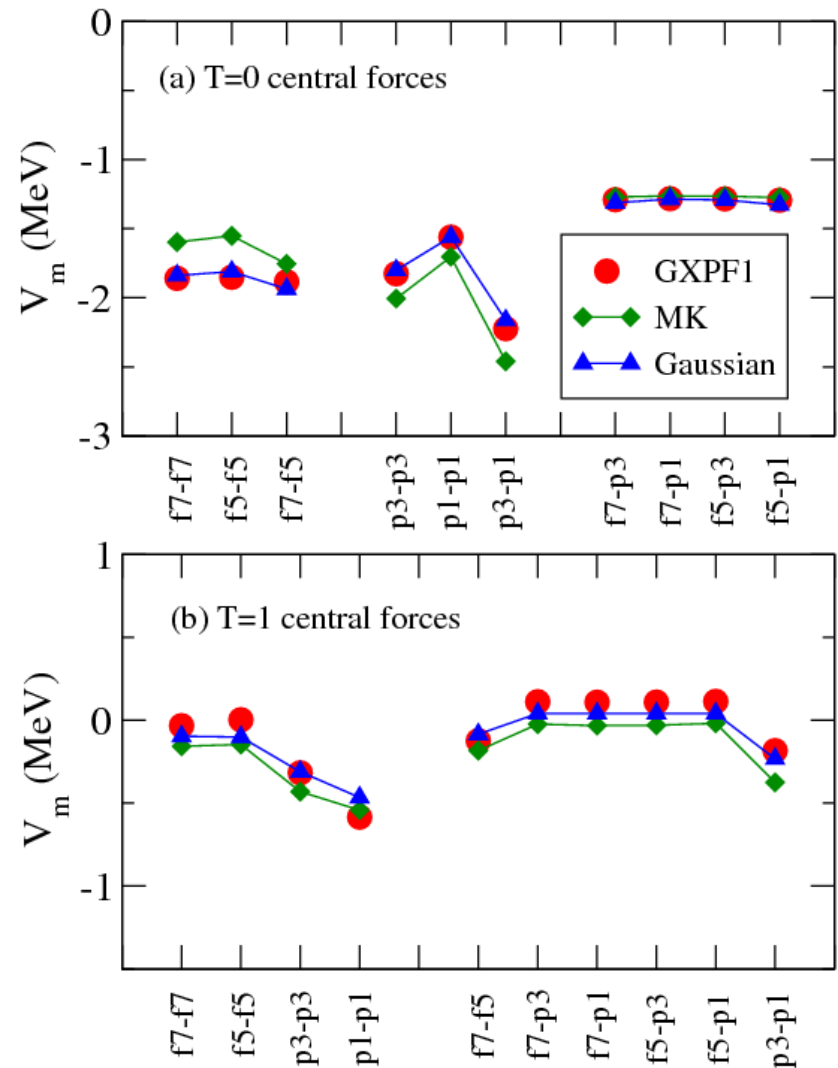
A new interaction for the sd-pf shell

- Components of the interaction
 - sd part + pf part + cross-shell part
 - USD as the sd part (with a slight modification as adopted in SDPF-M: changing magic number from N=16 to 20)
 - GXPF1B as the pf part (with a slight modification in the $f_{7/2}$ pairing and q -pairing matrix elements; improving the 2^+_1 of Si isotopes around N=22)
- **A newly constructed interaction** for the cross-shell interaction
 - Based on the monopole-based universal interaction picture
 - Consisting of central, LS (fixed to M3Y), and tensor ($\pi+\rho$) parts
 - Refined central force by including density dependence
 - Parameters of the central force are determined to fit the central monopole of GXPF1: **a natural continuation of GXPF1** to the cross shell

GXPF1 vs. Gaussian for central

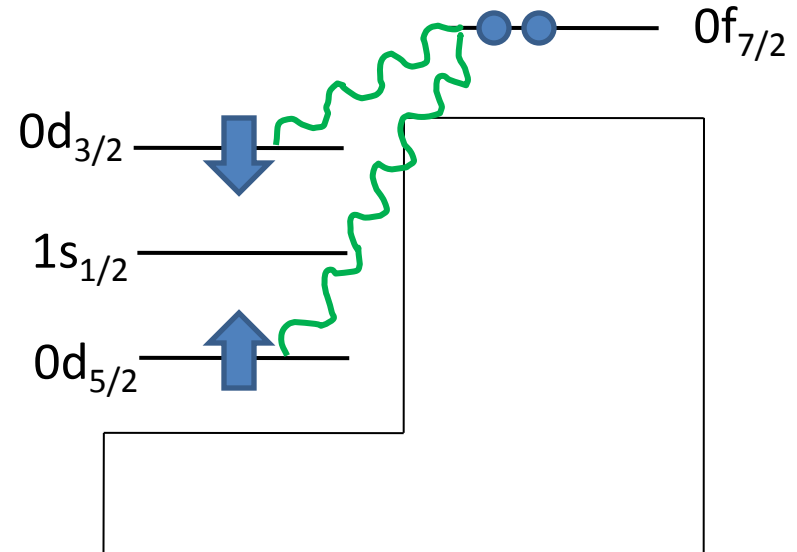
- Extracting the central of GXPF1
 - Spin-tensor decomposition
- Comparison with MK (Millener-Kurath): Yukawa
 - T=0 f-f: weaker due to the difference of range
 - T=0 p-p: stronger due to the lack of density dependence
 - T=1 overall: stronger due to different S=0 and S=1 ratio

Monopole centroids for the central force



Shell evolution from N=20 to 28

- The effect of the cross-shell interaction
 - $\pi(sd)$ orbits are of interest.
- Neutron: $f_{7/2}$
 - $V^m(f_{7/2}, sd)$
- To be discussed
 1. Z=16 gap: single hole states in ${}_{19}\text{K}$ isotopes
 2. Effects on collectivity: deformation in ${}^{42}\text{Si}_{28}$
 3. Reduction of the LS splitting: distribution of the spectroscopic factor



Monopole interaction in K levels

- $\pi 0d_{3/2}$ vs. $\pi 1s_{1/2}$ from N=20

to 28

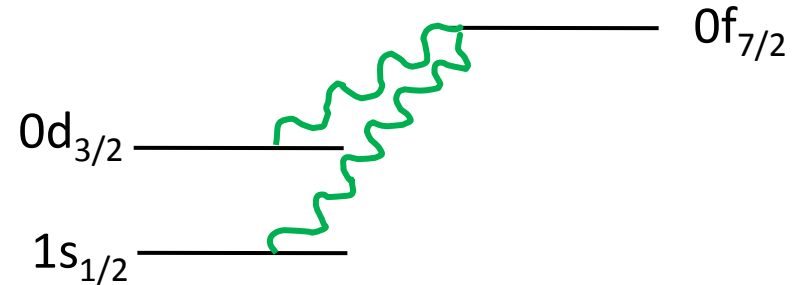
= $V^m(0f_{7/2}, 0d_{3/2})$ vs.

$V^m(0f_{7/2}, 1s_{1/2})$

- Central vs. tensor

- Both the central and the tensor contribute almost to the same extent.

➔ Sharp change of the gap



p-n monopole centroid (in MeV)

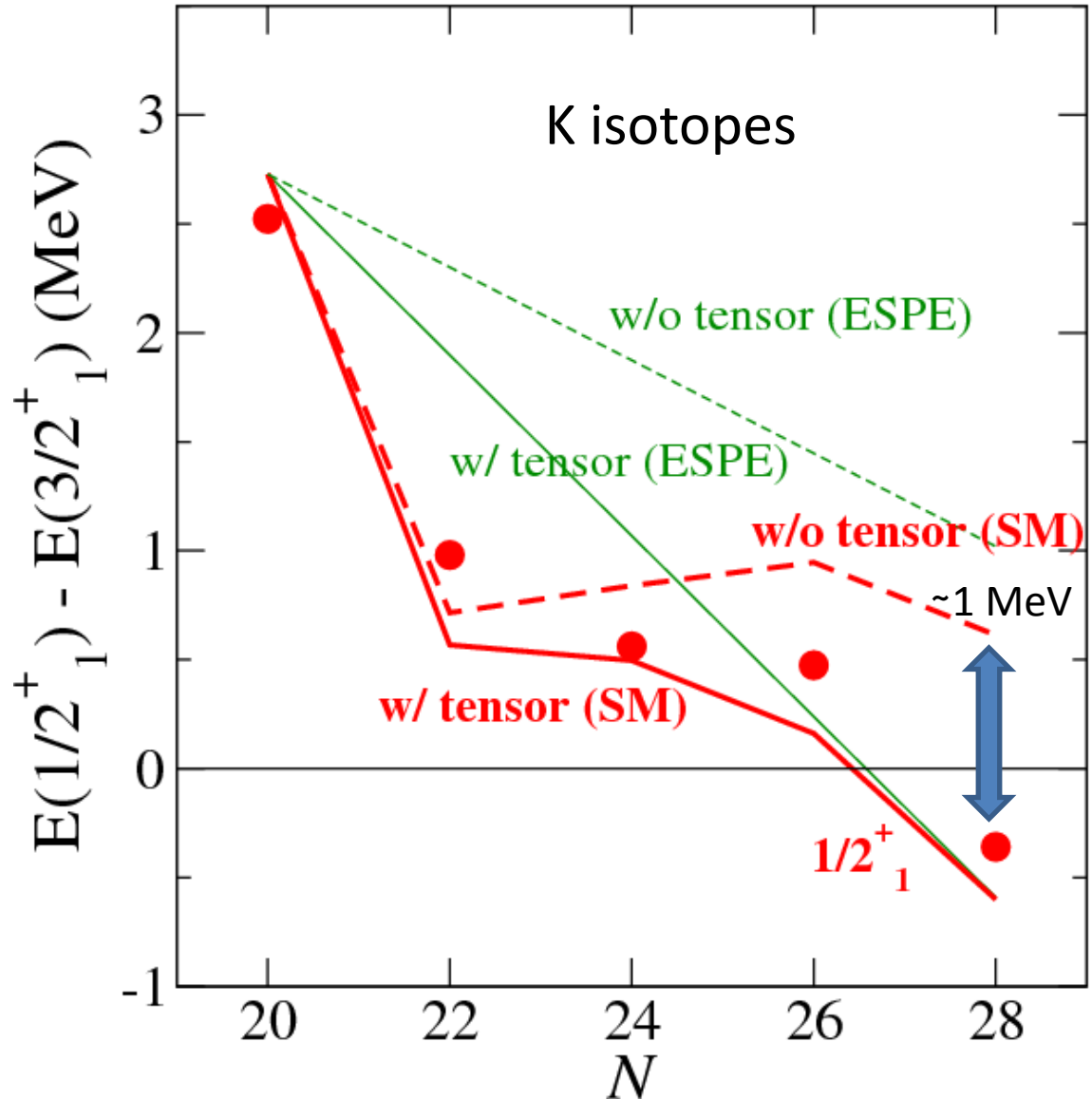
		$d_{3/2}$	$s_{1/2}$	difference
$f_{7/2}$	central	-1.10	-0.88	-0.22
	tensor	-0.21	0	-0.21

strength scaled at A=42

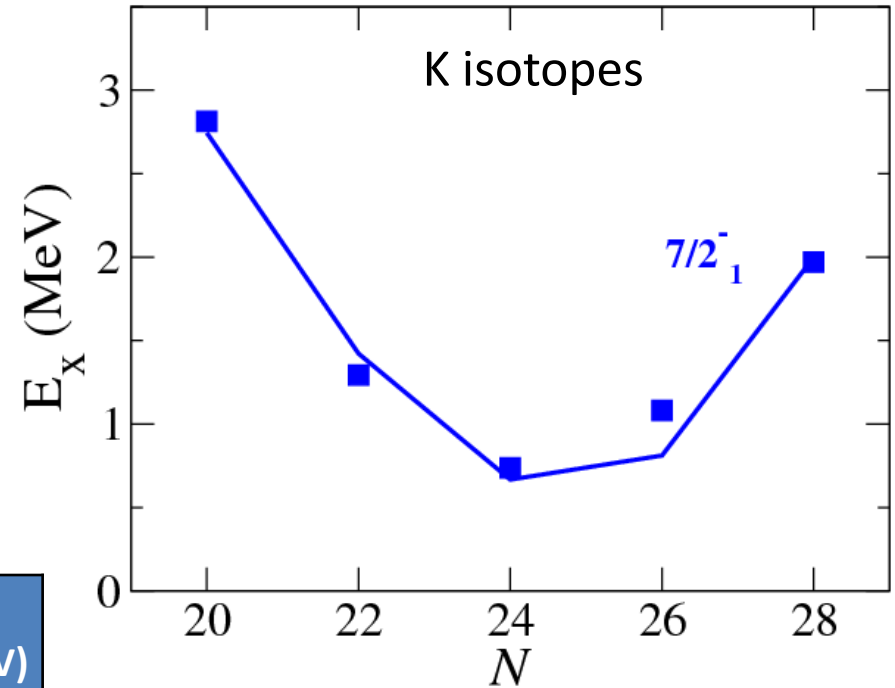
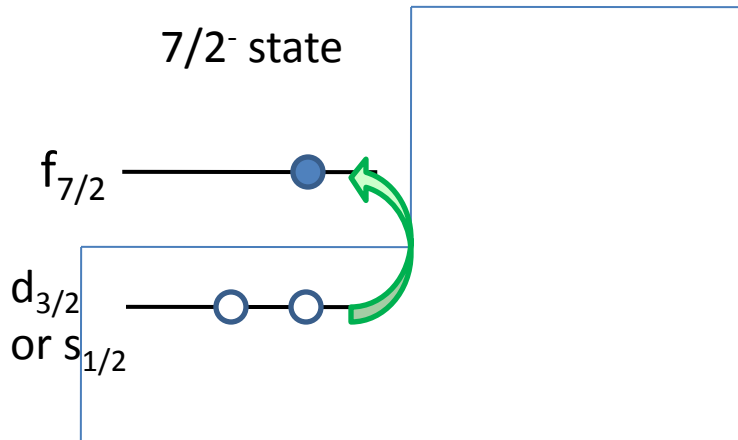
Evolution of $\pi d_{3/2}$ - $s_{1/2}$ gap in K isotopes

- Energy levels

- Significance of the tensor force is clear.
- Directly reflect the gap between $\pi(d_{3/2})$ and $\pi(s_{1/2})$ at $N=20$ and 28
- $1/2^+_1$ has a large mixing with $\pi(d_{3/2})$ \otimes $\nu(2^+)$ in $N=22, 24,$ and 26.



Unnatural parity states: probing Z=20 gap

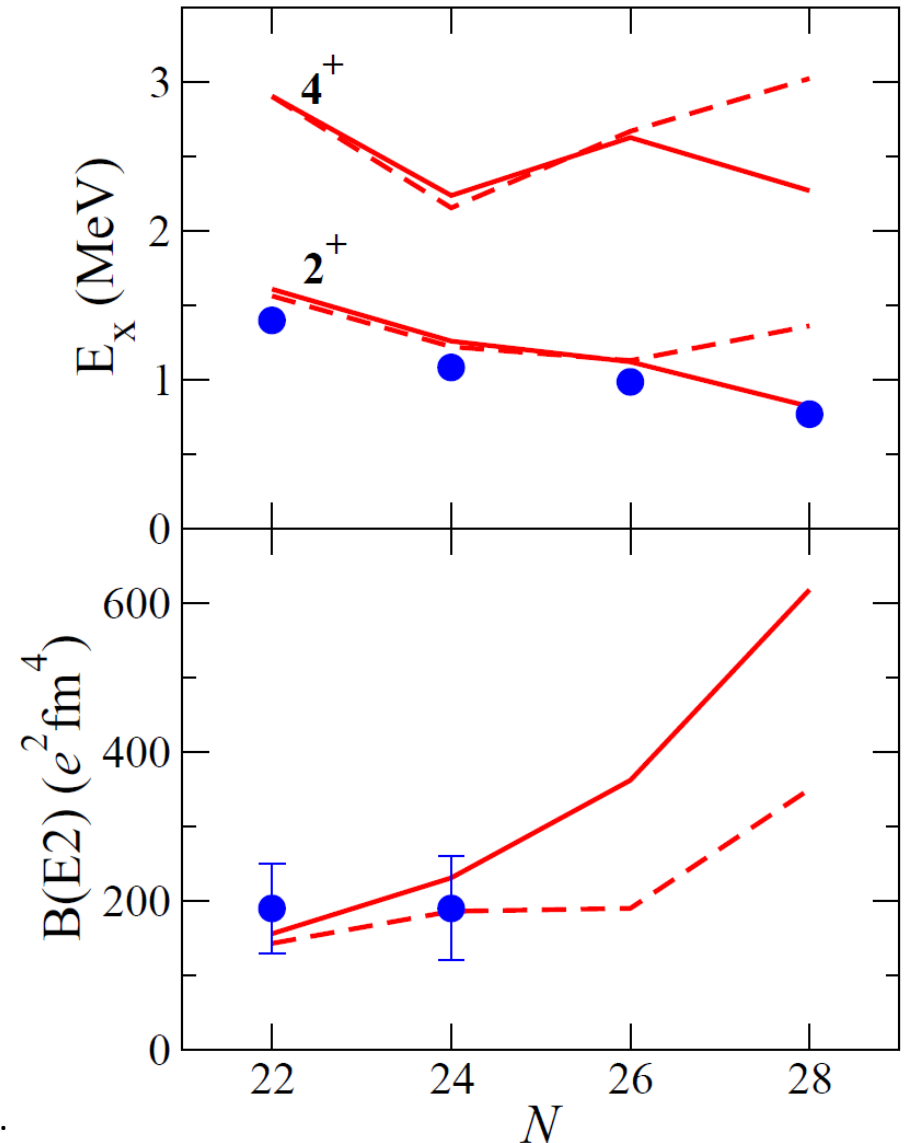


$^{47}\text{K}_{28}$	Ex.($7/2^-_1$) (MeV)	Effective shell gap (MeV)	Correlation energy (MeV)
Exp.	1.97		
Present	2.00	8.54	6.54
SDPF-NR	5.62	11.45	5.83

- Correlation energy: large but similar among interactions
- Effective shell gap: crucial for the level

Collectivity of Si isotopes: N=28 magicity

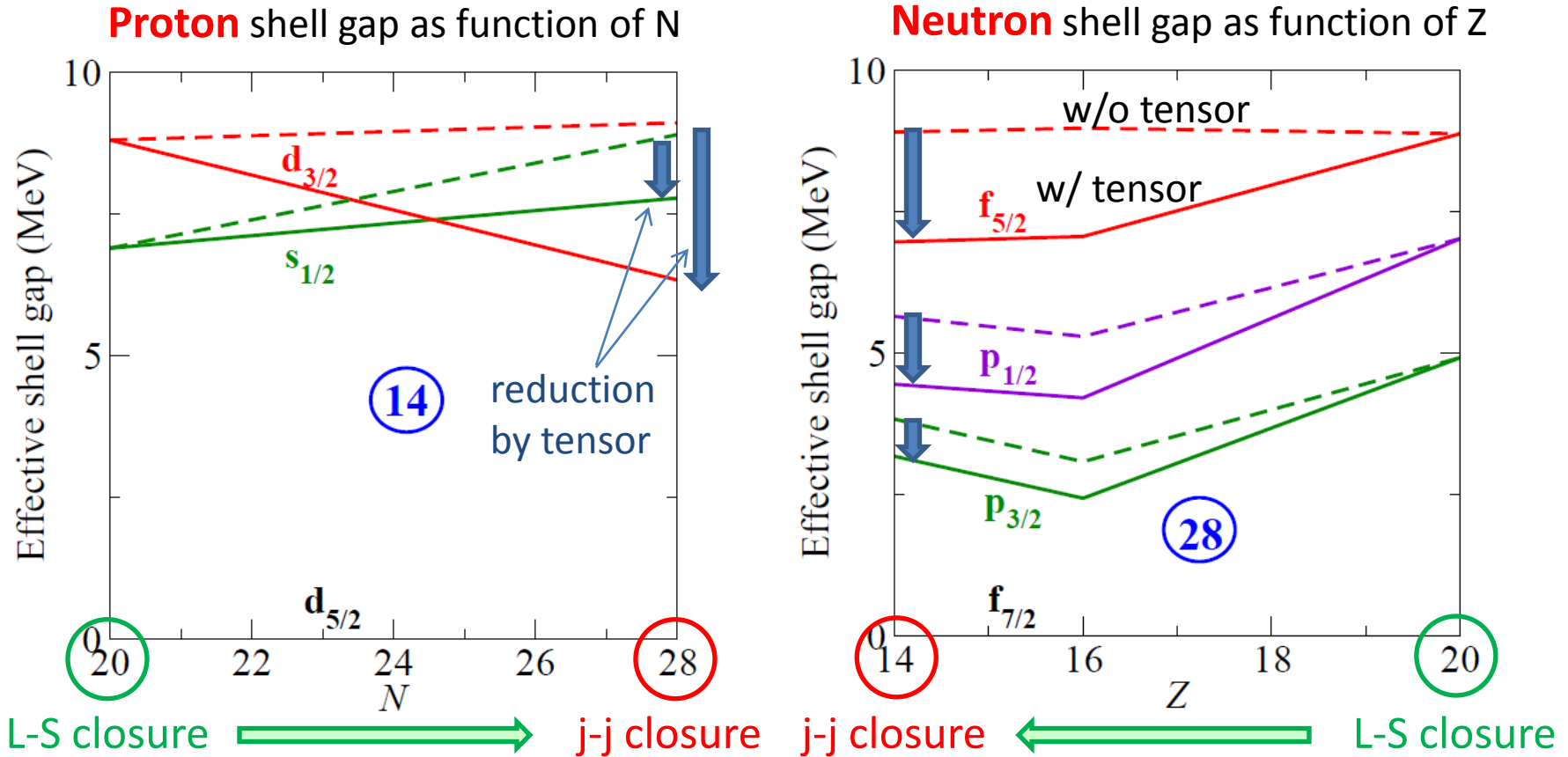
- Energy levels $N \leq 26$
 - 2^+_{1} is dominated by $\nu(f_{7/2})^2$
 - Pairing and q-pairing in $f_{7/2}$ are more sensitive.
- Large difference at $N=28$
 - Disappearance of the magic number



Exp.) ^{40}Si : C.M. Campbell et al., Phys. Rev. Lett. 97, 112501 (2006).

^{42}Si : B. Bastin et al. Phys. Rev. Lett. 99, 022503 (2007).

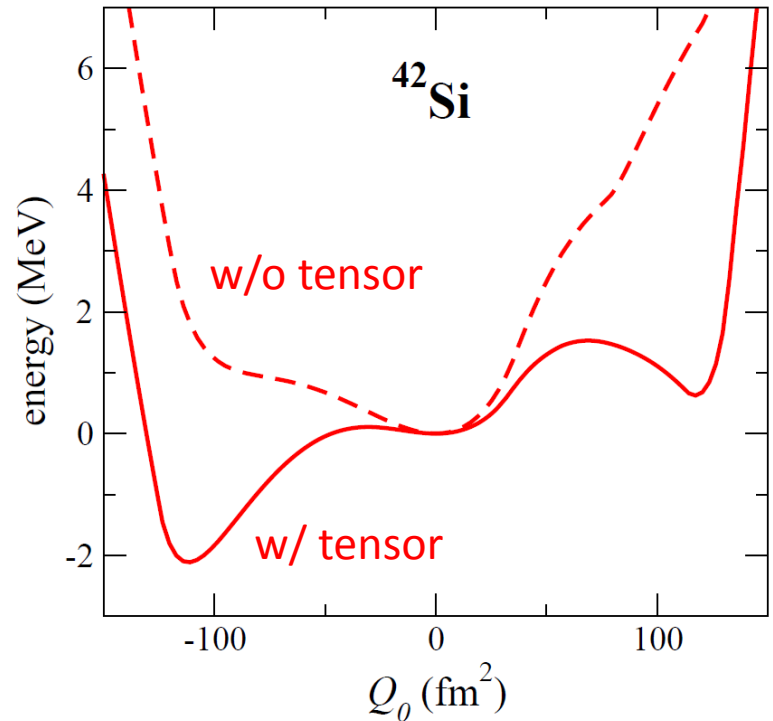
Comparison of the effective SPE



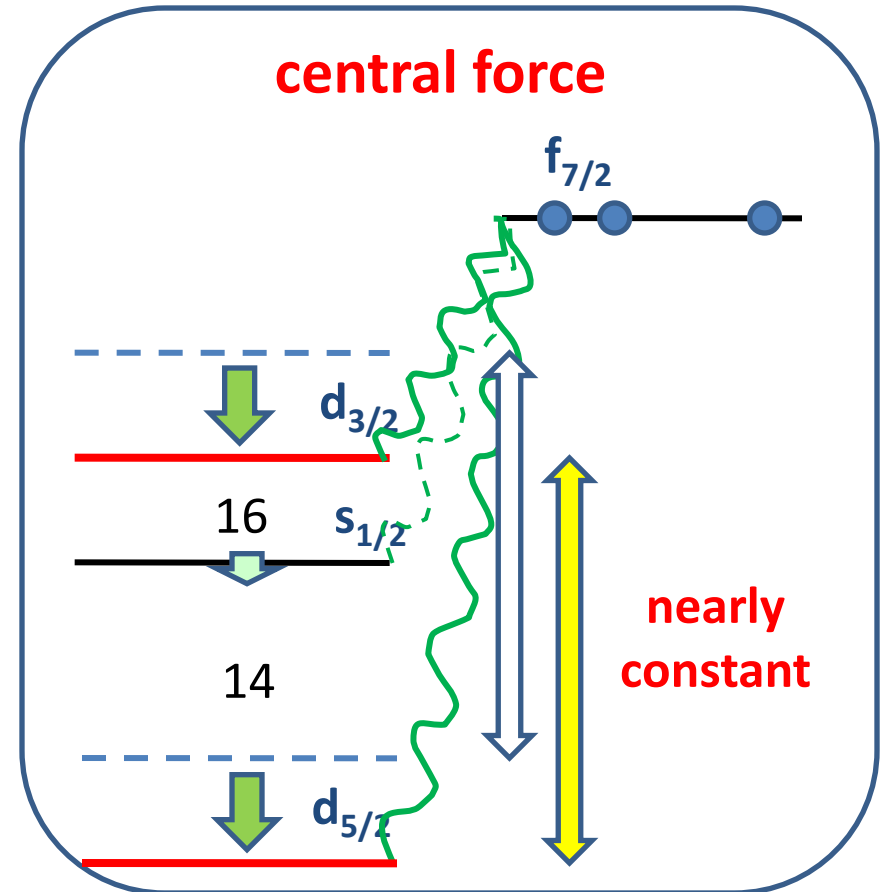
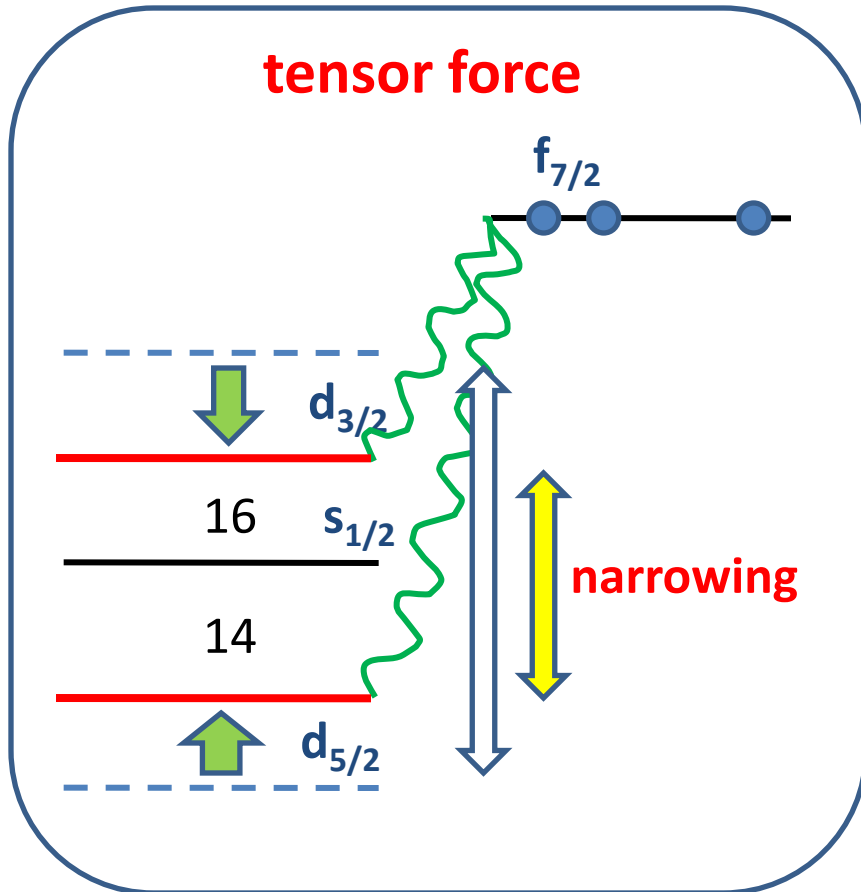
- **Coherent** quenching of proton and neutron shell gaps which increase toward the j-j closure

Potential energy surface (PES) for ^{42}Si

- PES: constrained (Q_0) Hartree-Fock calculation in the shell model space
 - Successful in the shape coexistence in ^{56}Ni (T. Mizusaki et al., Phys. Rev. C 59, R1846 (1999).)
- Effect of the tensor force: large
- Oblate deformed g.s. caused by the tensor
 - Consistent with calculated Q moment of the 2^+_{1} : $+23 \text{ e}^2\text{fm}^4$



Difference between tensor and central

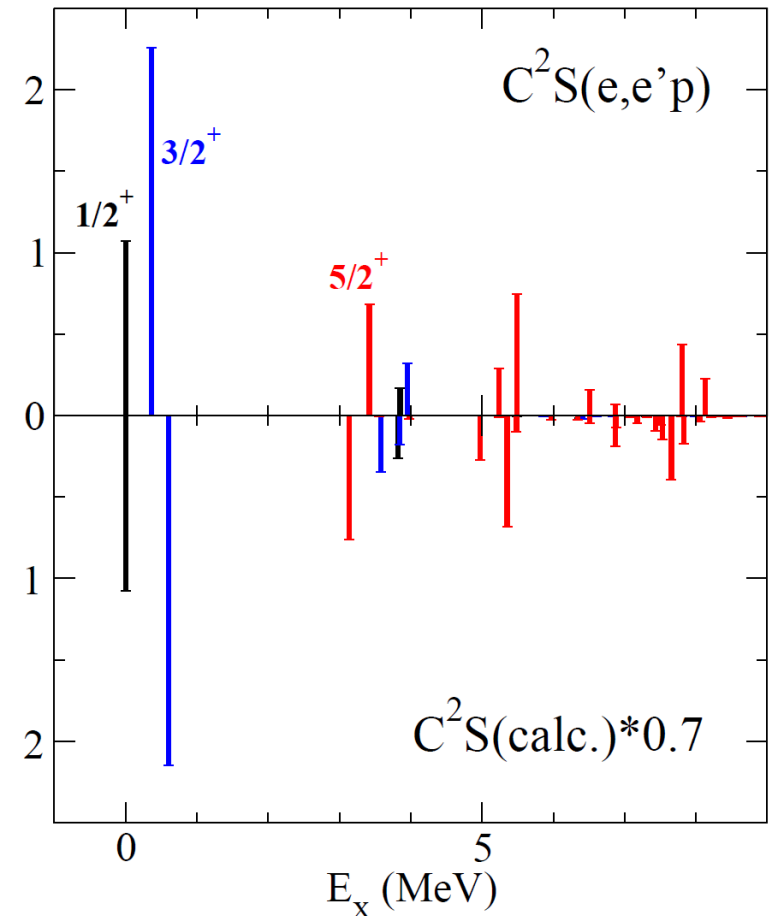


- Both tensor and central affect the reduction of the Z=16 gap.
- Almost only tensor contributes to **the reduction of the LS splitting.**

Spectroscopic factor for 1p removal from ^{48}Ca

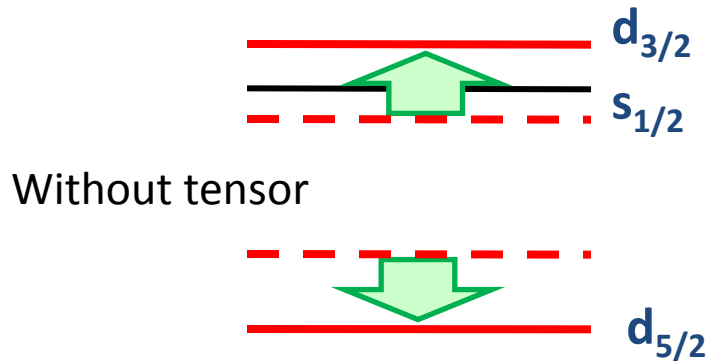
- $\pi d_{5/2}$ hole state
 - Ex.: high
 - Fragments into many states
- Spectroscopic factor
 - The centroid gives the single particle energy.
- Comparison between experiment and calculation
 - Quenching factor 0.7 is needed.
 - Very good : both position and strength

Present interaction (w/ tensor)



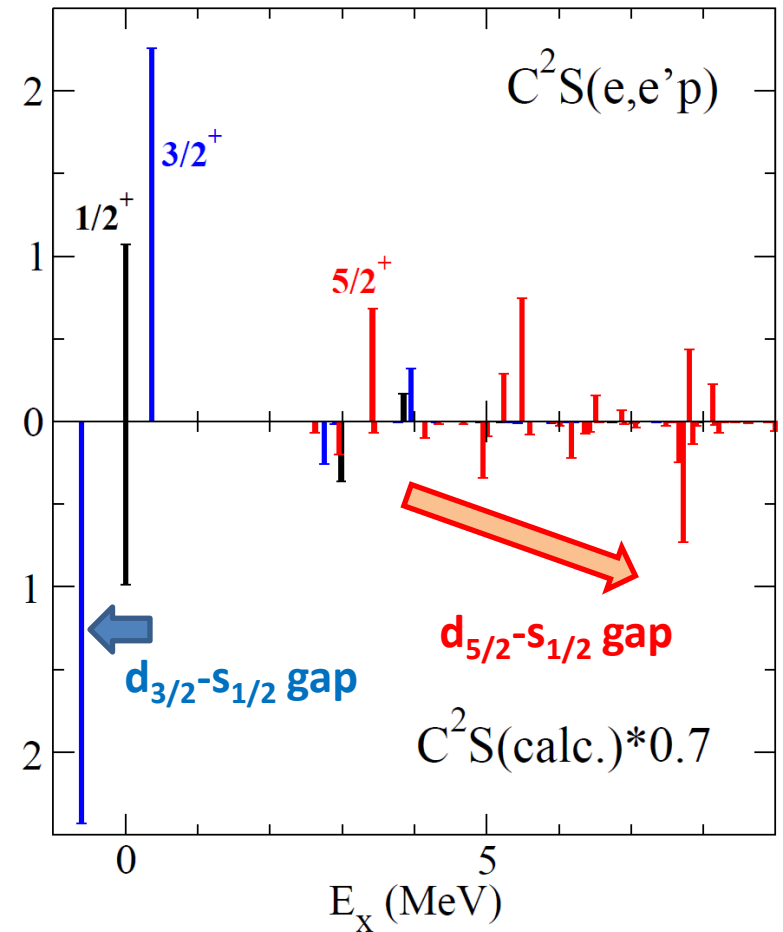
(e,e'p): G.J. Kramer et al., Nucl. Phys. A 679, 267 (2001).

What happens without the tensor force?



- $d_{3/2}$
 - The **position** of the single-hole state shifts to the left.
- $d_{5/2}$
 - $5/2^+$ levels exist from around 3 MeV, but the **strength** shifts to higher excitation energy.

w/o tensor in the cross shell int.

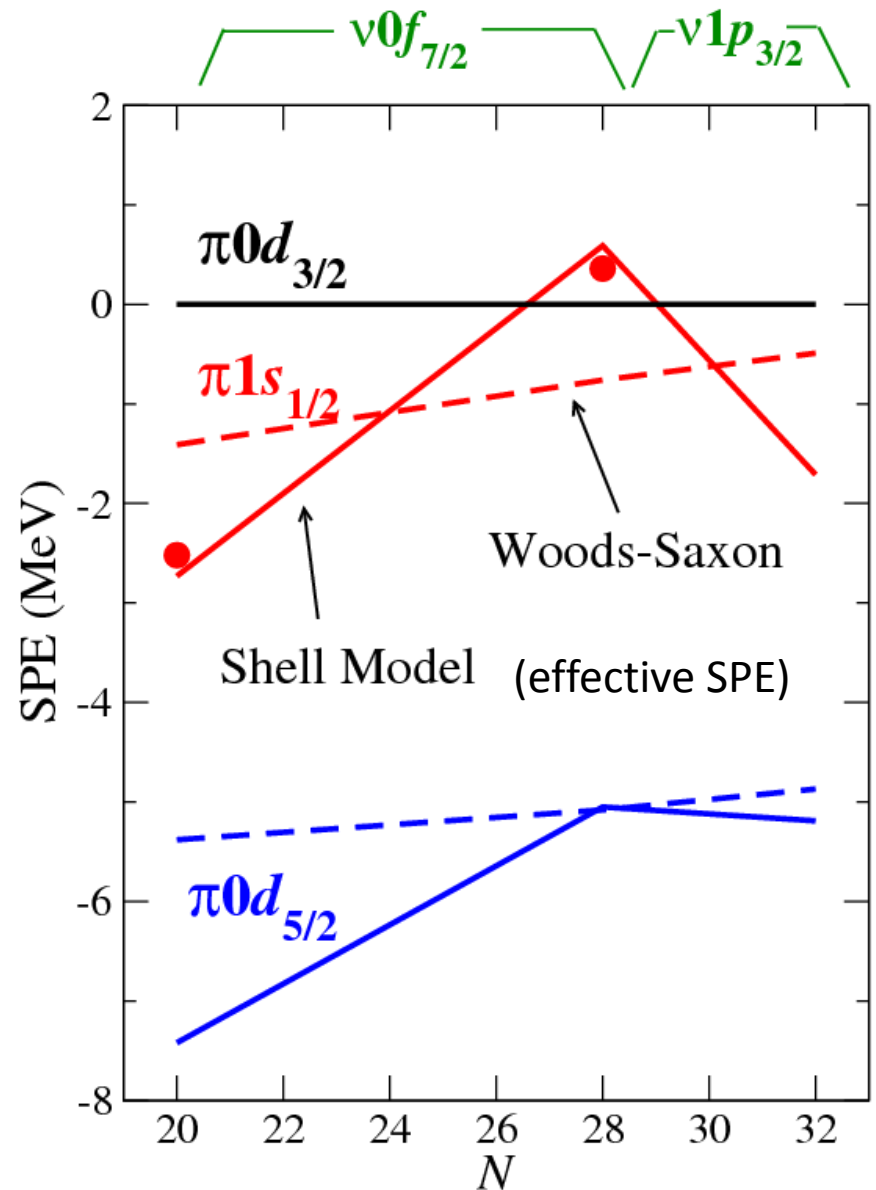


Comparison to Woods-Saxon potential

- Woods-Saxon
 - Very slow and monotonic change
 - Very small reduction of LS splitting from N=20 to 28



Independent of parameters used



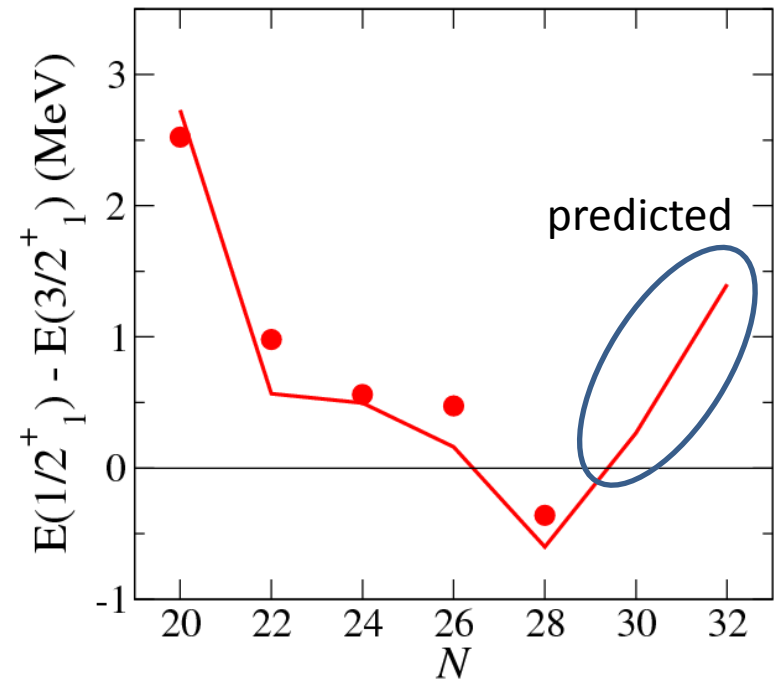
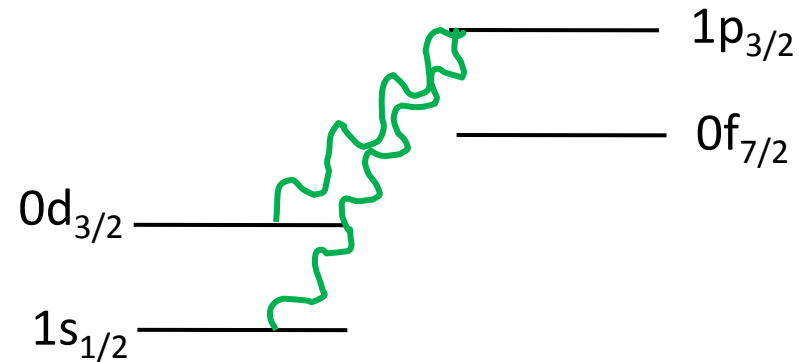
Shell evolution beyond N=28

- Fermi surface: $\nu 1p_{3/2}$
 - $V^m(1p_{3/2}, 0d_{3/2})$ vs. $V^m(1p_{3/2}, 1s_{1/2})$

		$d_{3/2}$	$s_{1/2}$	difference
$f_{7/2}$	central	-1.10	-0.88	-0.22
	tensor	-0.21	0	-0.21
$p_{3/2}$	central	-0.68	-1.15	+0.47
	tensor	-0.05	0	-0.05

The $1/2^+$ level is predicted to turn.

- Example of non-monotonic change



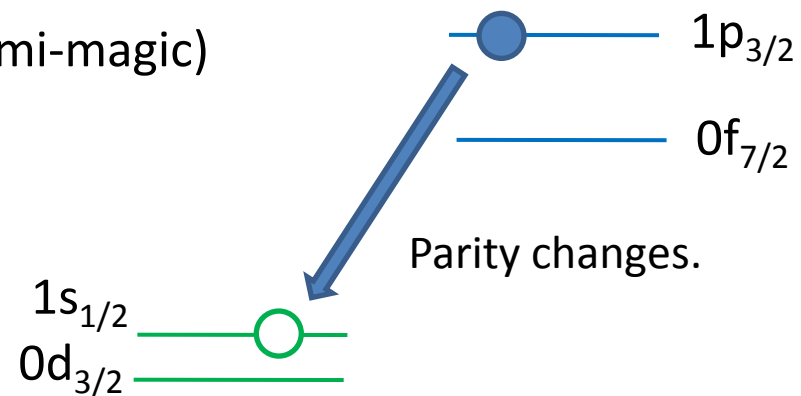
How to probe the change?

- No direct measurement of the spin/parity in the g.s. of K isotopes beyond N=28
- The only experimental data available: **β decay** to Ca isotopes
 - Parity of low-lying states: different between K and Ca
 - first forbidden decay

- **First forbidden decay as a probe of the ground state of K:**
promising

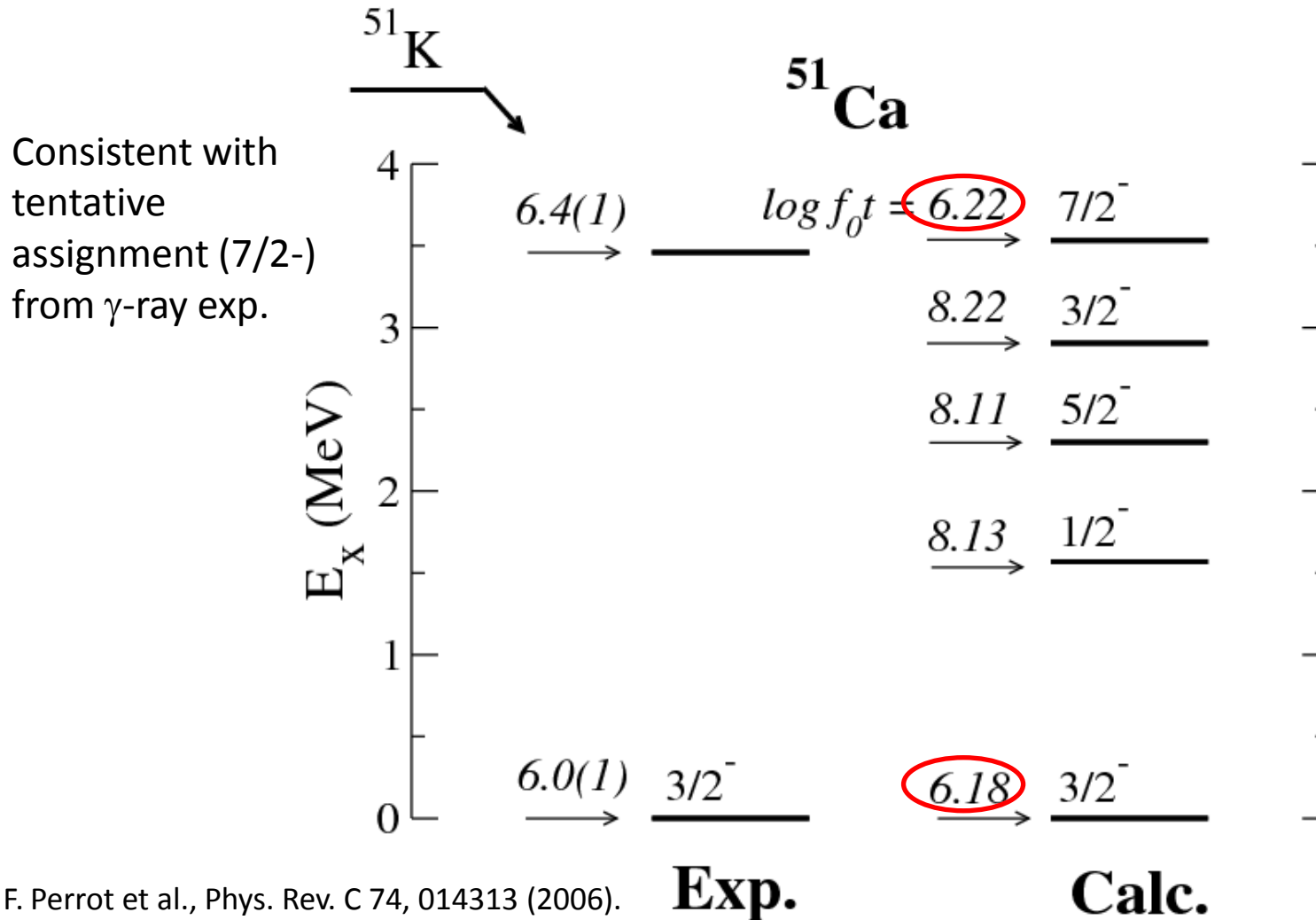
- Structure of daughter: Ca isotopes (semi-magic)

- Simple: ambiguity is small
- Very low level density:
one-to-one correspondence
to experiment



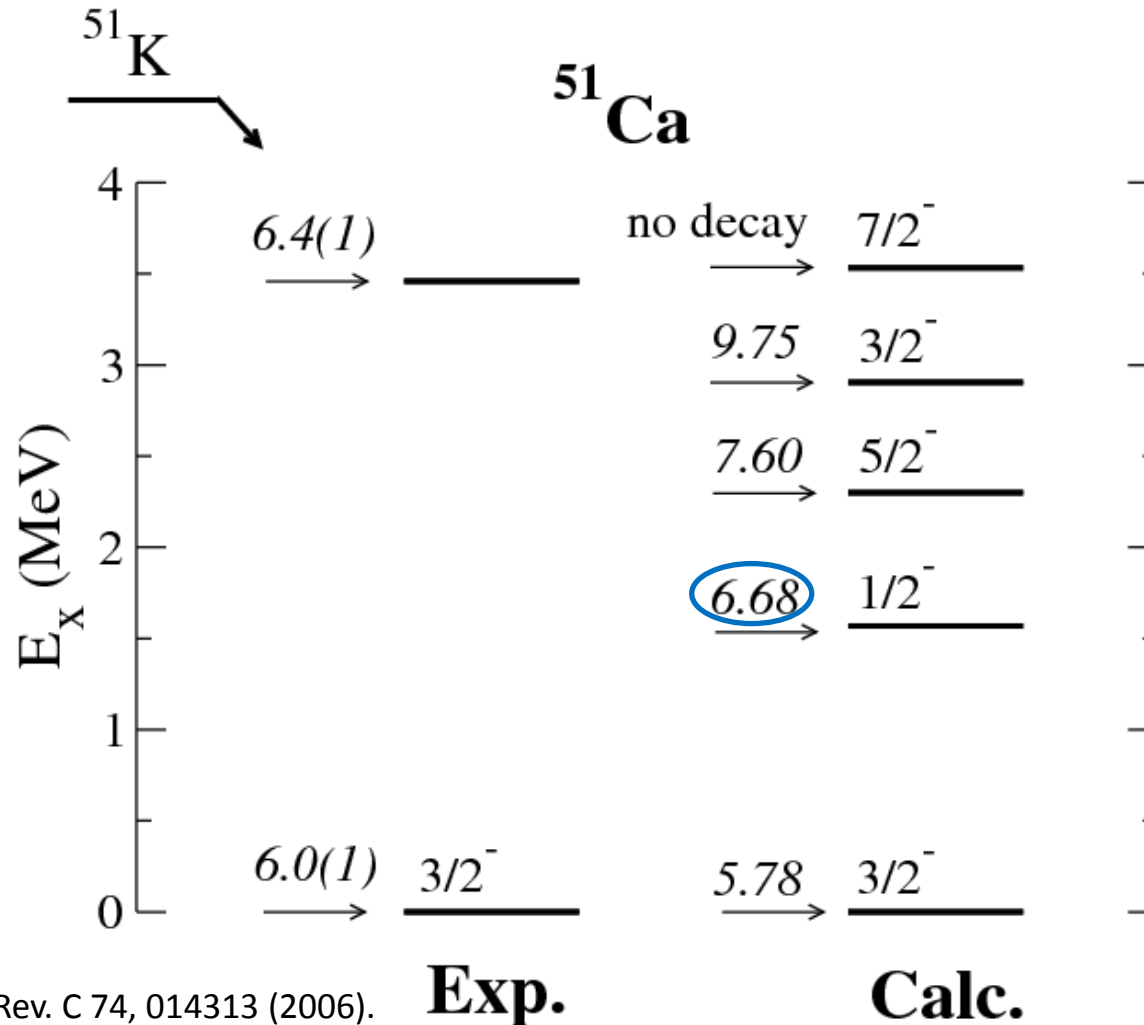
β decay of $^{51}\text{K}_{32}$: end of $\nu p_{3/2}$

- Ground state assumed: $3/2^+$



β decay of ^{51}K : end of $\nu p_{3/2}$

- Ground state assumed: $1/2^+$



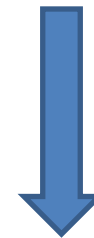
Monte Carlo shell model

- A tool to go beyond the conventional diagonalization method

$$\mathbf{H} = \begin{pmatrix} * & * & * & * & * & \cdot & \cdot \\ * & * & * & * & \cdot & \cdot & \cdot \\ * & * & * & \cdot & \cdot & \cdot & \cdot \\ * & * & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} \xrightarrow{\text{diagonalization}} \begin{pmatrix} \varepsilon_1 & & & & & & 0 \\ & \varepsilon_2 & & & & & \\ & & \varepsilon_3 & & & & \\ & & & \cdot & & & \\ & & & & \cdot & & \\ & & & & & \cdot & \\ 0 & & & & & & \cdot \end{pmatrix}$$

Conventional Shell Model
all Slater determinants

Huge matrix



$$\mathbf{H} \approx \begin{pmatrix} * & * & * & \cdot \\ * & * & * & \cdot \\ * & * & \cdot & \\ \cdot & \cdot & & \end{pmatrix} \xrightarrow{\text{diagonalization}} \begin{pmatrix} \varepsilon'_1 & & 0 \\ & \varepsilon'_2 & \\ 0 & & \cdot \end{pmatrix}$$

Monte Carlo Shell Model
bases important for a specific eigenstate

Small matrix

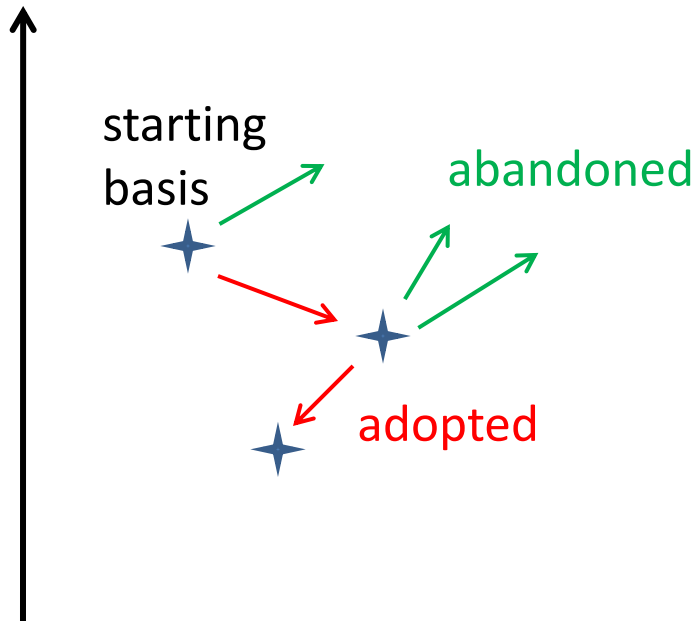
by selecting a good set of basis states in a stochastic way

Basis state: Slater determinants (in most cases), pair condensed basis (demonstrated in medium-heavy region), or quasi-particle state (not implemented yet) with symmetry restoration

Rough idea of generating MCSM bases

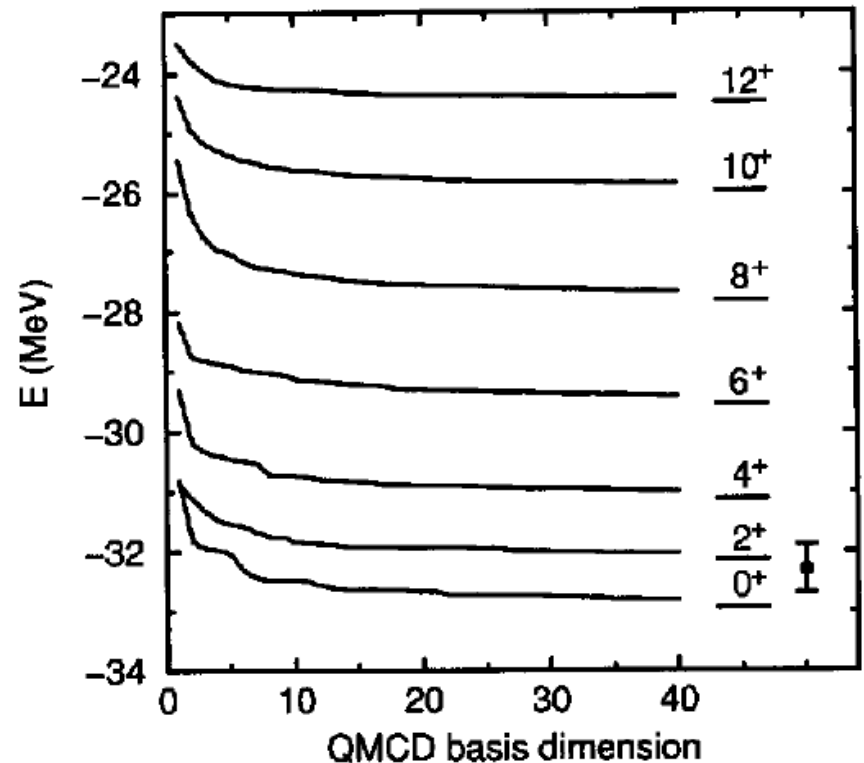
- Trial and error

Energy (obtained by diagonalization)



A linear combination of **a few tens of bases with symmetry projection** is very close to the exact solution.

^{48}Cr in pf shell, $2 \cdot 10^6$ m-scheme dimension



Successful in pf shell, “island of inversion”, and Ba regions

Computing environment

Present: Alpheet-2 since 2002



176 cores, alpha chip ~1GHz
~350 GFlops

Japanese next-generation
supercomputer
available 2012, **10 PFlops(?)**



次世代スーパーコンピュータ施設 完成イメージ図



Why a new MCSM code?

- To make use of up-to-date computers
 - Some limitations in the old code:
 - Relying on obsolete parallel-computing library (i.e., PVM)
 - Basis representation: not flexible (completely different code between Slater det. version and pair condensed basis version)
 - Only isospin conserving interaction can be handled.

Remove those restrictions



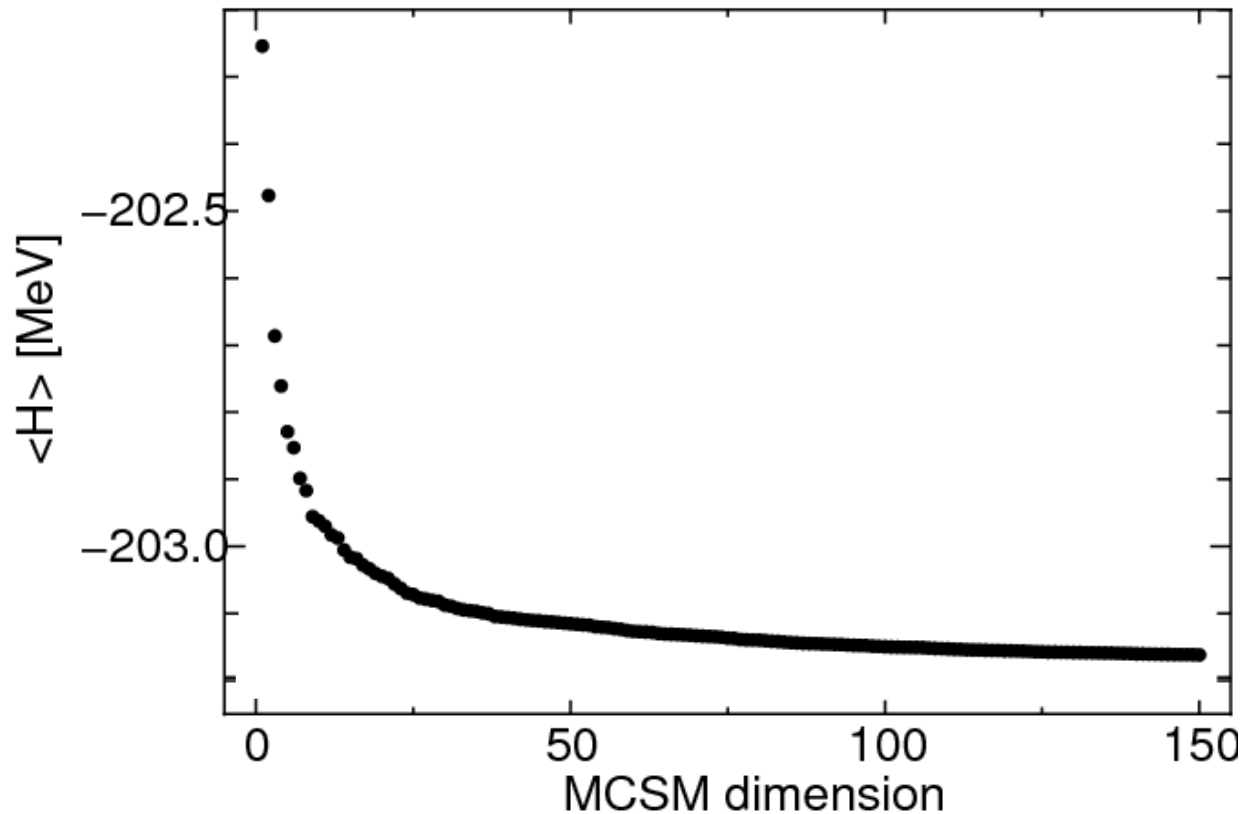
Applicability must be expanded.

+ some advances

1. A new algorithm to make calculation faster (by Utsuno)
2. An “extrapolation method” to evaluate the exact energy is implemented.
(by Shimizu)

How far from the exact solution?

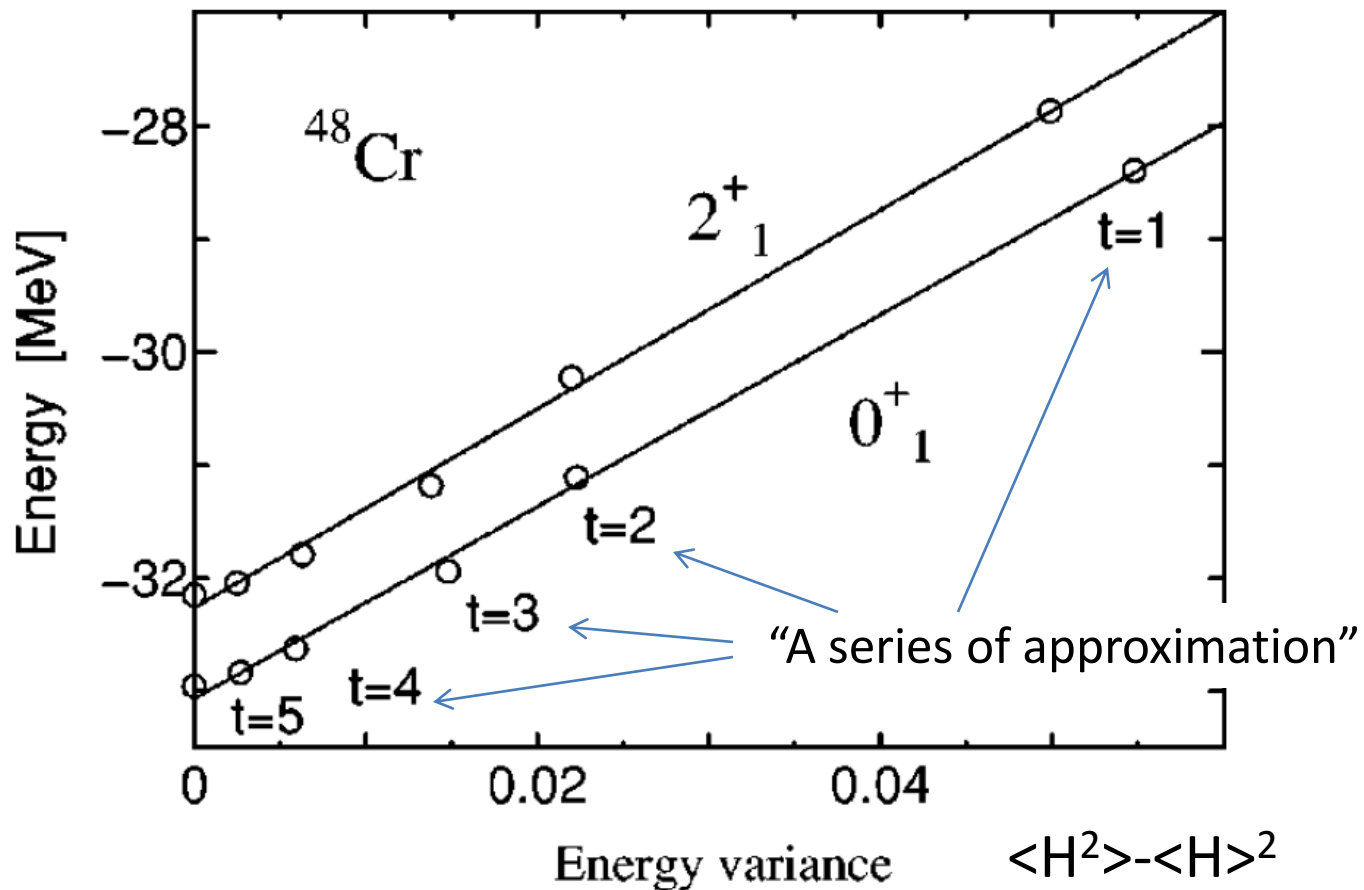
^{56}Ni in pf shell, 0^+_1 , 10^9 m-scheme dimension



- Very small difference between 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

- Based on strong correlation between energy and its variance
 - Demonstrated by Mizusaki in the framework of conventional shell model



Is it easy to apply to MCSM?

- Need to compute $\langle H^2 \rangle$
 - Conventional shell model
 $|\Psi\rangle = H|\Phi\rangle$ is able to be calculated because $|\Phi\rangle$ is a superposition of **all** the Slater determinants. $\langle H^2 \rangle = \langle \Psi | \Psi \rangle$
 - MCSM
Basis representation: a finite number of Slater determinants
 $|\Psi\rangle$ cannot be expressed as a **finite** number of Slater determinants.
It is necessary to evaluate $\langle H^2 \rangle$ directly.



Too time consuming to perform in a straight way

Reduction of the loop

Most time-consuming part

$$\sum_{ijkl\alpha\beta\gamma\delta} \bar{v}_{ijkl} \bar{v}_{\alpha\beta\gamma\delta} \rho_{ki} \rho_{lj} \rho_{\gamma\alpha} \rho_{\delta\beta} + \dots$$

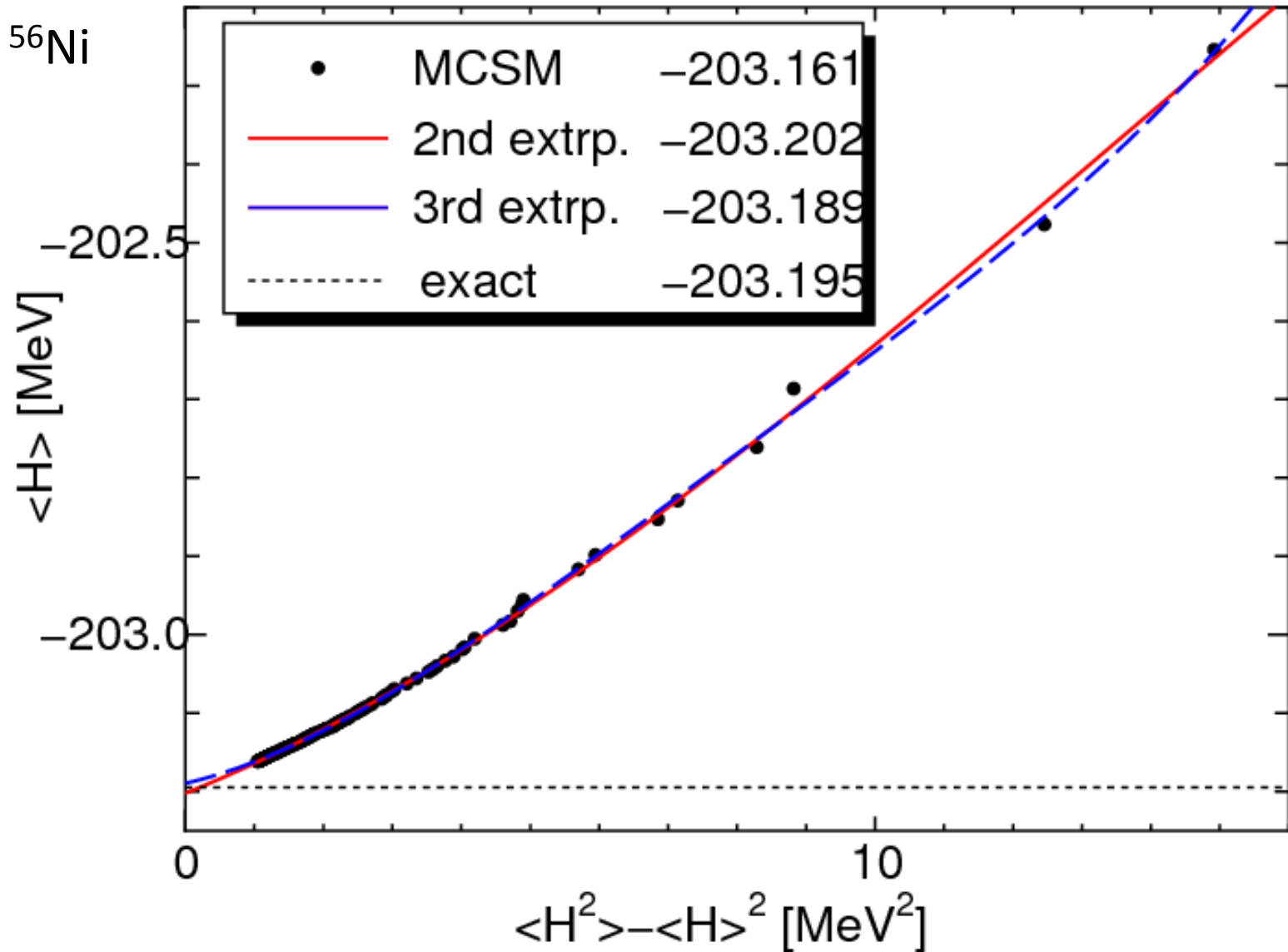
eightfold loop (i,j, ... runs single-particle states)



Reduced to sixfold loop

It is feasible to evaluate $\langle H^2 \rangle$ now!

An example of the extrapolation method



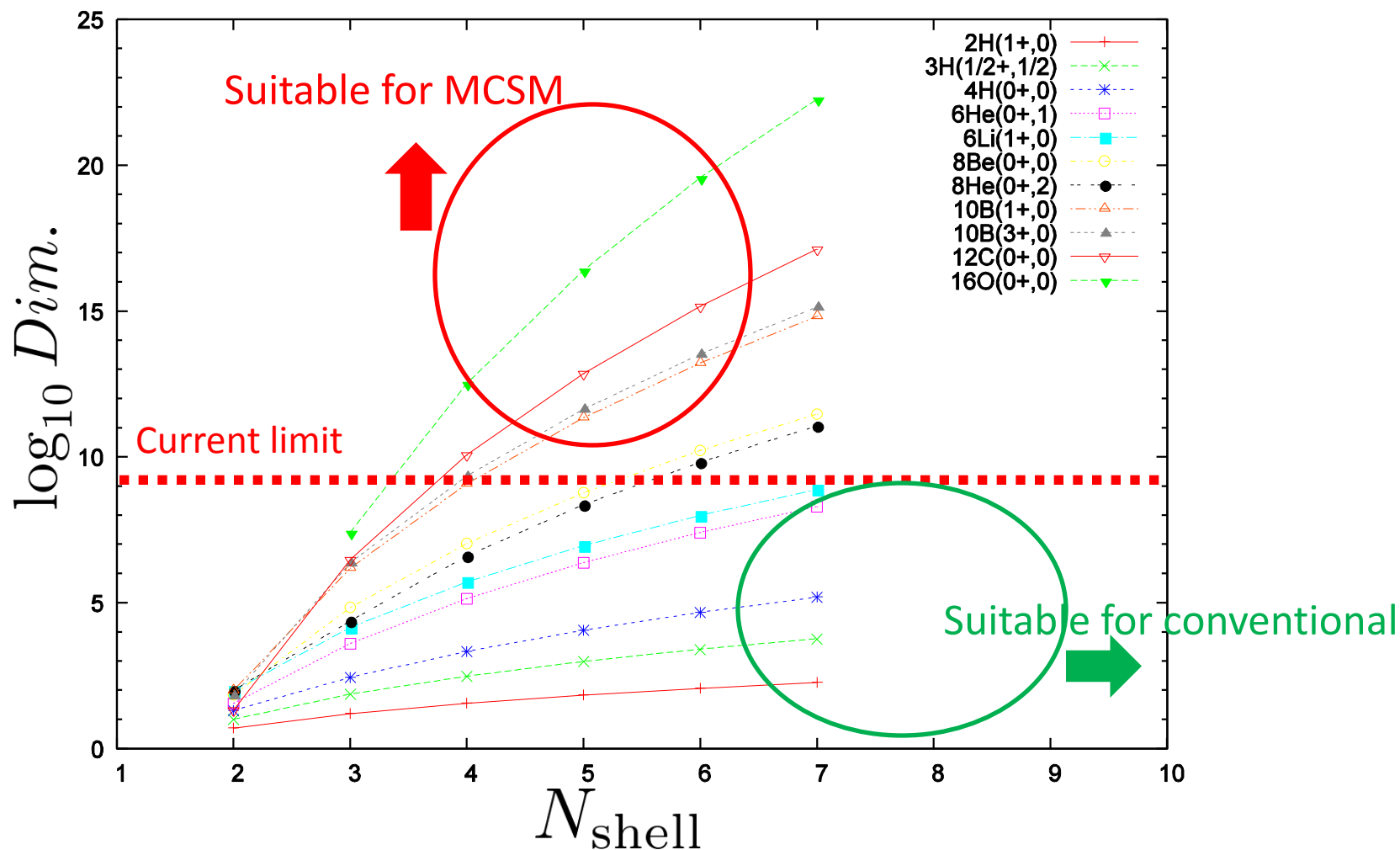
Application to the *ab initio* calculation

- No inert core assumed and many valence orbits taken
 - Large single-particle space: very challenging both for conventional approach and for MCSM
 - Computational difficulty
 - **Conventional approach**: proportional to dimension
 $\sim N C_n$: N =# of single-particle states and n =# of particles
 - **MCSM**: proportional to # two-body matrix elements
 $\sim N^4$; mildly depends on n



The difference makes different advantage.

What can be done?

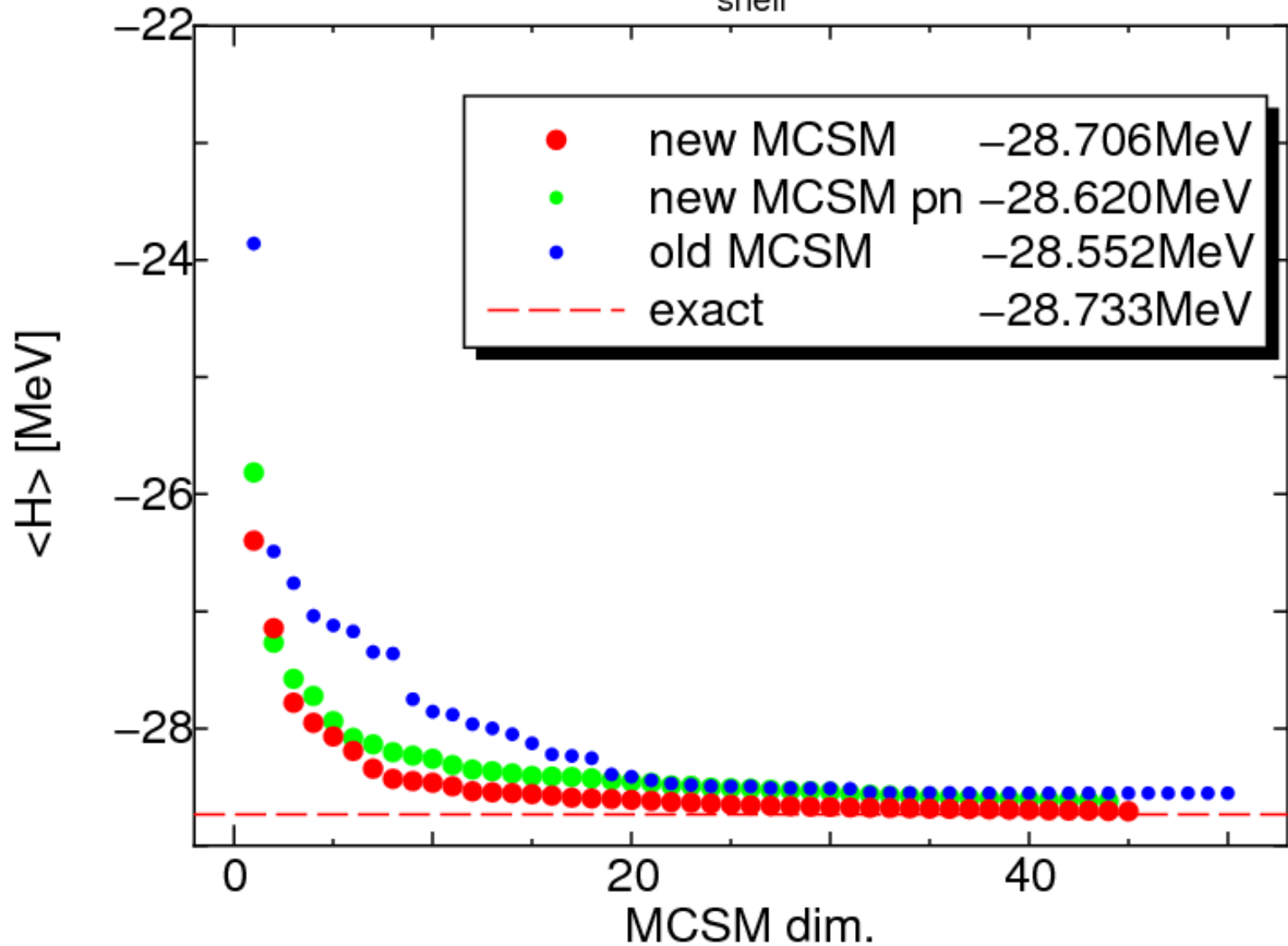


MCSM
➔

- Heavier nuclei
- Multi-particle multi-hole excited states

Benchmark calculation

${}^4\text{He}$ JISP16 $N_{\text{shell}}=4$ $hw=25\text{MeV}$



Summary

- I reported recent progress on the description of shell evolution and status of the development of a new Monte Carlo shell model code.
- Shell evolution
 - An effective interaction = bare tensor force + simple Gaussian central force, called monopole-based universal interaction, works quite well.
 - Its descriptive power is demonstrated around $N=28$.
 - Non-monotonic shell evolution, i.e., expanding and shrinking shell gap, is predicted for the proton shell beyond $N=28$.
- MCSM
 - Aiming at running on the next generation supercomputer in Japan, a new MCSM code has been developing.
 - Some advances such as extrapolation method are shown.