HPCI project field 5
“The origin of matter and the universe”

2014/06/05 ARIS2014
at Ito Hall, Tokyo

K computer

# Frontier of Nuclear Shell-Model Calculations and High-Performance Computing

CENTER *for*
NUCLEAR STUDY

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Y. Tsunoda (Tokyo), and T. Yoshida (CNS)

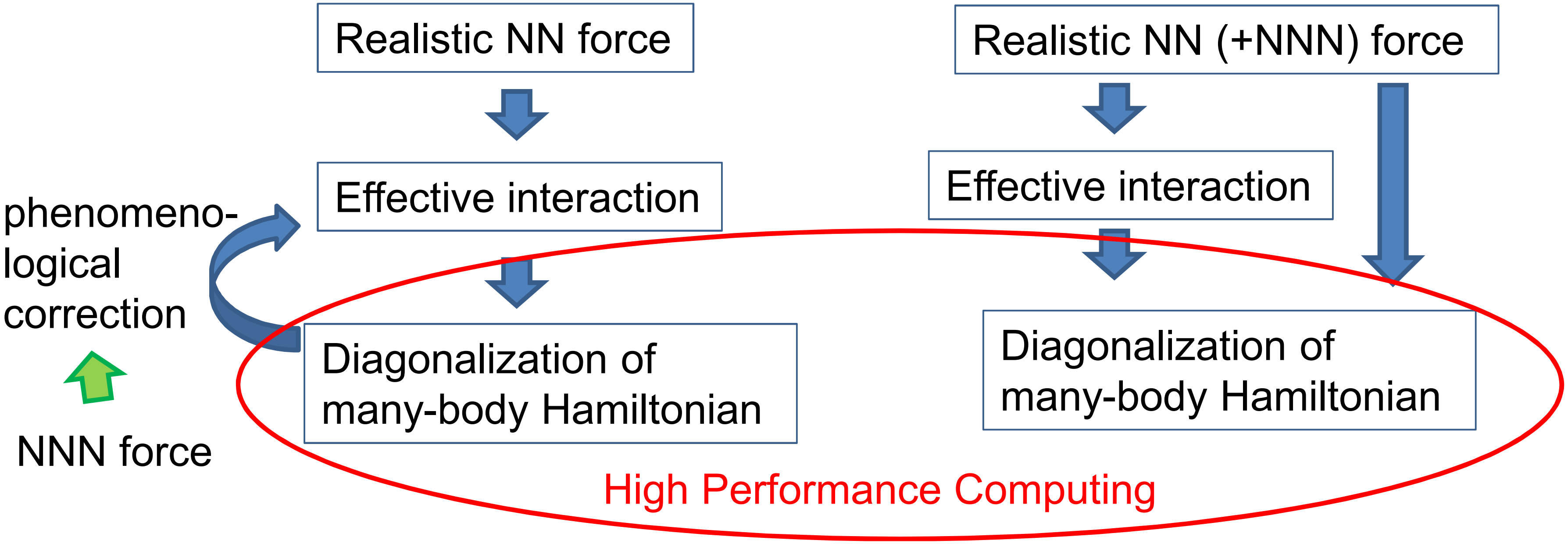
# Recipe for shell-model calculations

large-scale shell-model calc.

model space: valence shell (+ extention)

no-core shell model

excitation energy (Nmax hw)



Realistic NN force

Effective interaction

Diagonalization of many-body Hamiltonian

phenomeno-logical correction

NNN force

Realistic NN (+NNN) force

Effective interaction

Diagonalization of many-body Hamiltonian

High Performance Computing

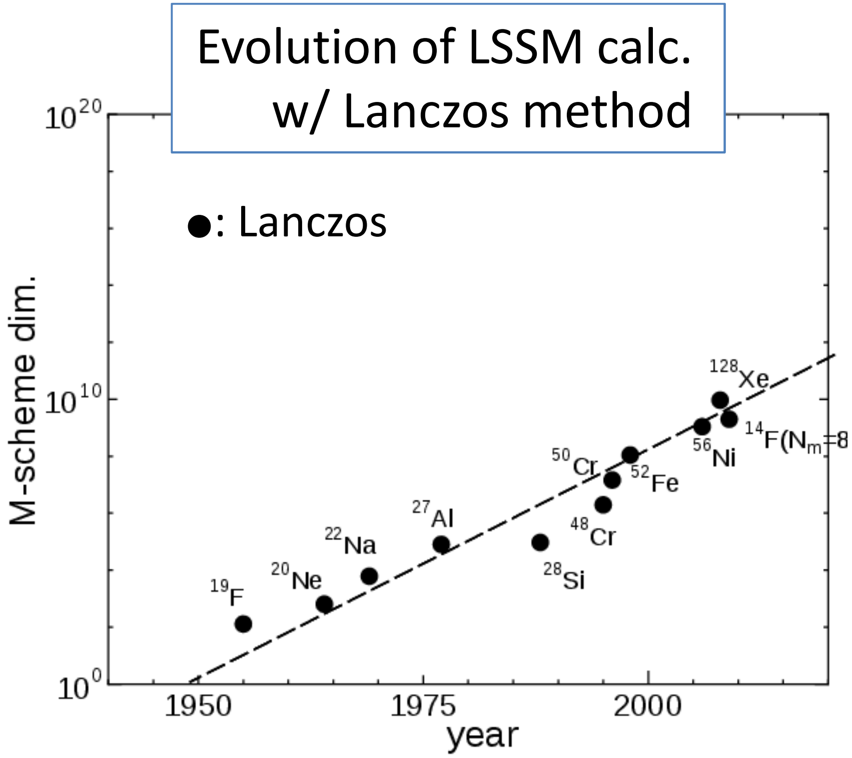
$$|\Psi\rangle = \sum_m v_m |m\rangle \qquad \sum_{m'} \langle m|H|m'\rangle v_{m'} = E|m\rangle$$

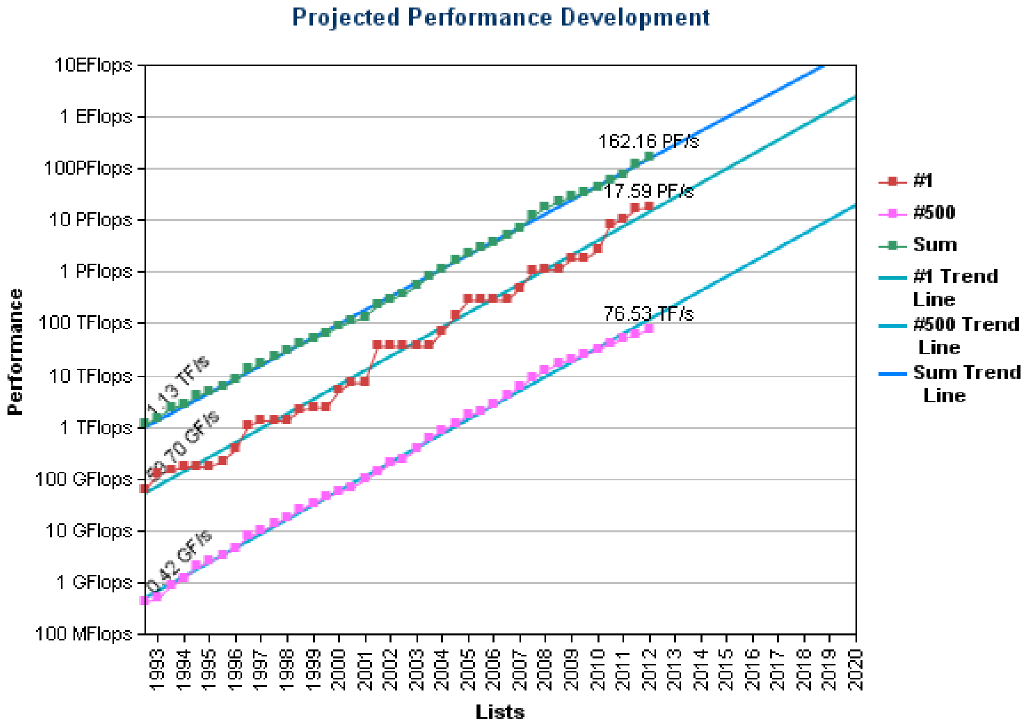
$|m\rangle$ : configuration, “spherical” Slater determinant of harmonic oscillator

The number of $|m\rangle \approx \frac{1}{f}\begin{pmatrix} N_p \\ Z \end{pmatrix}\begin{pmatrix} N_p \\ Z \end{pmatrix}$

Hamiltonian matrix is sparse
⇒ Lanczos algorithm

# Frontier of large-scale shell-model calculations


Evolution of LSSM calc.
w/ Lanczos method



- The maximum dimension of the *M*-scheme Hamiltonian matrix of the LSSM evolve exponentially as the performance development of supercomputers
- Present limitation ≈ $10^{10\text{-}11}$ (as expected by the extrapolation in 2000)

e.g. $^{68}$Ni in pf+g9/2+d5/2 $5 \times 10^{15}$ → 2040 for $10^{15}$ dim.?

# Large-scale shell model calculations

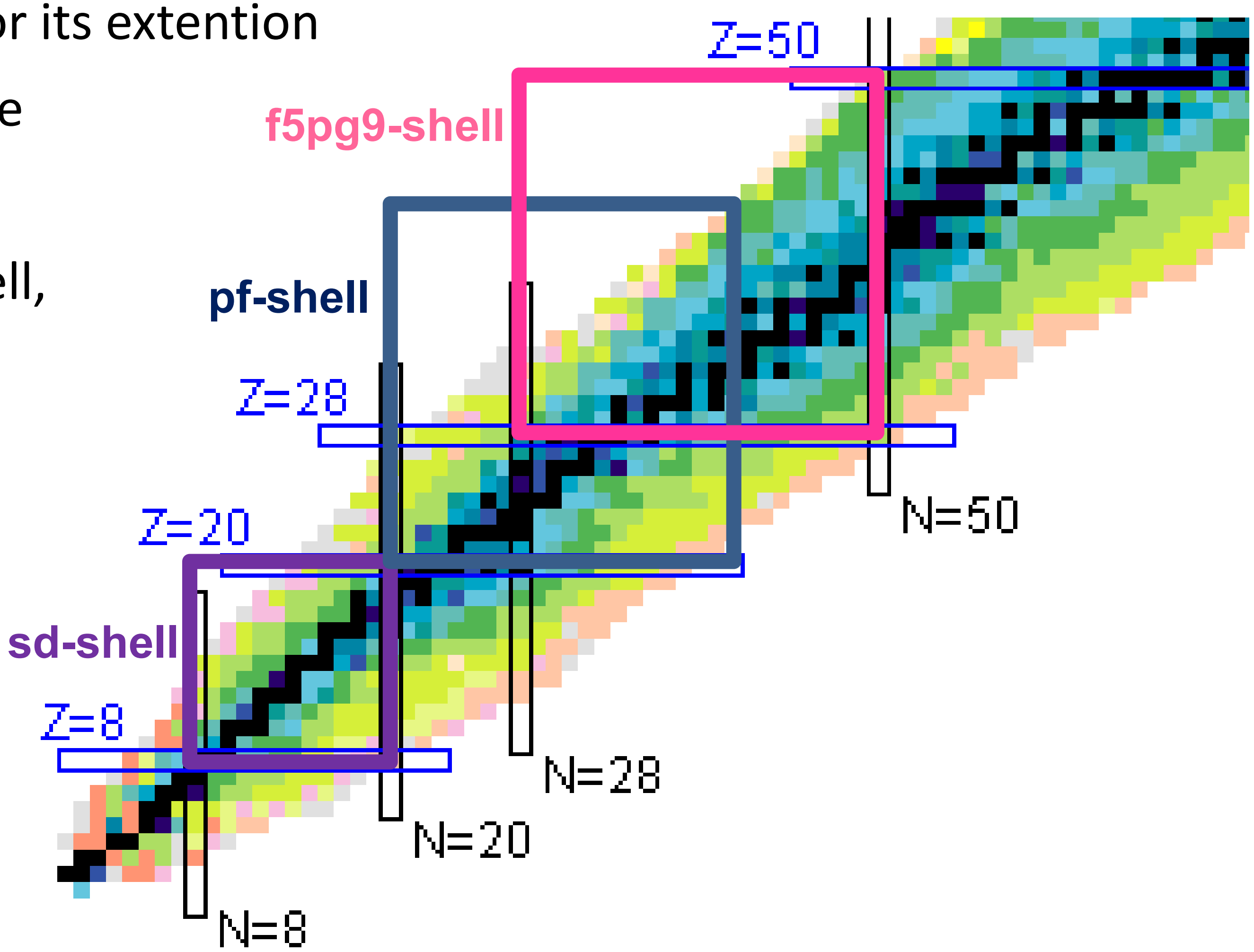
valence shell or its extention

as model space

*sd* shell, *pf* shell,

*f5pg9* shell

diagonalizable

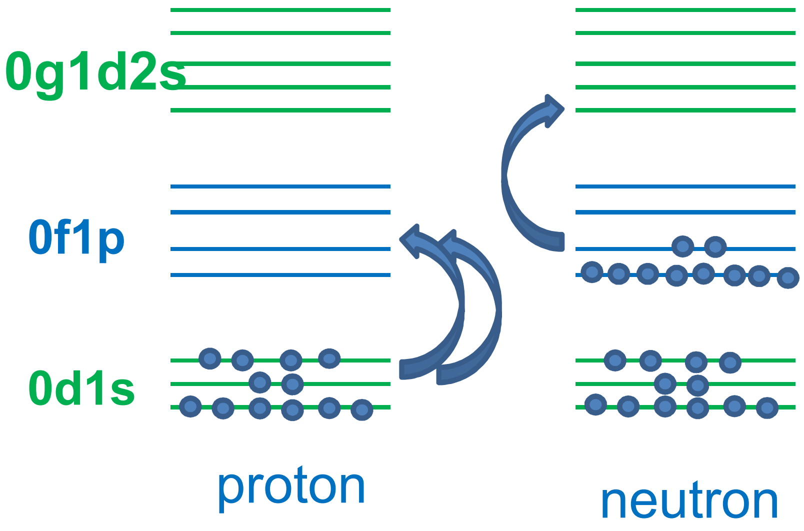


$^{60}$Zn in pf-shell : 2x10$^{9}$
$^{78}$Y in f5pg9-shell : 1.3x10$^{10}$

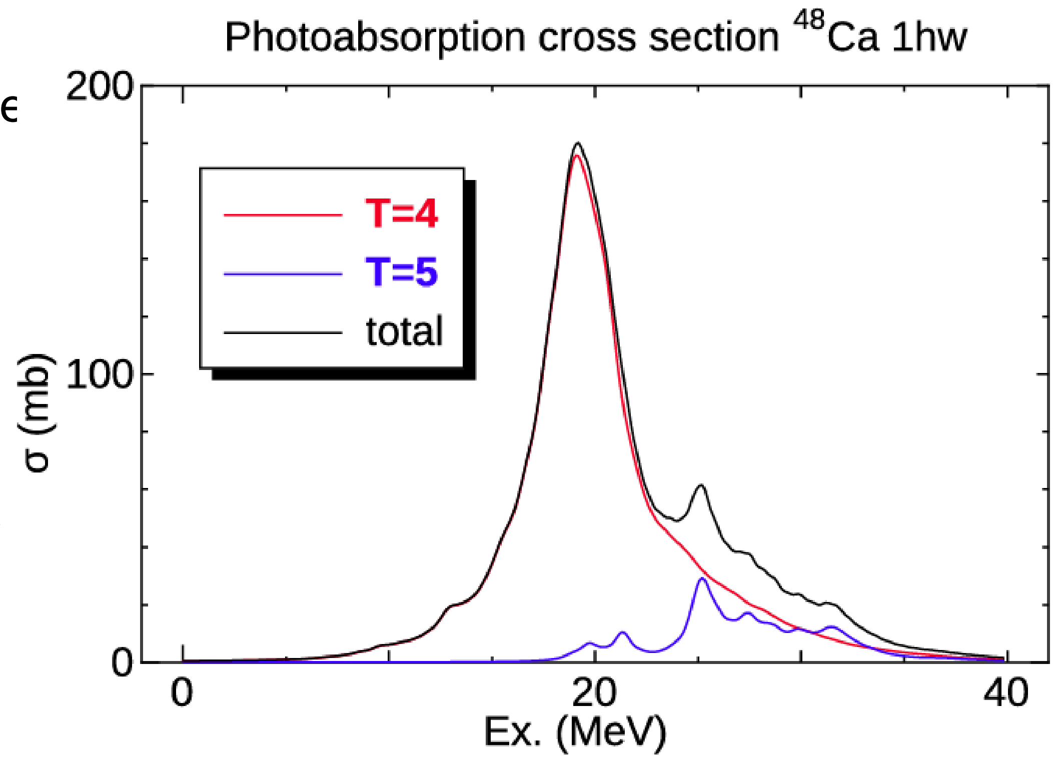
# Example of the large-scale shell-model calculations

NS, Y. Utsuno, S. Ebata, T. Otsuka, M. Honma and T. Mizusaki, in preparation

1hw/3hw sd-pf-sdg shell calculations for negative-parity states of Ca isotope to describe E1 excitations



We develop *M*-scheme shell-model code with Lanczos method for massive parallel computation "KSHELL".



**1hw : upto 1hw excitation in sd-pf-sdg shell**

**$4.1\text{x}10^6$ M-scheme dim.** at PC

**(1+3)hw: up to 3hw excitation in sd-pf-sdg shell**

**$1.2\text{x}10^{10}$ M-scheme dim.** at supercomputer

# HPCI Strategic Program for Innovative Research

by MEXT, Japan FY2011 – FY2015

to facilitate efficient use of K computer and HPC

- Strategic 5 Fields:
  - Field1: “Supercomputational Life Science”
  - Field2: “Computational Materials Science Initiative”
  - Field 3: “Projection of Planet Earth Variations for Mitigating Natural Disasters”
  - Field 4: “Industrial Innovation”
  - Field 5: “The origin of matter and the universe”
    - lattice QCD
    - Nucleus ← Our group
    - Supernova Explosion
    - Early Star Formation

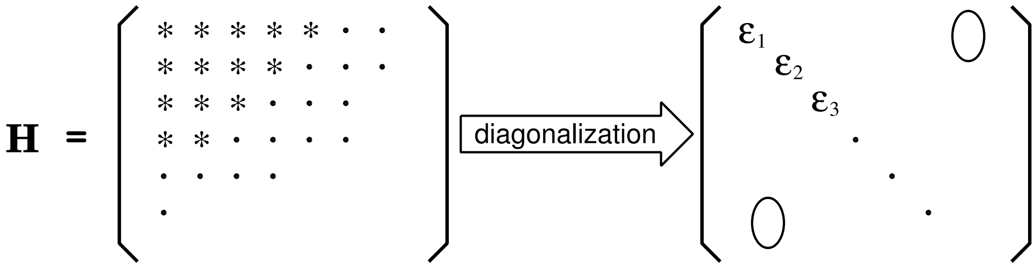
Head: Takaharu Otsuka (Tokyo)

nuclear shell-model calculations using Monte Carlo shell model

# Monte Carlo Shell Model

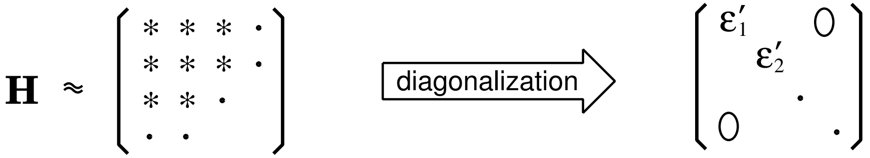
Otsuka, Honma, Mizusaki, Shimizu, Utsuno, PPNP47, 319 (2001)

a tool to go beyond the conventional Lanczos diagonalization method
for Large-Scale Shell Model calculations



**Conventional Shell Model**
all Slater determinants

Stochastically selected basis



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

**Monte Carlo Shell Model**
bases important for a specific eigenstate

$\hat{h}(\sigma)$ one-body Hamiltonian

σ... auxiliary field

random numbers

$$\left|\Psi\right\rangle = \sum_{k=1}^{N_{MCSM}} f_k P^{J,\pi} \left|\phi_k\right\rangle$$

MCSM basis, deformed Slater det.

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

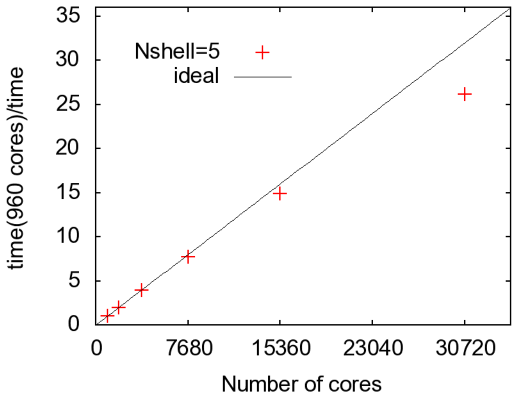
Wave function is described as a linear combination of *J*-projected deformed Slater determinants.
Increase MCSM dimension, or number of deformed Slater det. till energy converges.

# “Advanced” Monte Carlo Shell Model towards K computer

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

PC cluster
100CPU

Parallel efficiency



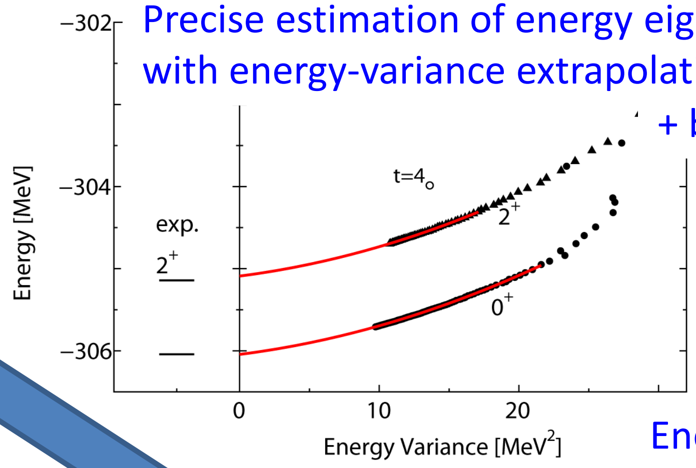
OpenMP+MPI hybrid parallel
100,000 cores

NS, T. Abe, Y. Tsunoda, Y. Utsuno, T. Yoshida, T. Mizusaki, M. Honma and T. Otsuka, Prog. Theor. Exp. Phys. **2012** 01A205 (2012).

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

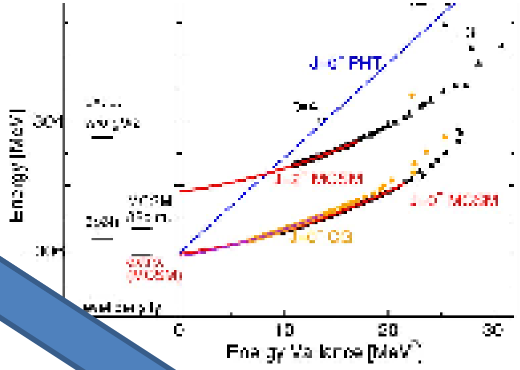
Precise estimation of energy eigenvalues with energy-variance extrapolation

+ basis reordering technique

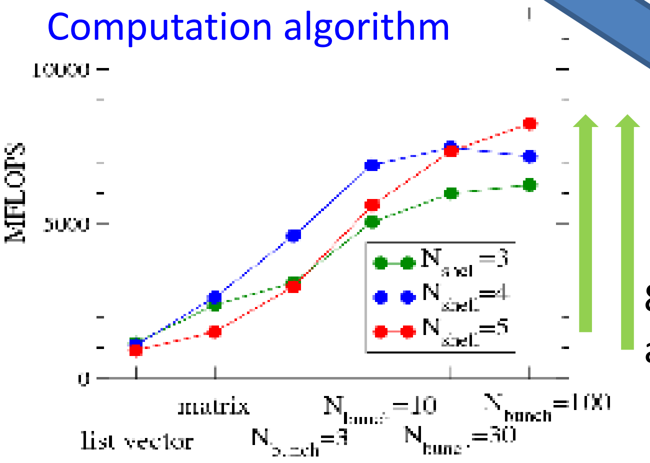


NS et al., Phys. Rev. C **85** 054301(2012).

Energy gradient for optimization of wave function



Computation algorithm

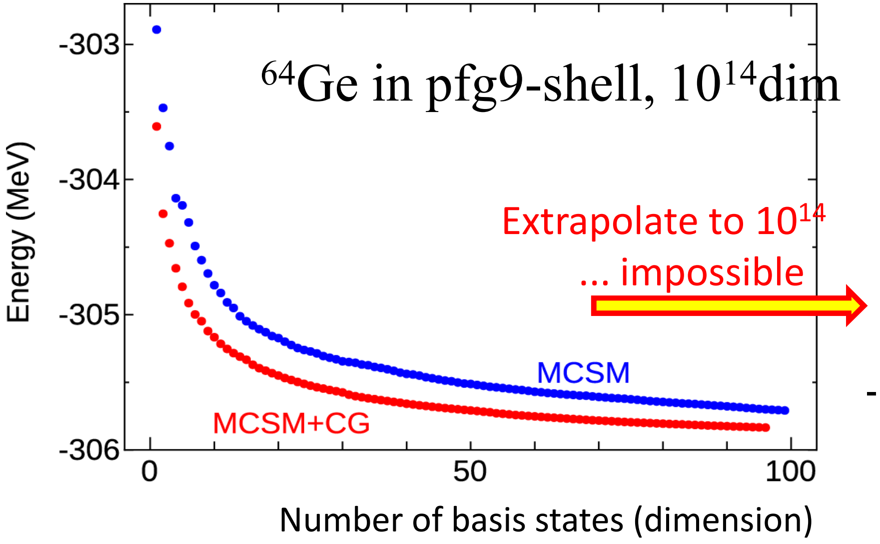


8 times
acceleration

Y. Utsuno, NS, T. Otsuka, and T. Abe, Comp. Phys. Comm. **184** 102 (2013).

K computer

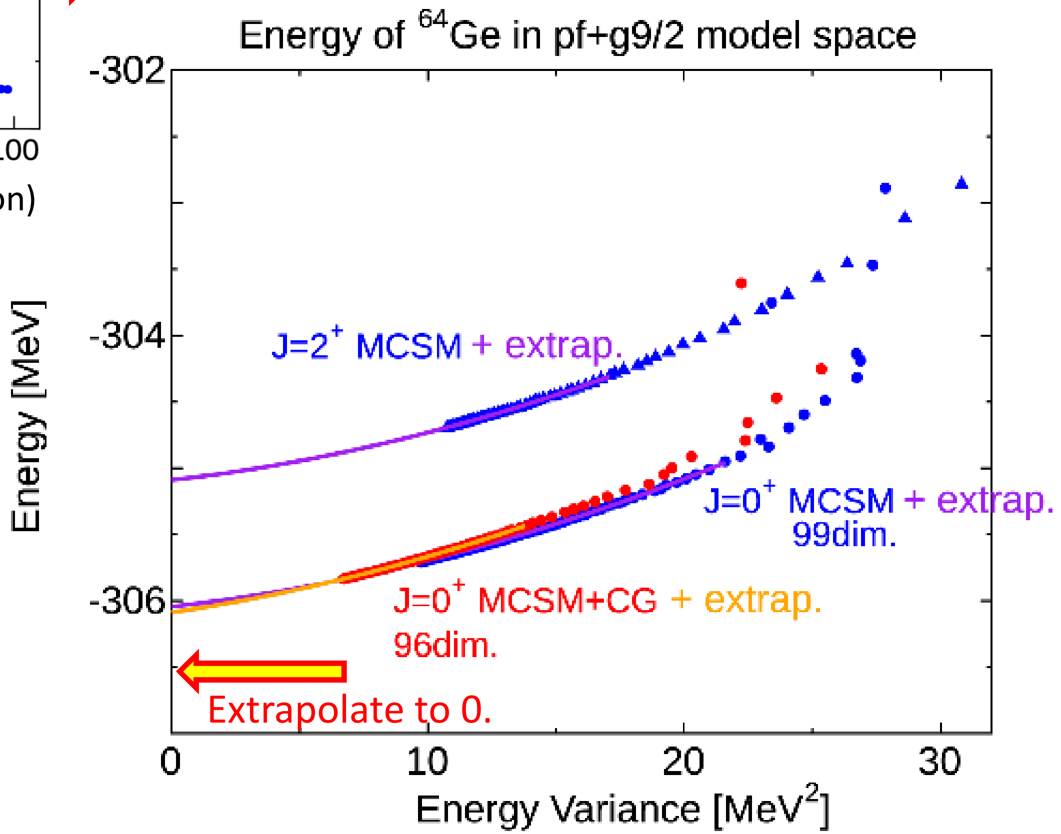
# Energy variance extrapolation in the MCSM: $^{64}$Ge in *pfg9*-shell

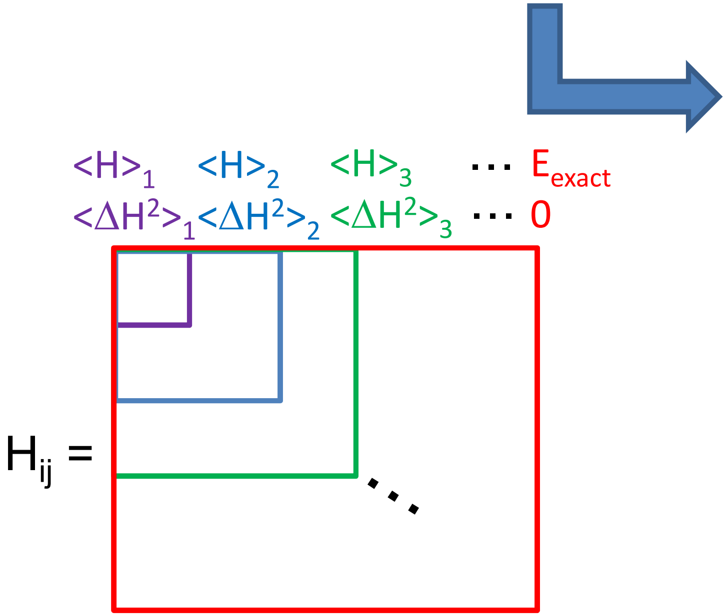


Energy variance : $\langle \Delta H^2 \rangle = \langle H^2 \rangle - \langle H \rangle^2$

As the number of basis states increases, the approximated w.f. approaches the exact one and the energy variance approaches zero.

Extrapolate towards $\langle \Delta H^2 \rangle \to 0$





# Advantages of the MCSM

- computation intensive, rather small memory access, small I/O ... good at massive parallel computation

*M*-scheme Lanczos method vs MCSM wave function

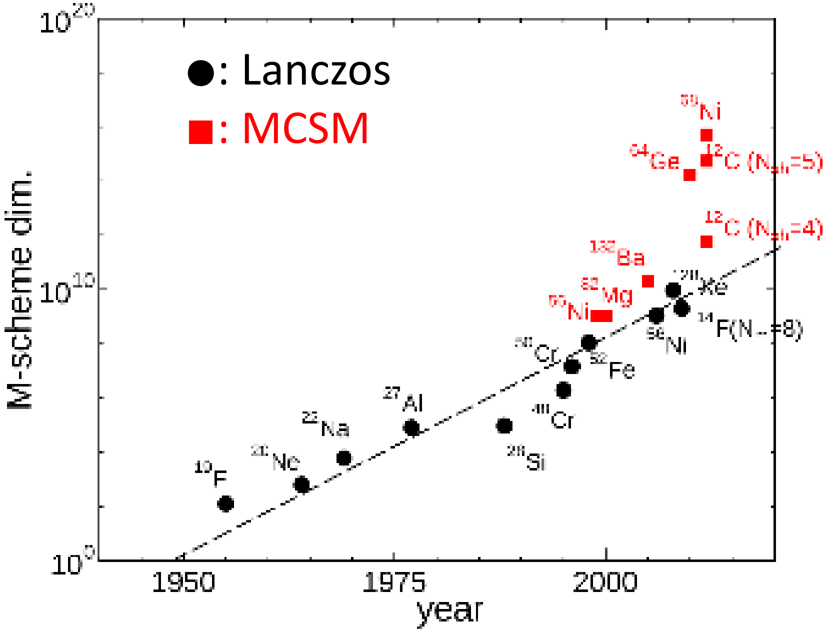
discretized integral of Euler’s angle

$$|\Psi\rangle = \boxed{\sum_{m=1}^{\sim 10^{10}} f_k} |\phi_m\rangle \qquad |\Psi\rangle = \sum_{k=1}^{N_{MCSM}\sim 100} f_k \boxed{P^{J,\pi}} |\phi_k\rangle$$

huge memory and disk I/O

- overcome the limitation of Lanczos method

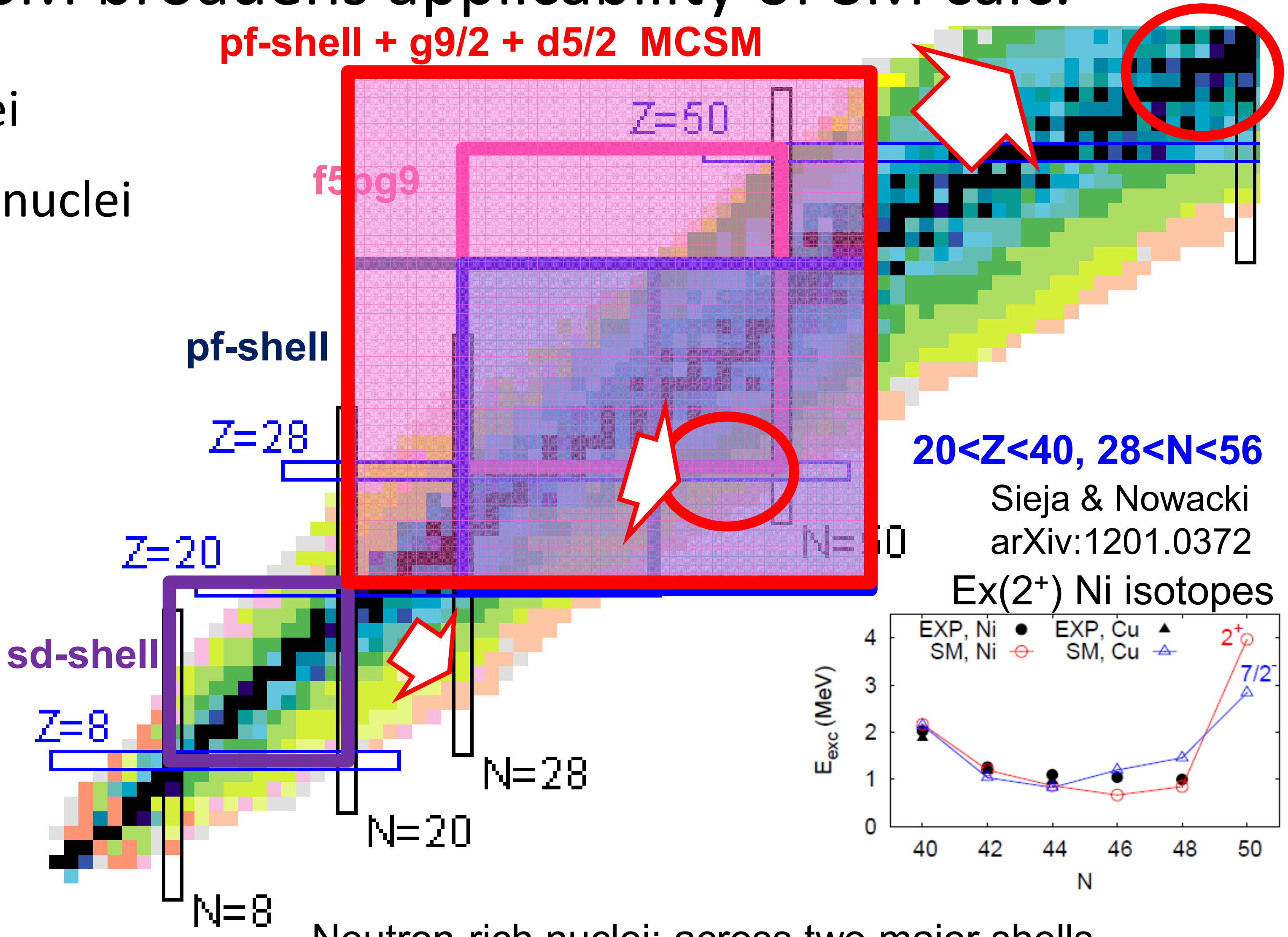
- analyze “intrinsic” wave function and shape
  (discussed later)



# MCSM broadens applicability of SM calc.

heavier nuclei

neutron-rich nuclei



**20<Z<40, 28<N<56**

Sieja & Nowacki

arXiv:1201.0372

Ex(2$^+$) Ni isotopes

Neutron-rich nuclei: across two major shells

⇒ proton neutron different model space

+ truncation

⇒ full isospin-invariant space + MCSM

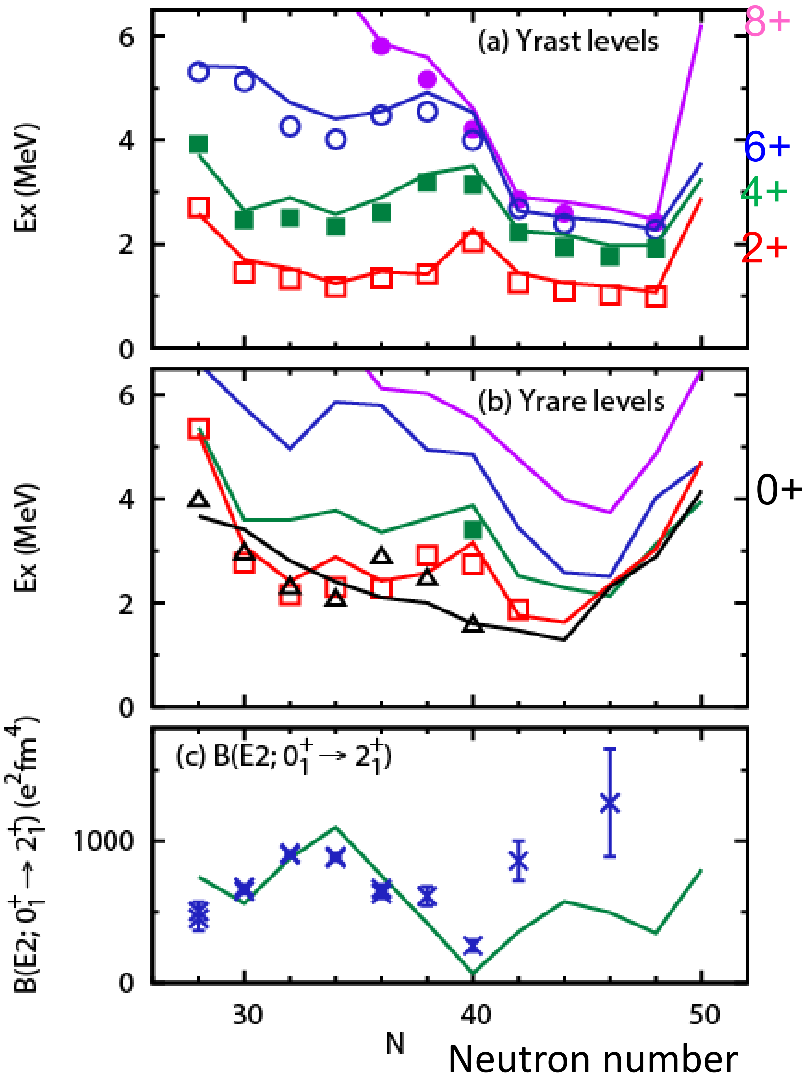
Y. Tsunoda AS2-A037, S. Suchyta PS2-A039, Y. Utsuno oral

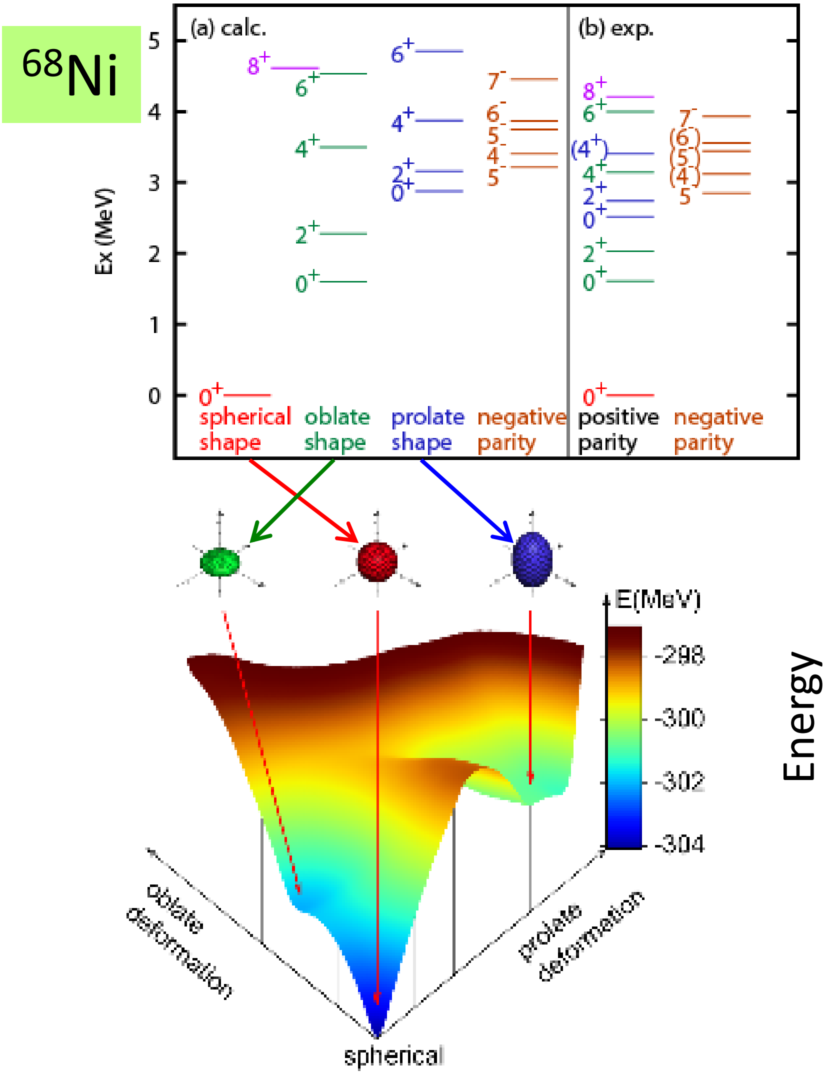
# Neutron-rich Ni isotopes and shell evolution

Exp.: S. Suchyta PS2-A039

pf-shell + g9/2, d5/2 orbits w/o truncation
... 5.1 x $10^{15}$ M-scheme dim.

Y. Tsunoda, T. Otsuka, NS, M. Honma and Y. Utsuno, PRC 89, 031301(R) (2014)





# $^{68}$Ni $0^+$ states ⇔ different shapes

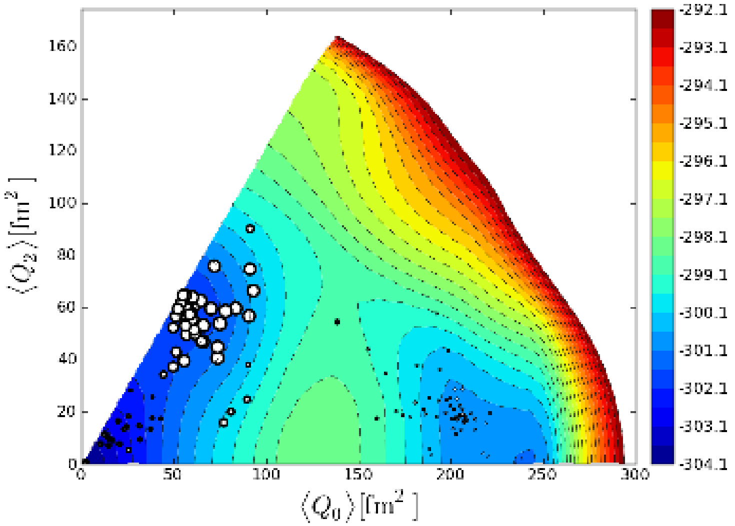
MCSM w.f. $|\Psi\rangle = \sum_{k=1}^{N_{MCSM}\sim 100} f_k P^{J,\pi} \boxed{|\phi_k\rangle}$

PES is calculated by Q-constraint Hartree-Fock calc.

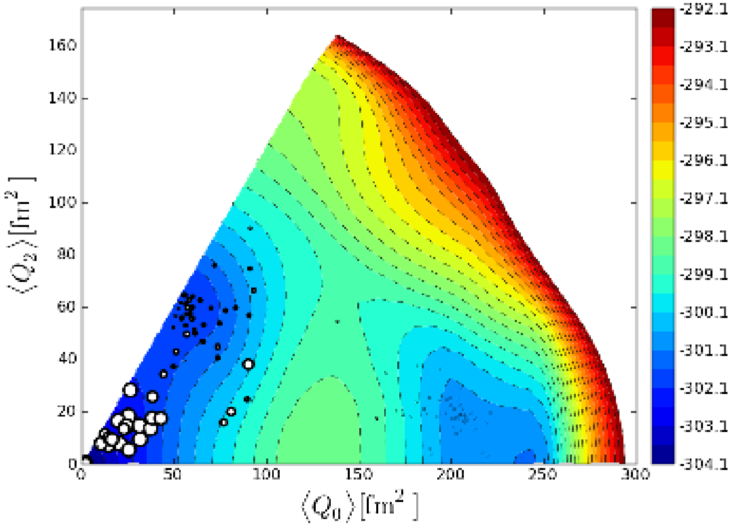
Location of circle : quadrupole deformation of $|\phi_k\rangle$

Area of circle : overlap probability $\frac{1}{N_k}\left|\langle\Psi|P^{J,\pi}|\phi_k\rangle\right|^2$

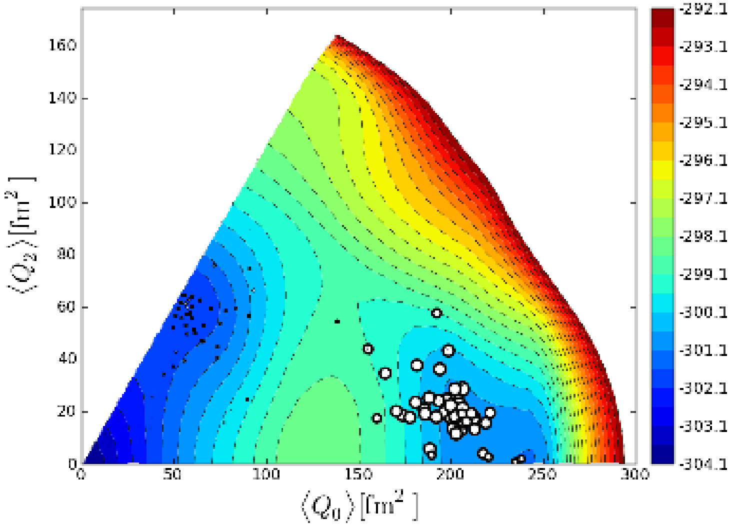
$0^+_2$ : oblate β ~ -0.2



$0^+_1$ : spherical β ~ 0

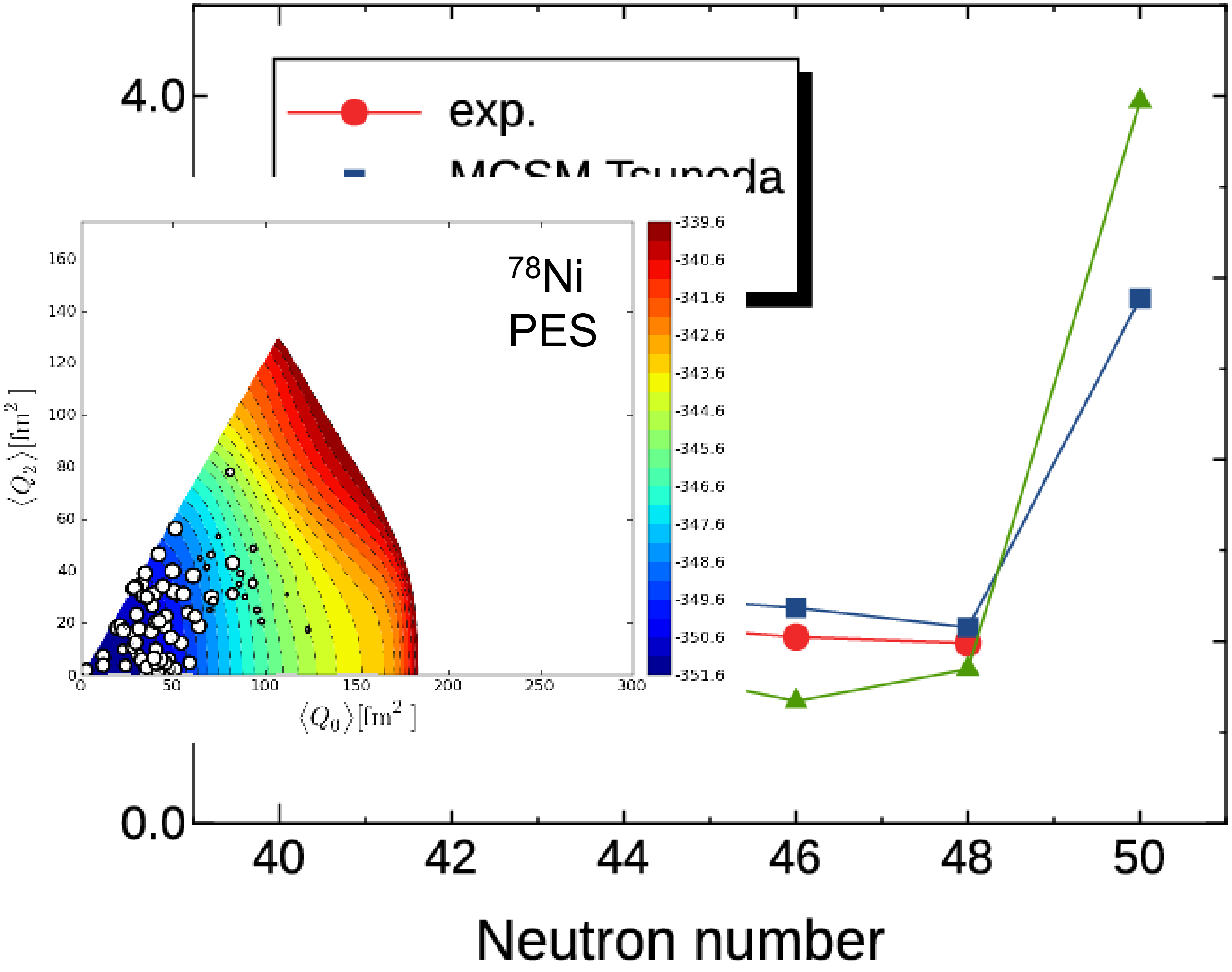


$0^+_3$ : prolate β ~ +0.4



# Towards $^{78}$Ni : prediction

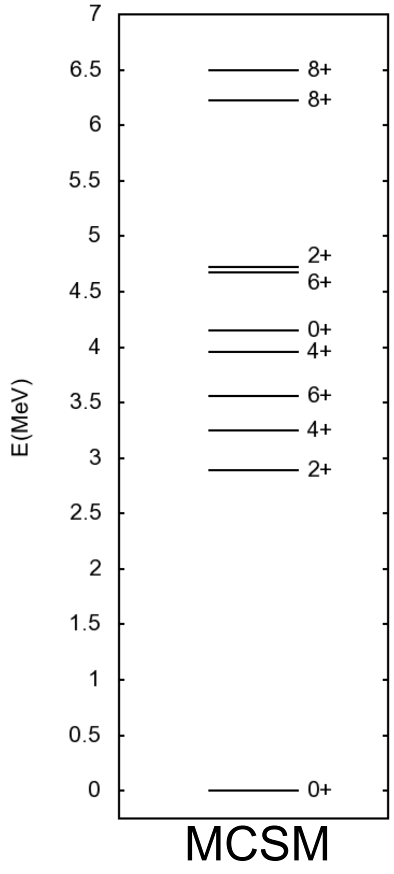
Excitation energies of Ni isotopes



Z=28, N=50

How magic?

Both SM results give large 2+ energy

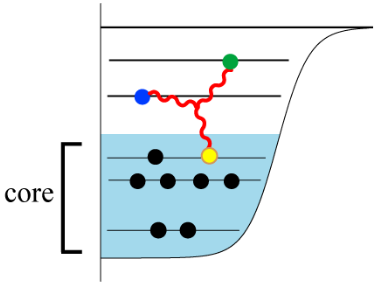


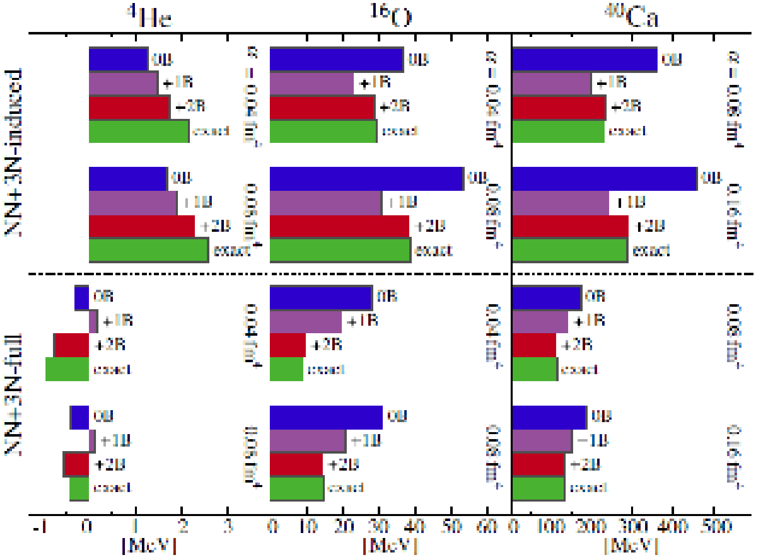
SM: Sieja and Nowacki, arXiv:1201.0373 π pf, ν f5pg9d5

MCSM: Y. Tsunoda *et al.,* PRC 89 031301(R) (2014) full pfpg9d5

# Towards SM calc. w/o phenomenological correction

## 3-body force into normal ordered 2-body force



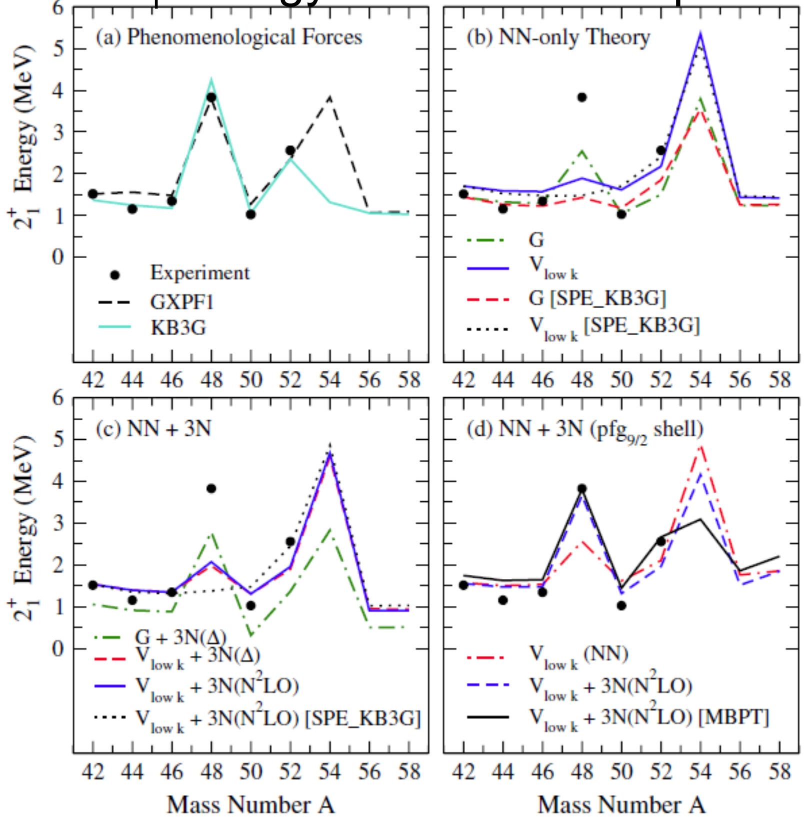


Normal ordered 2-body force is good approximation for no-core SM

Ref. R. Roth et al., PRL 109, 052501

Phenomenological fit of SM interaction
← 3-body force origin

$2^+_1$ Energy of calcium isotopes



SM calc. w/o phenom. correction

Normal ordered 2-body force

Ref. J. Holt, T. Otsuka, A. Schwenk and T. Suzuki, JPG 39 085111 (2012)

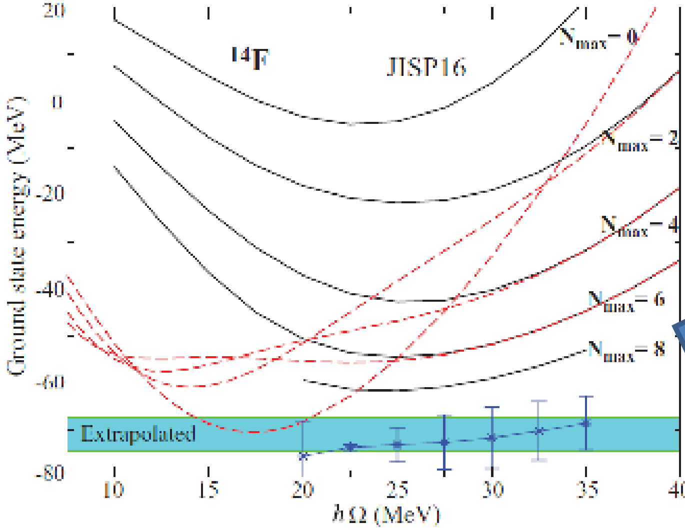
# No-core shell model

Importance Truncated NCSM

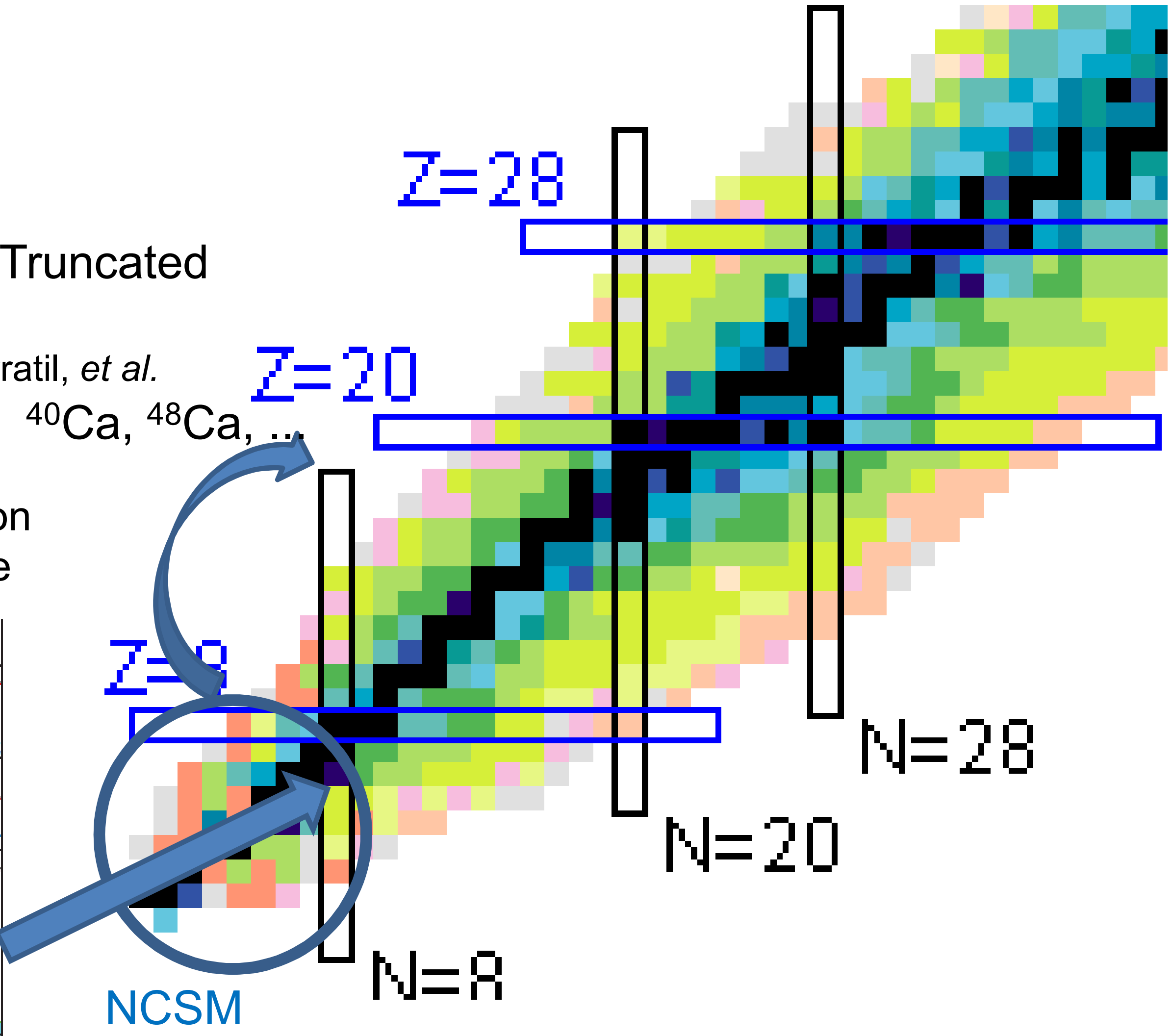
R. Roth, P. Navratil, *et al.*

$^{40}$Ca, $^{48}$Ca, ...

Excitation energy ($N_{max}hw$) truncation
Extrapolation to infinite model space



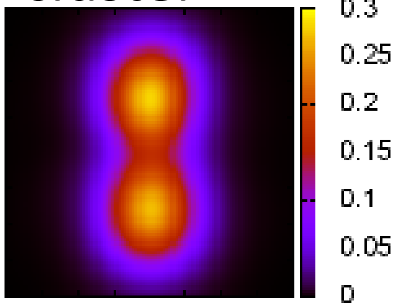
P. Maris, J. P. Vary and A. Shirokov
PRC 79, 014308 (2009)



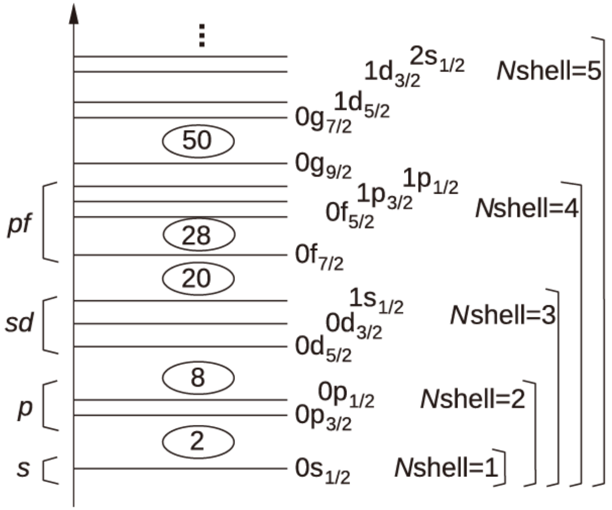
NCSM and reaction ... S. Quaglioni *et al.*

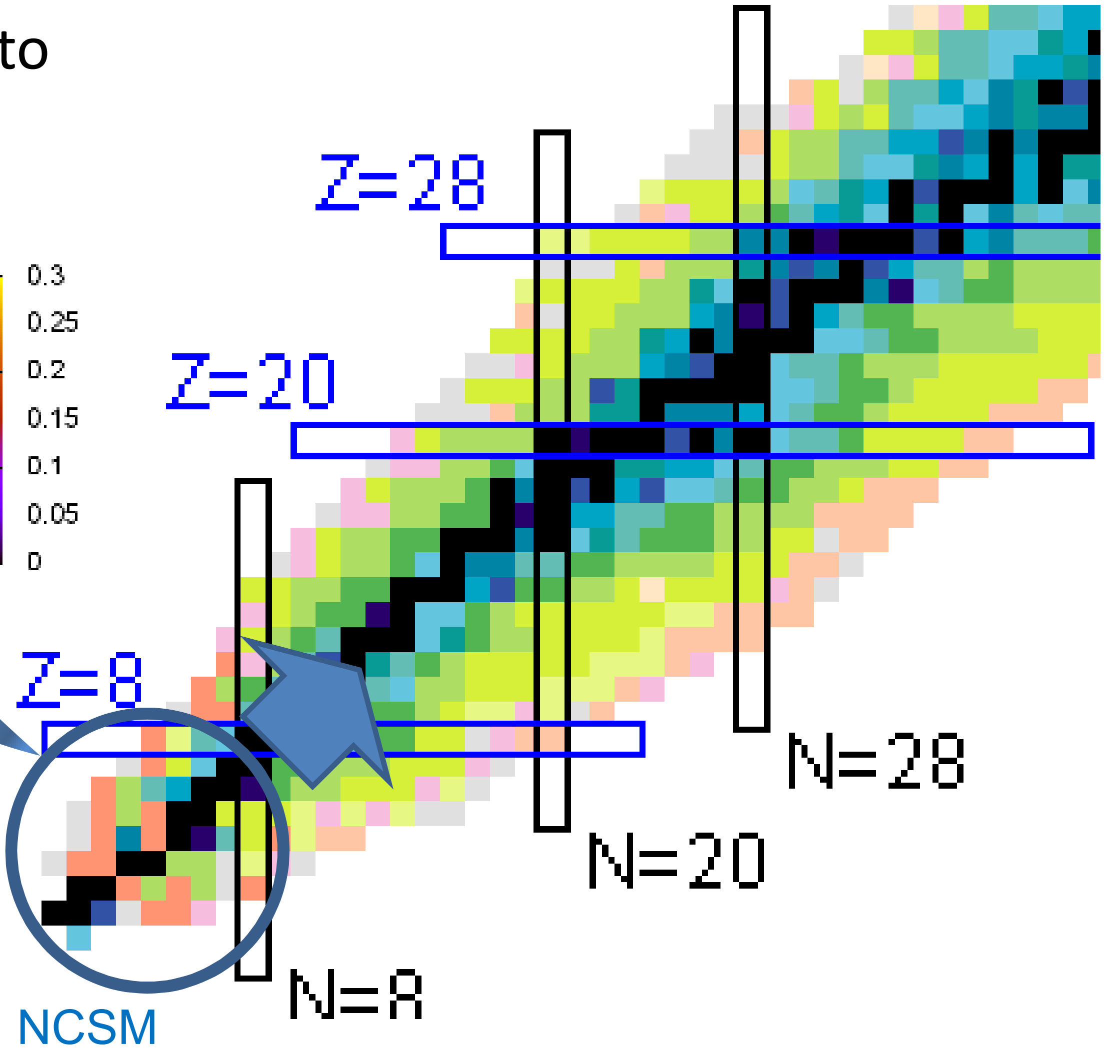
# MCSM for no-core shell model calc.

- Enhance the applicability to heavier region by MCSM
- Description of cluster structure by MCSM



- $N_{shell}$ truncation





truncation by single-particle energy

T. Abe, P. Maris, J. Vary *et al.*, AS2-A018

# Extrapolation to infinite model space based on EFT

$$\lambda_{sc} = \sqrt{m\hbar\omega/(N+3/2)} = \lambda^2/\Lambda$$
$$\Lambda = \sqrt{m(N+3/2)\hbar\omega}$$

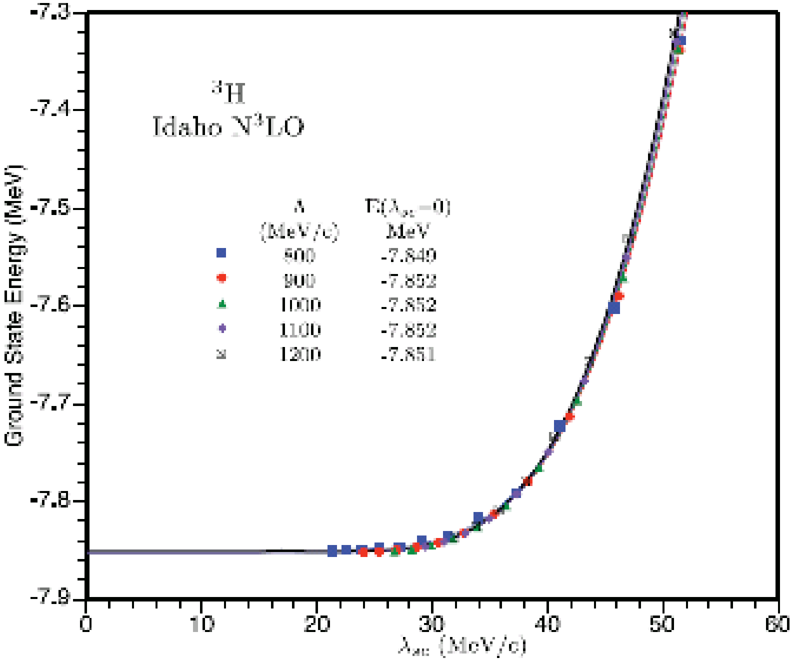
## MCSM

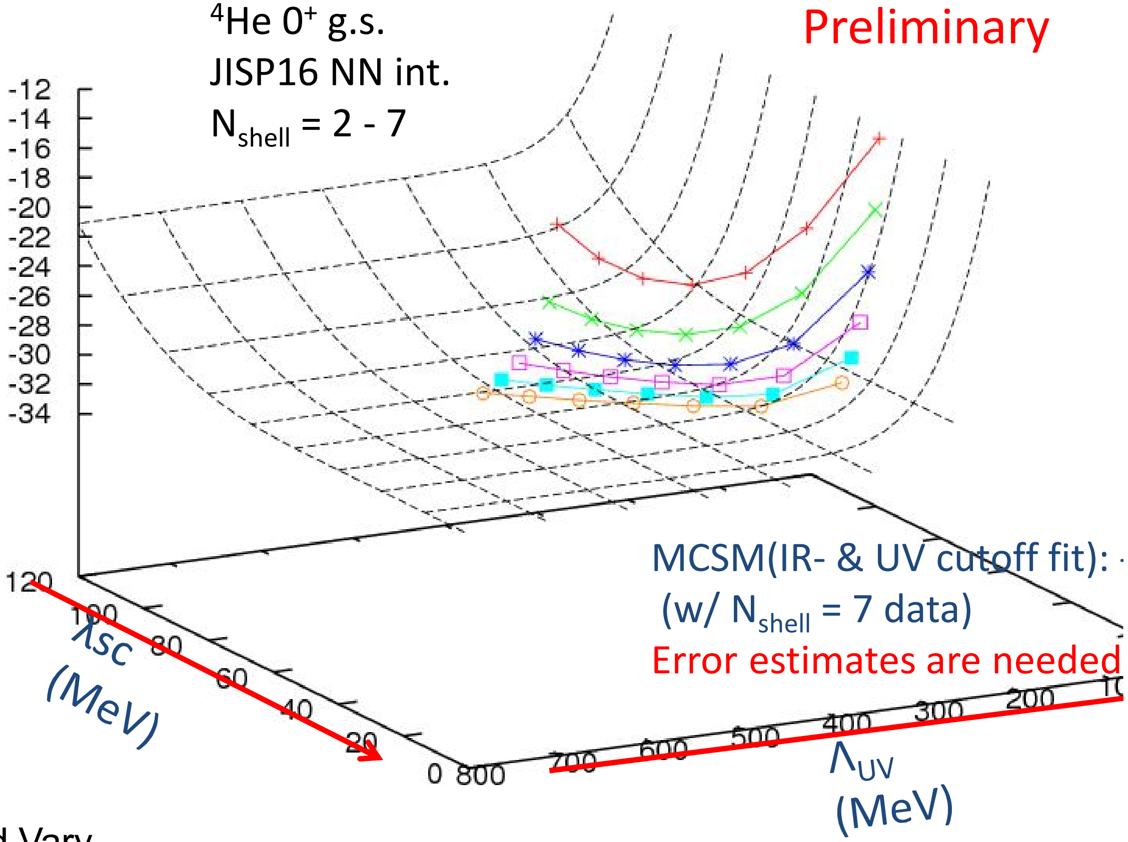
Excitation energy ($N_{nshell}$) truncation

$$E(\lambda,\Lambda) = E(\lambda=0,\Lambda=\infty) + a\exp(-b/\lambda) + c\exp(-\Lambda^2/d^2)$$

## NCSM

Excitation energy ($N_{max}hw$) truncation





$^4$He $0^+$ g.s.
JISP16 NN int.
$N_{shell}$ = 2 - 7

Preliminary

MCSM(IR- & UV cutoff fit):
(w/ $N_{shell}$ = 7 data)
Error estimates are needed

Ref. Coon, Avetian, Kruse, van Klock, Maris and Vary
PRC 86 054002 (2012)

On going: $^8$Be($0^+$), $^{12}$C($0^+$), $^{16}$O($0^+$), …

T. Yoshida Poster AS2-A005

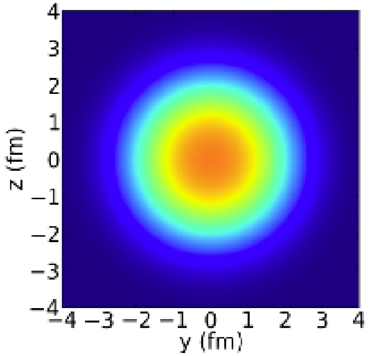
# Density profile of the MCSM wave function

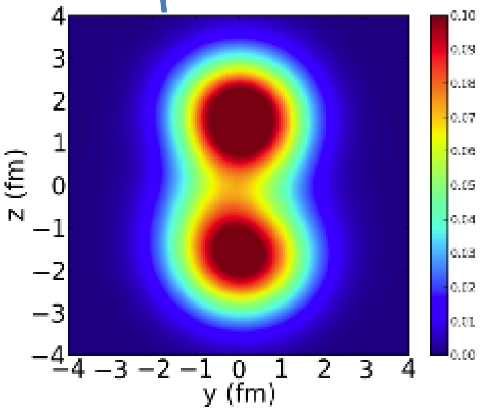
Density distribution of the ground state $J^\pi = 0^+$ of 8Be

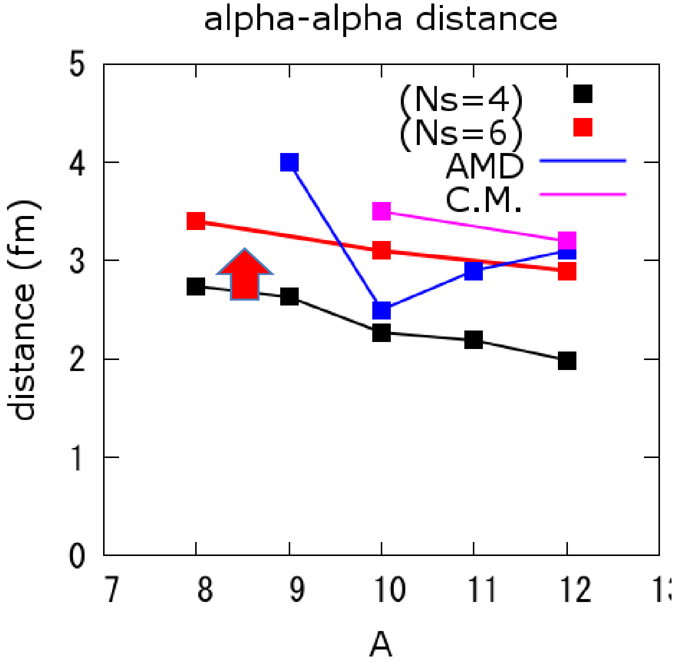
$$\left|\Psi\right\rangle = \sum_{k=1}^{N_{MCSM}} f_k P^{J,\pi} \left|\phi_k\right\rangle = P^{J,\pi} \boxed{\left( \sum_{k=1}^{N_{MCSM}} f_k \left|\phi_k\right\rangle \right)}$$

laboratory-frame
(spherical sym.)

"Intrinsic"
framework

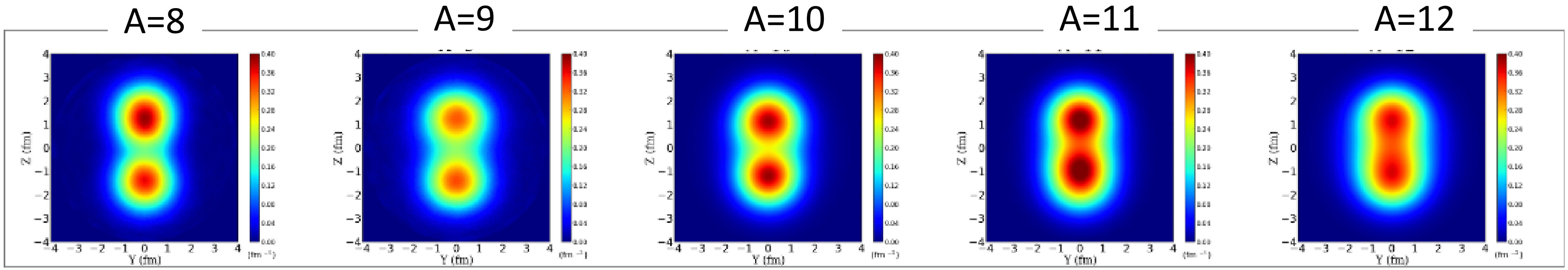






[AMD: Y.Enyo et al. PRC 2003 ]
[C.M. : M.Ito, N.Itagaki et al, PRL 2008]

## Matter density of Be isotopes JISP16 interaction



# Summary

- HPCI project promotes nuclear physics. In HPCI Field 5 Subject 2, we developed the “advanced” MCSM to run on K computer
  - energy-variance extrapolation, code R&D
  - unified description of neutron-rich Ni isotopes, shell evolution and shape coexistence
  - test the feasibility of no-core MCSM and propose a new method to draw the density profile
- MCSM purvey analysis of “intrinsic” shapes and their mixing, which enlighten cluster structure and shape coexistence.

# Collaborators

**HPCI project, Field 5**

- Takaharu Otsuka (Tokyo) Co-chair
- Takashi Abe (Tokyo) Poster AS2-A018
- Shuichiro Ebata (Hokkaido) Poster PS2-B022
- Michio Honma (Aizu)
- Yoritaka Iwata (CNS, Tokyo) Poster PS2-A061
- Takahiro Mizusaki (Senshu Univ.)
- Tomoaki Togashi (CNS, Tokyo) Poster PS2-A035
- Naofumi Tsunoda (CNS, Tokyo)
- Yusuke Tsunoda (Tokyo) Poster PS2-A037
- Yutaka Utsuno (JAEA) Oral Jun/3
- Tooru Yoshida (CNS, Tokyo) Poster PS2-A005

- James Vary (Iowa)
- Pieter Maris (Iowa) ICNT workshop, next week

Thank you !