

Study of medium-mass nuclei by large-scale shell model calculations

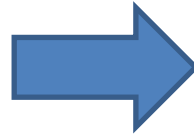
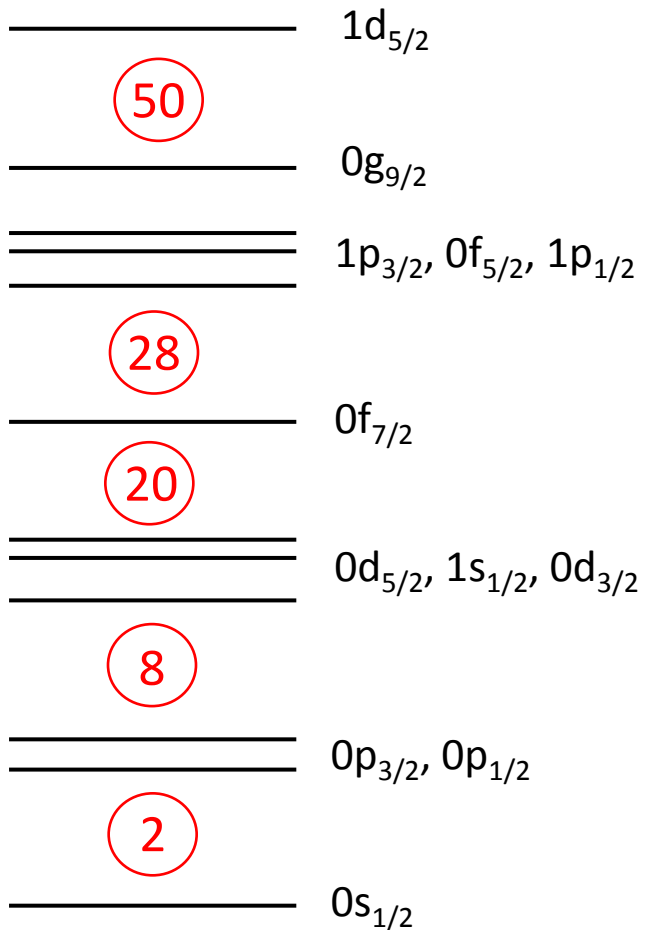
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Motivation

Shell structure
in **stable nuclei** ($Z \sim N$)



Different structure
in **exotic nuclei** ($Z \ll N, Z \gg N$)

Some **magic numbers** disappear
New magic numbers appear

Magic number nucleus: **closed shell**
Ground state has **spherical** shape
Excited states are **higher**



open shell nucleus:
Nucleus can have **deformed** shape
Excited states are **lower**

Motivation

Phenomena in **exotic nuclei** ($Z \ll N$, $Z \gg N$)

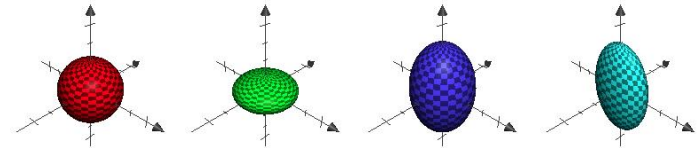
Evolution of shell structure

Size of shell gaps changes

Magicity becomes strong/weak

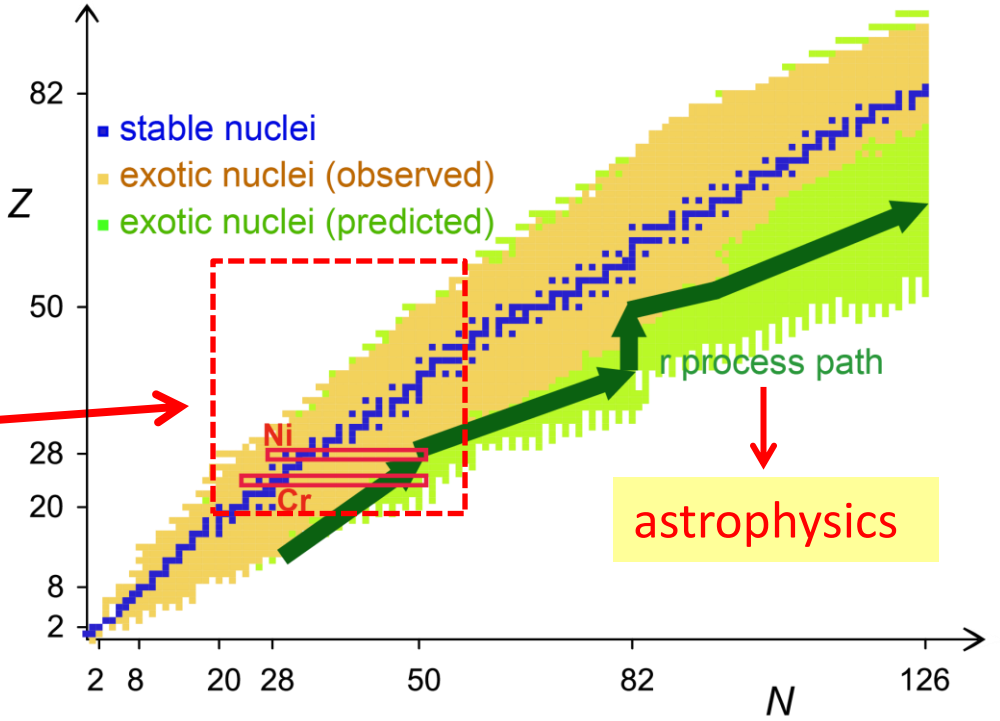
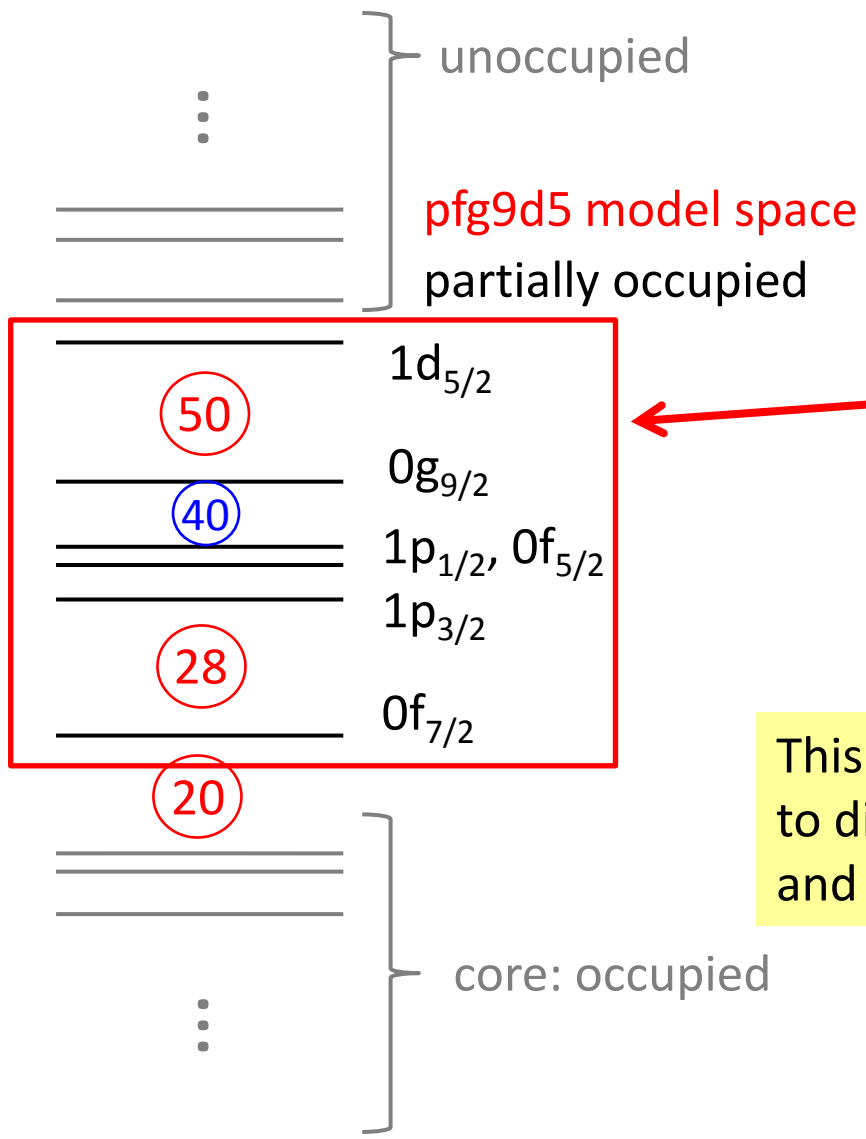
Shape coexistence

States of different shape coexist



Necessity of **large-scale calculations**
in large model space

Shell model calculation

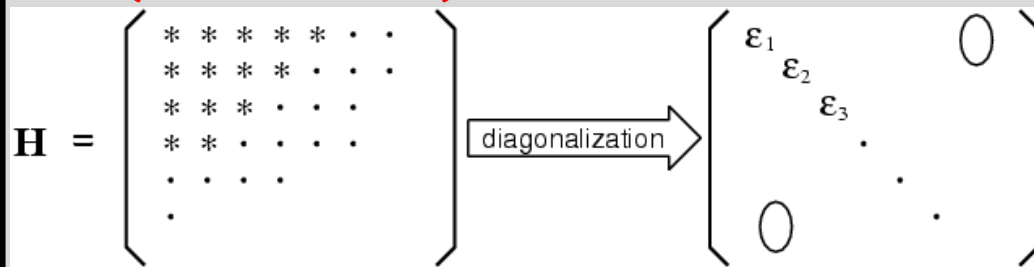


This model space is wide enough to discuss how **magic numbers 28, 50** and **semi-magic number 40** are retained/broken

Our effective interaction consists of microscopic and empirical interactions

Monte Carlo shell model (MCSM)

More than 10^{15} (in our model space)



Conventional Shell Model
all Slater determinants

Direct diagonalization is impossible in large model space

about 100



Monte Carlo Shell Model
bases important for a specific eigenstate

In MCSM, we diagonalize small Hamiltonian matrix constructed from **MCSM bases**

T. Otsuka *et al.* PPNP47, 319 (2001)

$$|\Psi_N\rangle = \sum_{n=1}^N \sum_{K=-J}^J f_{n,K}^{(N)} P_{MK}^{J\pi} |\psi_n\rangle$$

eigenstate

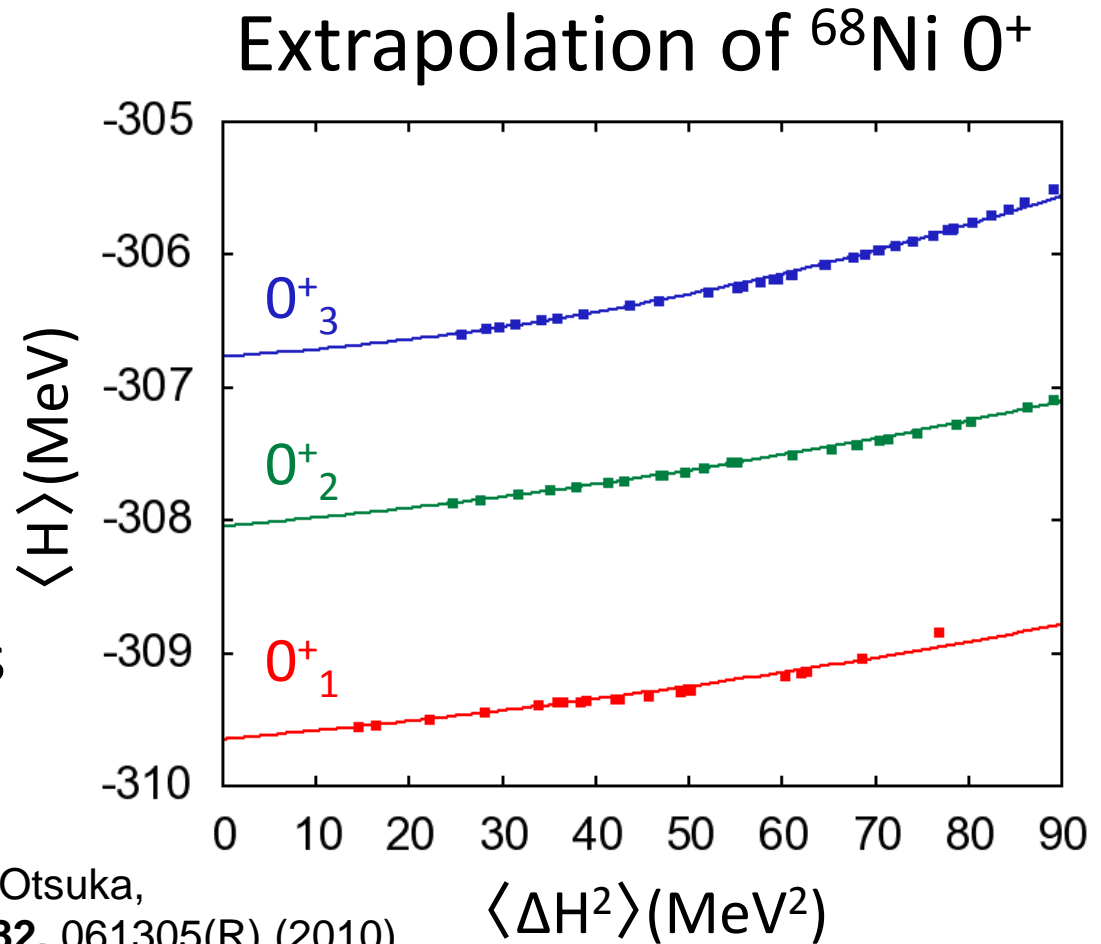
angular-momentum,
parity projection

Generated to minimize eigenenergies using quantum MC + variational method

Slater determinant

Energy-variance extrapolation

- Second-order extrapolation using energy variance
 $\langle \Delta H^2 \rangle = \langle H^2 \rangle - \langle H \rangle^2$
- Points are calculated with each number of bases



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

Based on T. Mizusaki and M. Imada,
Phys. Rev. C **65**, 064319 (2002); **67**, 041301(R) (2003)

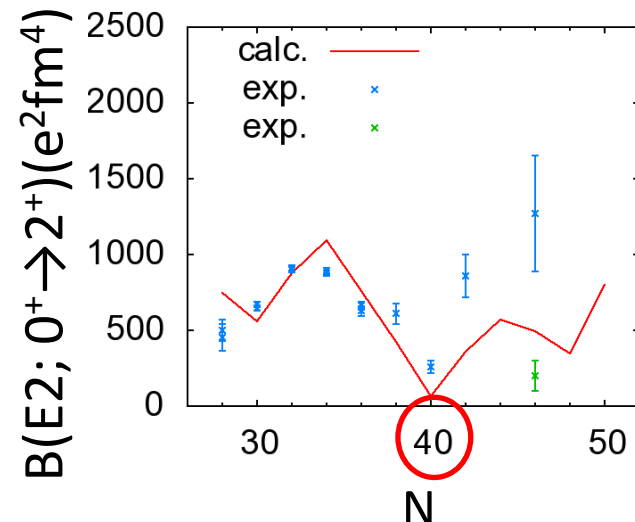
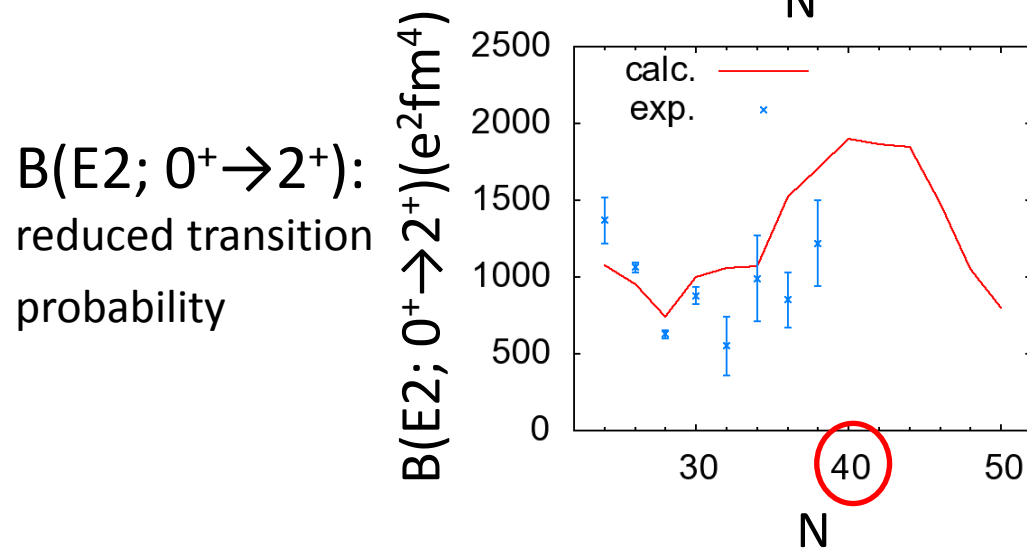
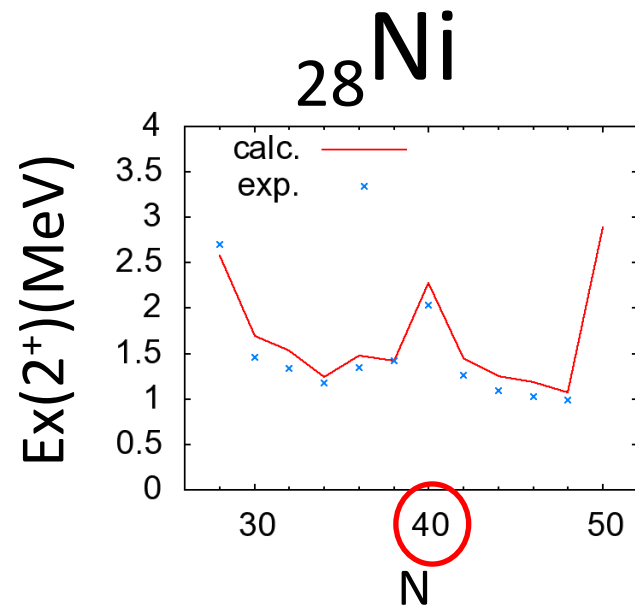
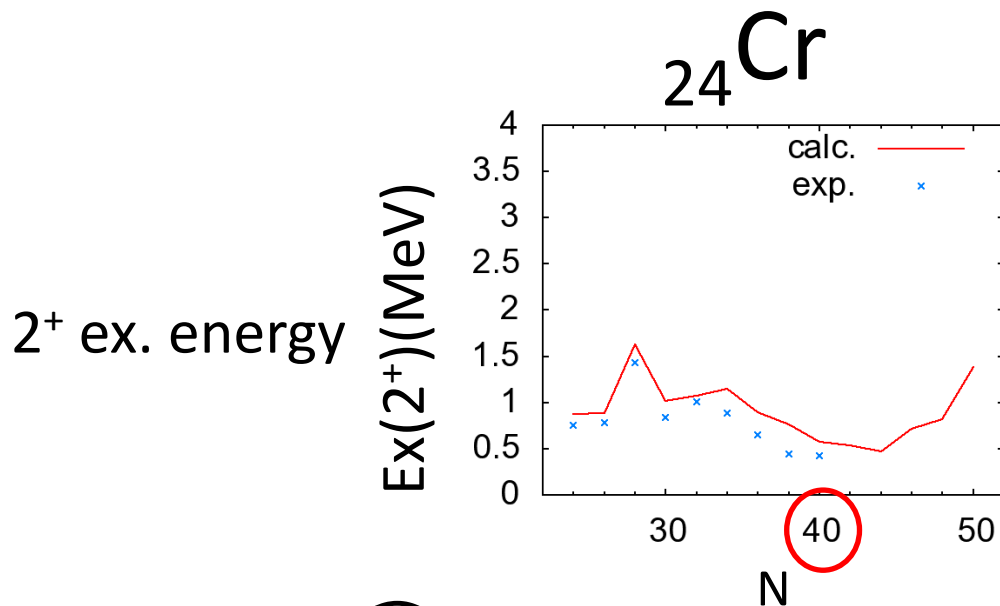
Parallel calculation

- Computational bottleneck is **integration over 3D rotations** to restore the angular momentum
⇒ # of total mesh points $\sim 50,000$
- Calculated parallelly for each mesh point
- Calculated on **K computer** (AICS),
FX10 (U. Tokyo),
and T2K Open Supercomputer
(U. Tokyo, U. Tsukuba)
- 14 hours, 7680 CPU cores for $^{68}\text{Ni } 8^+$ (K computer)



K computer

Results of Cr and Ni



- x B. Pritychenko, et al., arXiv:1102.3365v2 (2011)
- x de Angelis, private communication

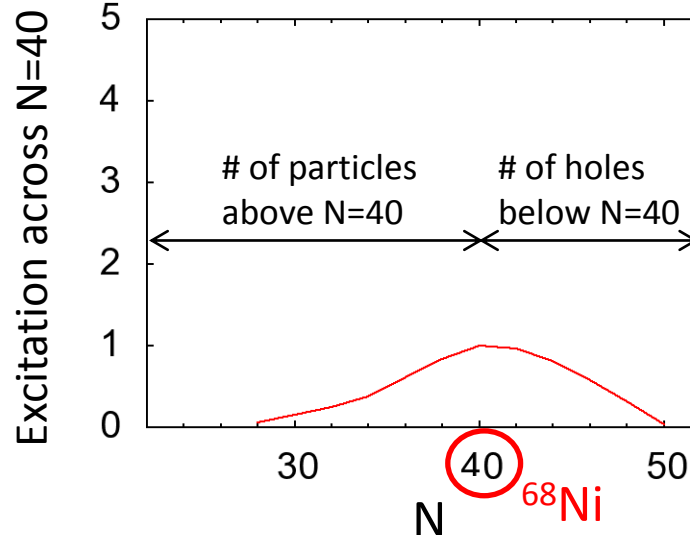
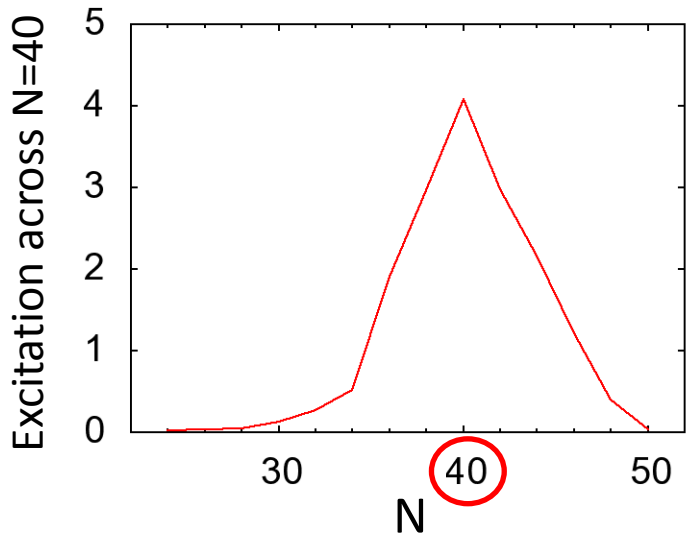
Neutron excitation across N=40 gap

^{24}Cr

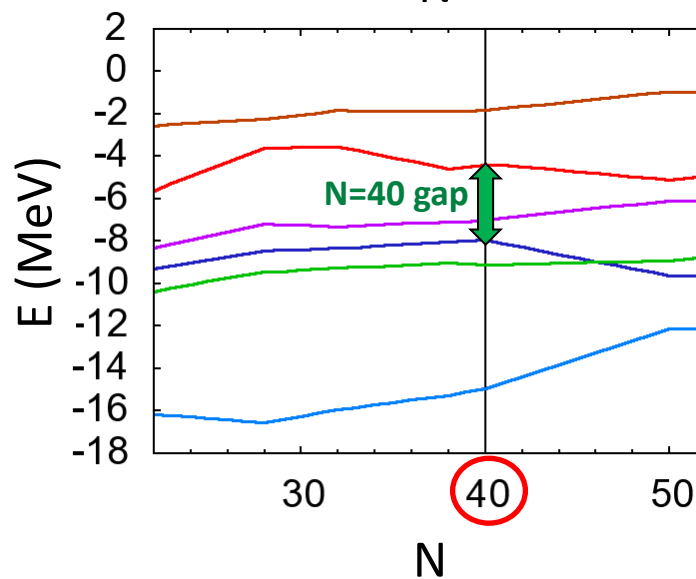
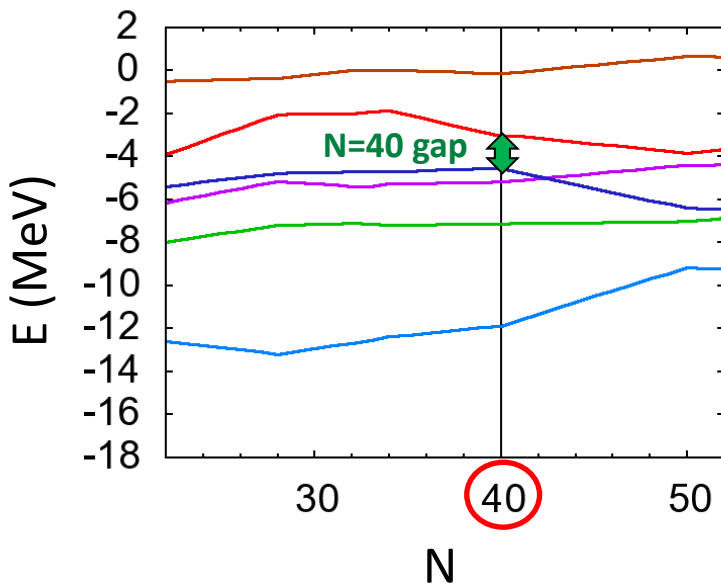
Change of
N=40 magicity

^{28}Ni

of neutrons excited across N=40 (0^+_{11})



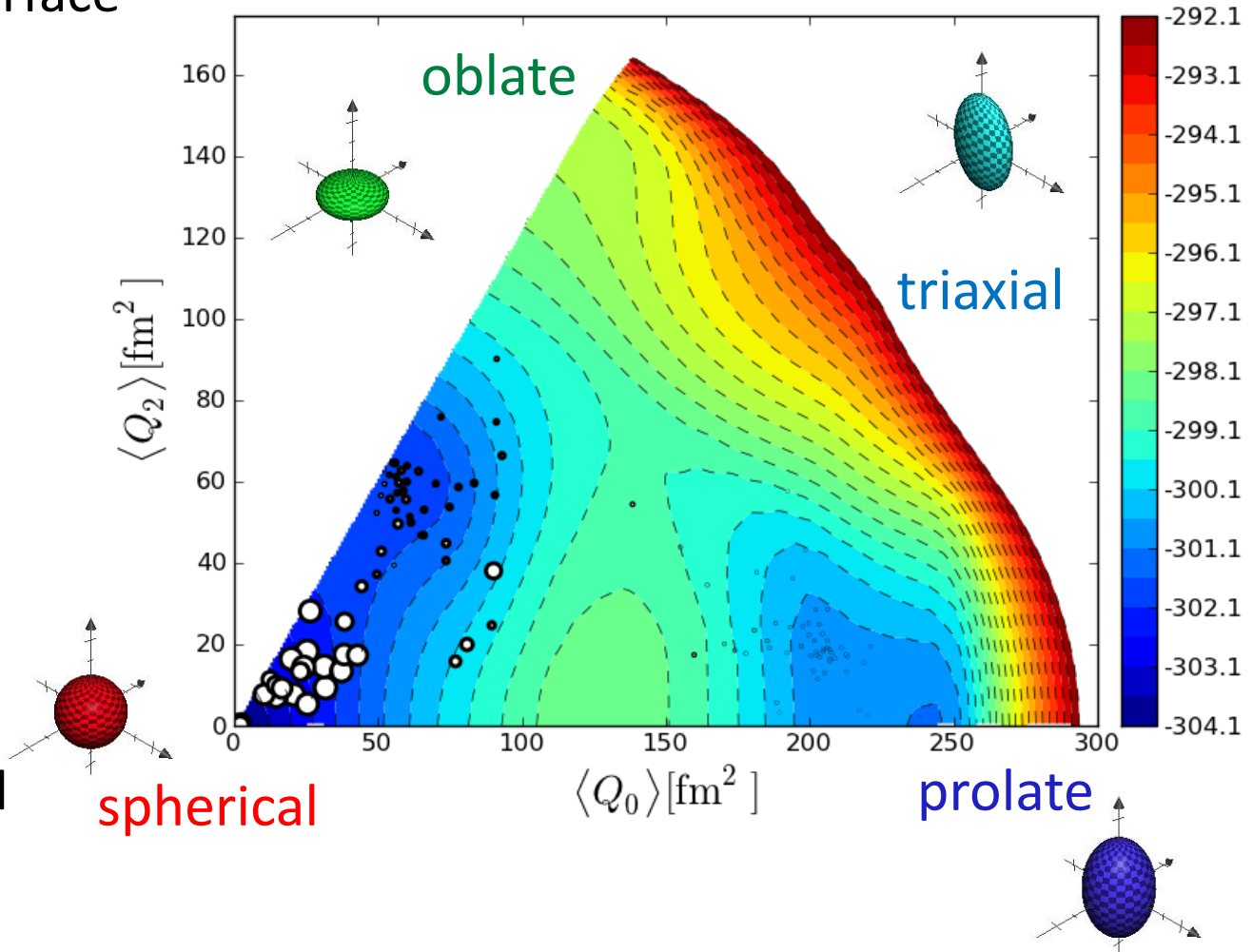
Neutron effective single-particle energy



PES (energy contour plot of various shapes)

0^+_1 state of ^{68}Ni ($Z=28, N=40$)

- Potential energy surface (PES) is calculated by Constrained HF
- **Location of circle:** quadrupole deformation of unprojected MCSM basis
- **Area of circle:** overlap probability between each projected basis and wave function



^{68}Ni 0^+ states \Leftrightarrow different shapes

We diagonalize
the quadrupole moment
to get principal axes

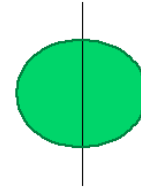
β : deformation parameter

$\beta > 0$: prolate

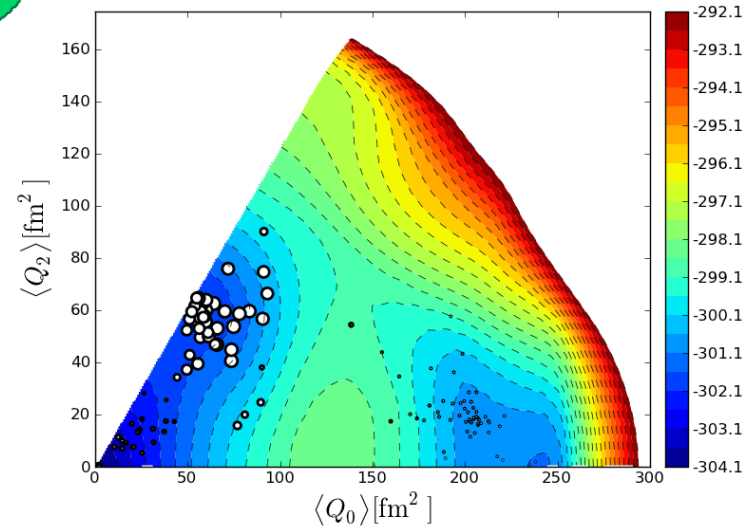
$\beta = 0$: spherical

$\beta < 0$: oblate

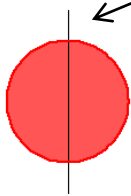
Shape
coexistence



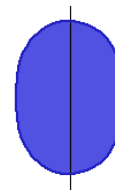
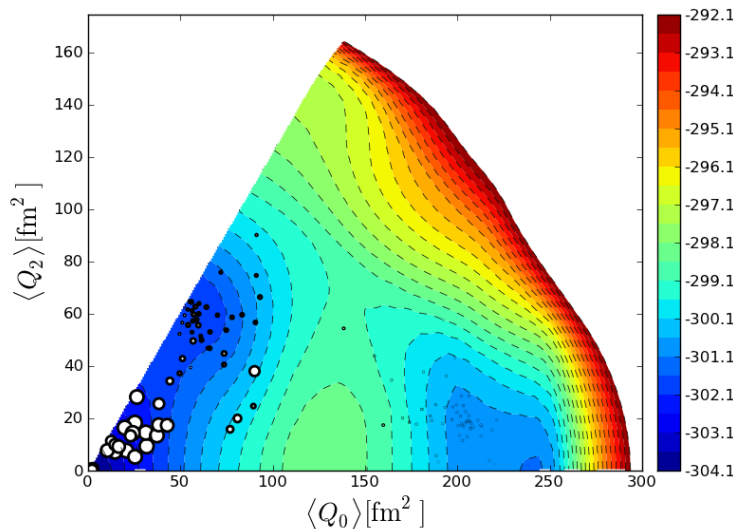
0^+_2 : oblate $\beta \sim -0.2$



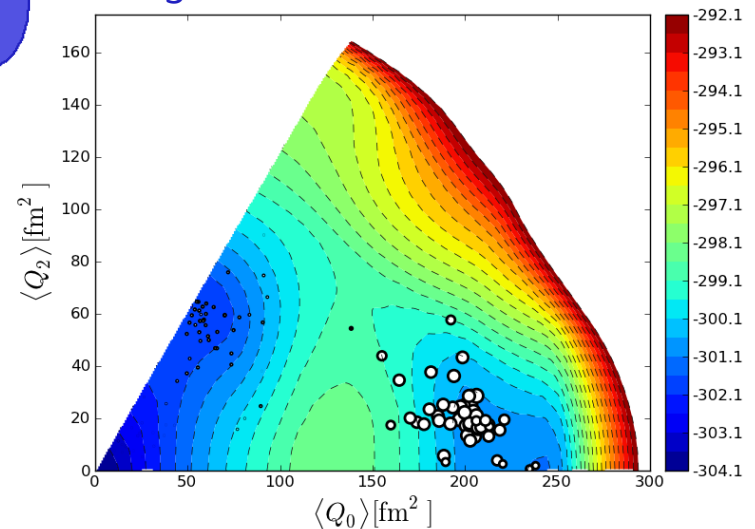
symmetry axis



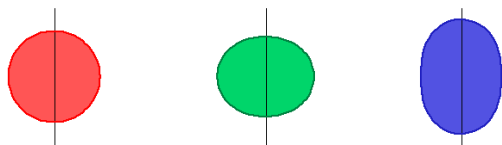
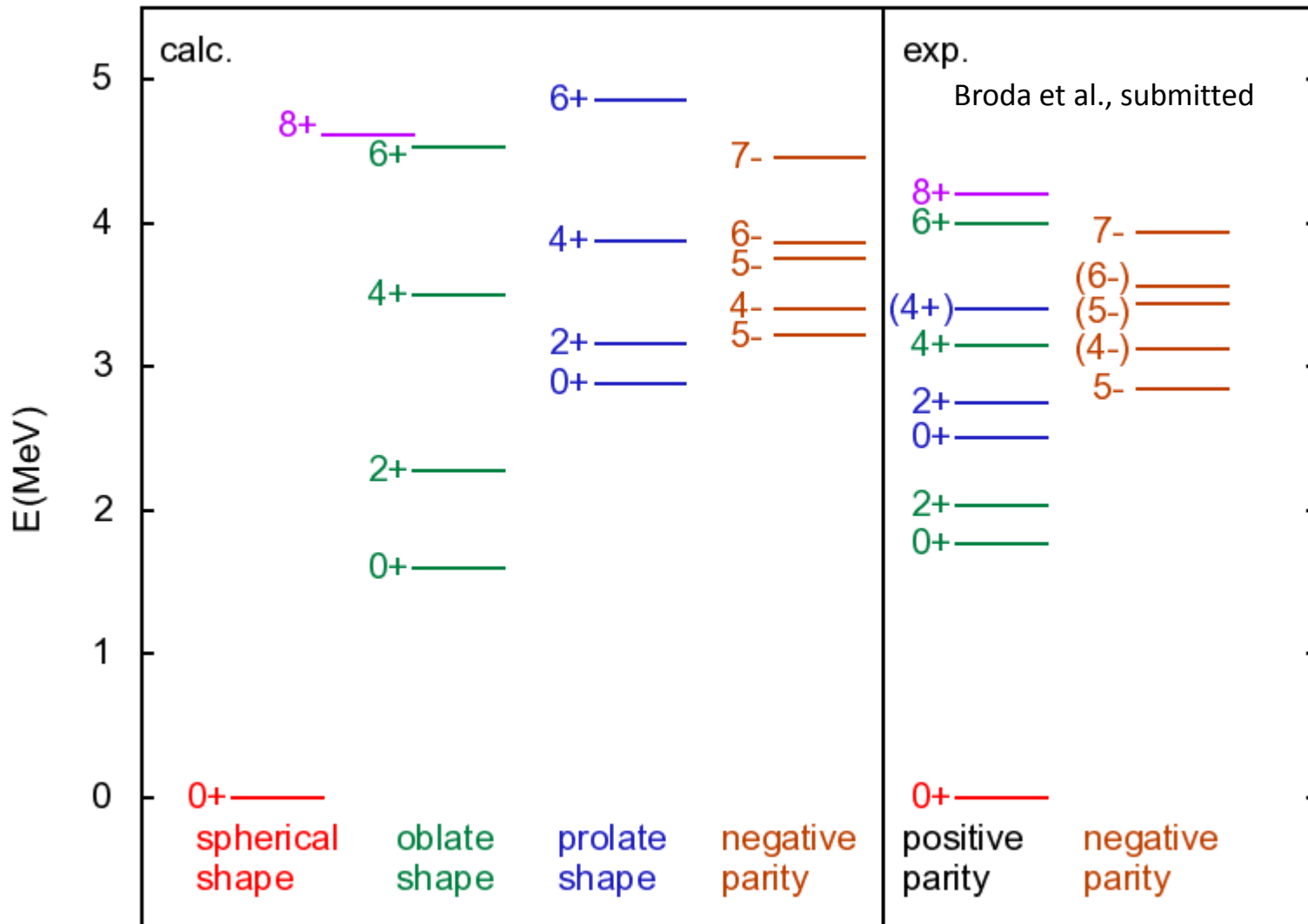
0^+_1 : spherical $\beta \sim 0$



0^+_3 : prolate $\beta \sim +0.4$



Level scheme of ^{68}Ni



Colors are determined from the calculation

Summary

- MCSM calculations for Cr, Ni nuclei in pfg9d5-shell
- Analysis of nuclear shape by using overlap and deformation of MCSM bases

- N=40 magicity changes between Cr and Ni
- Three 0^+ states of ^{68}Ni \leftrightarrow three **different shapes** within 3 MeV (shape coexistence)
- Calculated excitation energies of ^{68}Ni agree with experiments

↳ Unified description by using the same Hamiltonian due to large-scale calculation