Nuclear deformations and radial structure in the nuclear shell model

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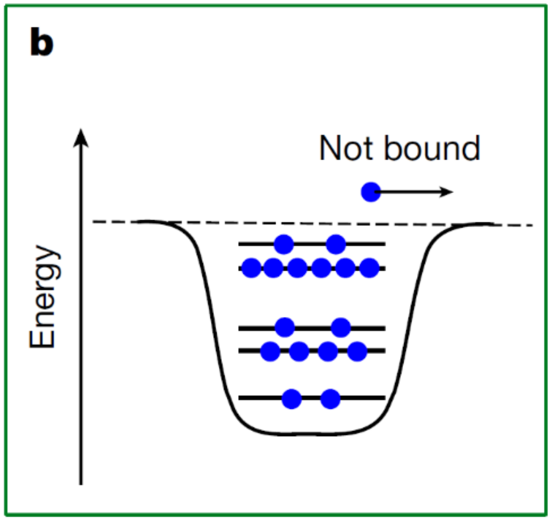
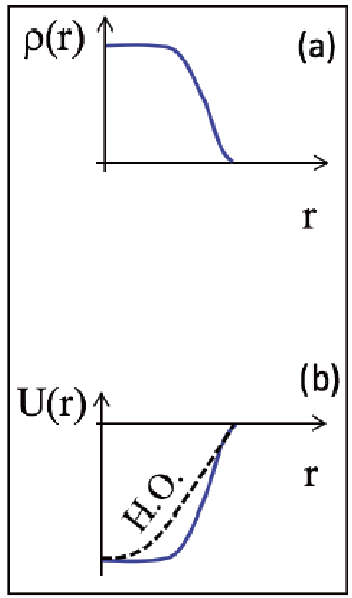
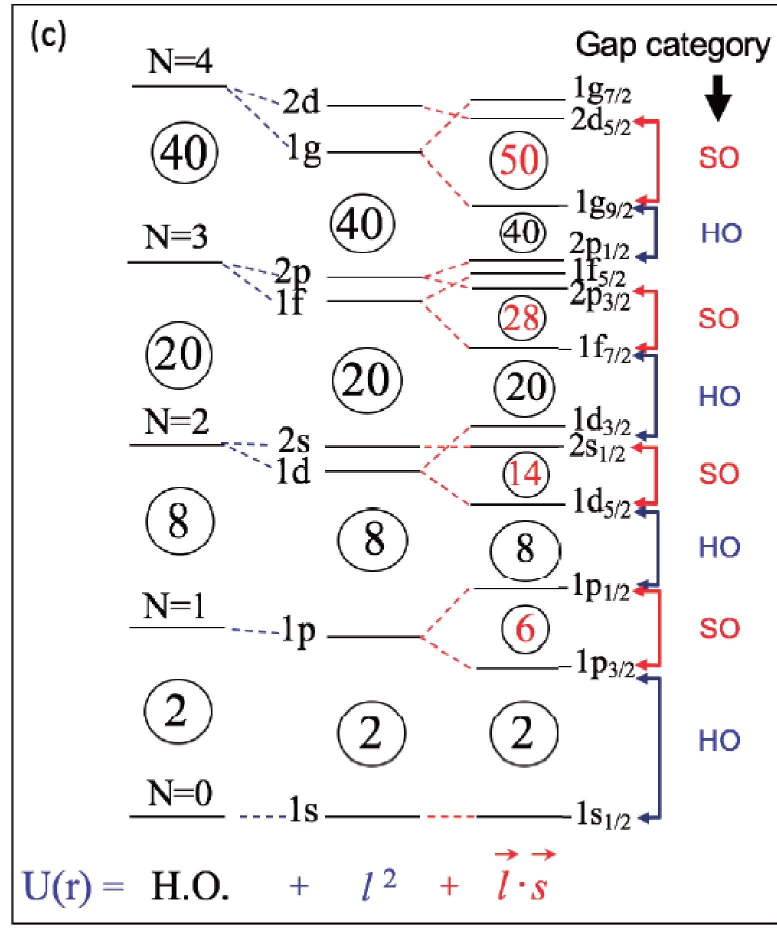
Shell model







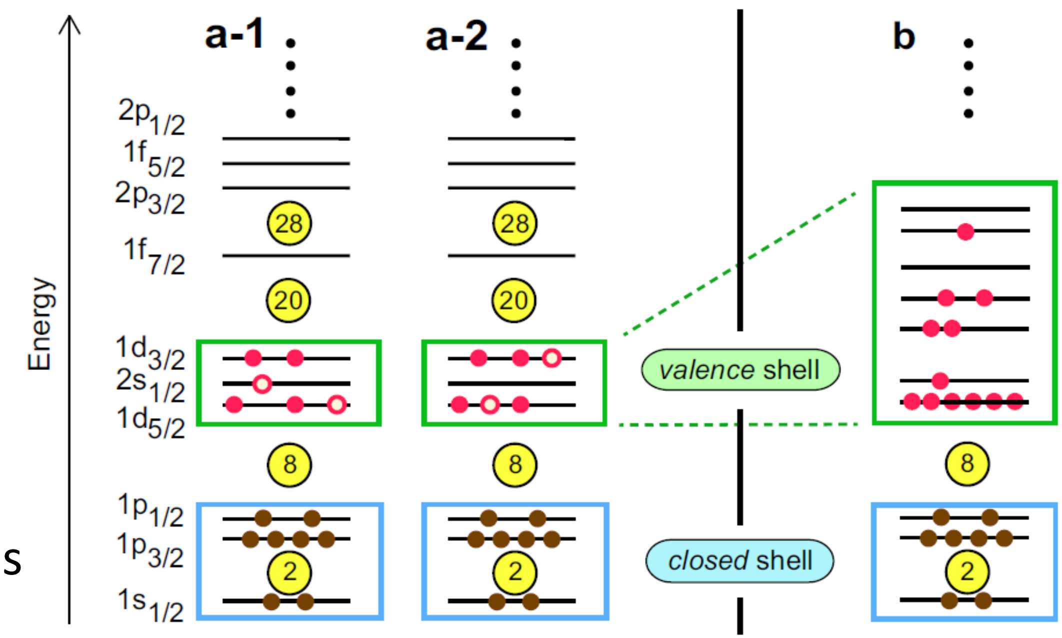
- Nucleons are in a mean potential produced by other nucleons
- Single-particle orbits make shell structure and magic numbers appear

Shell model calculation

- We consider many configurations of nucleons in the valence shell (model space)
- We represent eigenstates of the effective interaction as a superposition of such configurations

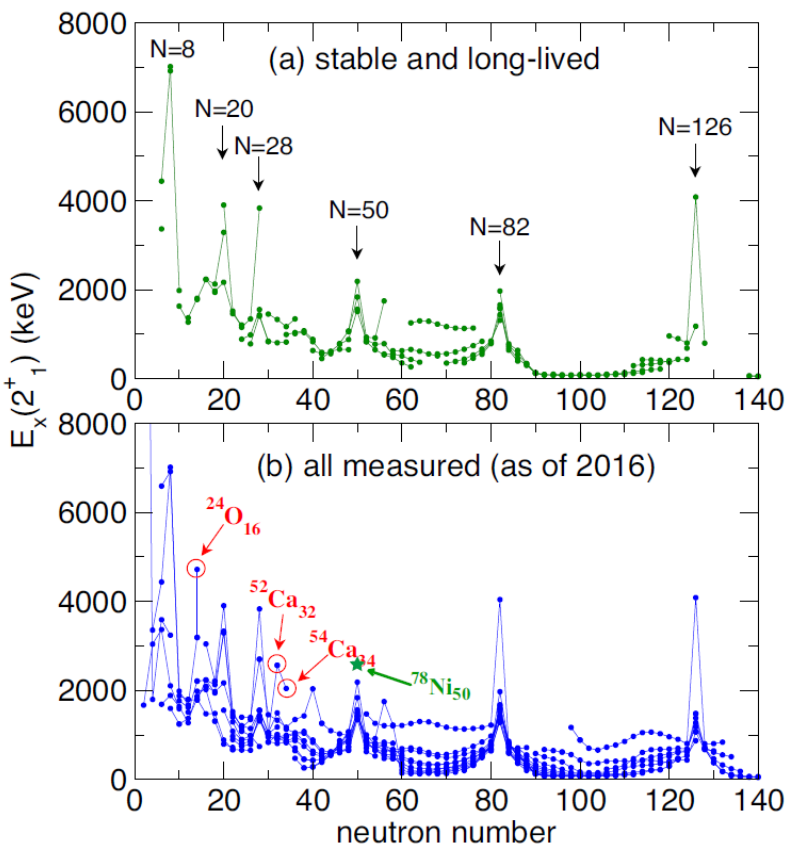
$$H = \sum_i t_i c_i^\dagger c_i + \sum_{i<j,k<l} v_{ijkl} c_i^\dagger c_j^\dagger c_l c_k$$

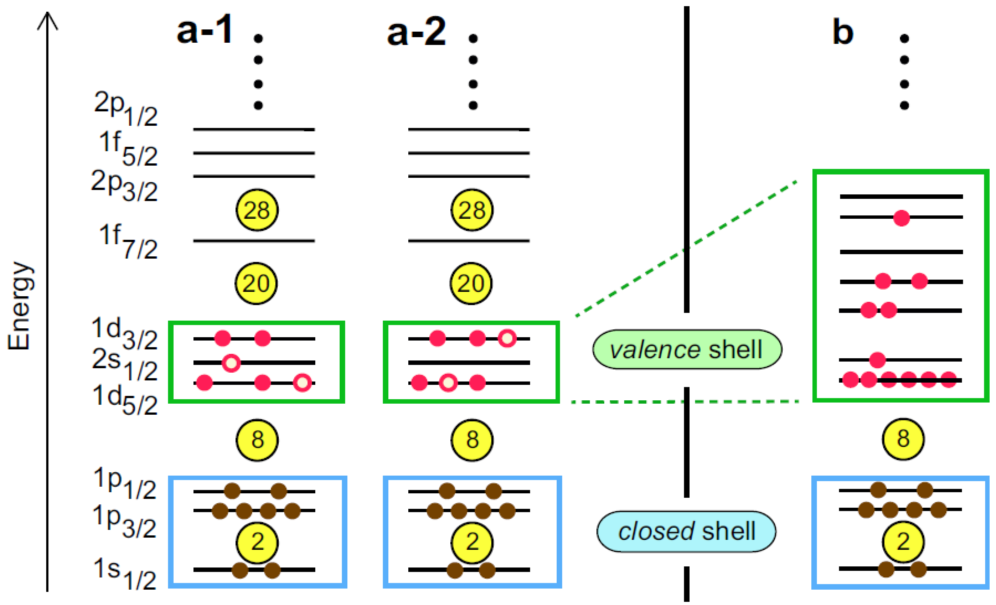
- Effective interaction is important to describe nuclear properties
- Effective interactions are derived microscopically or phenomenologically
- Several shell-model calculation codes are available and non-experts can perform calculation if effective interaction is available and model space is small



Shell evolution: change of shell structure

2+ excitation energy

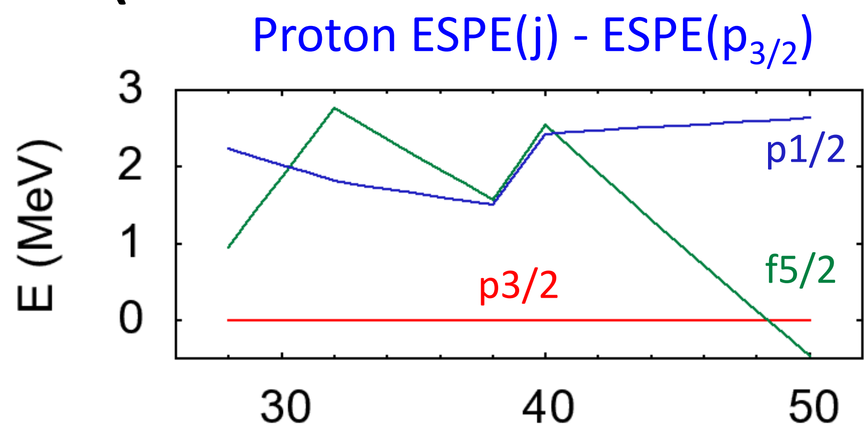


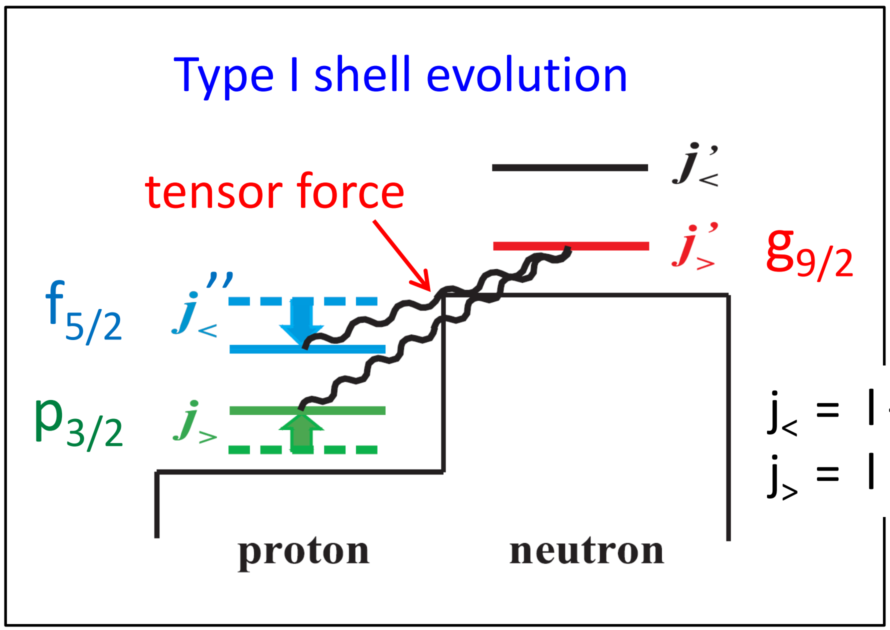


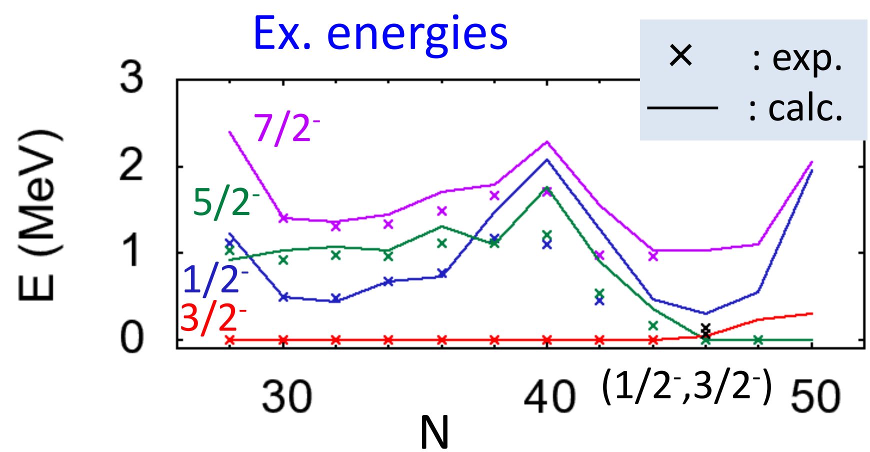
Large valence shell (model space) is needed

Cu isotopes (Z=29)

- proton $p_{3/2}$-$f_{5/2}$ level crossing from N = 40 to N = 50 (type I shell evolution)
- Calculated states show agreement with experiments, although they are not pure single-particle states.

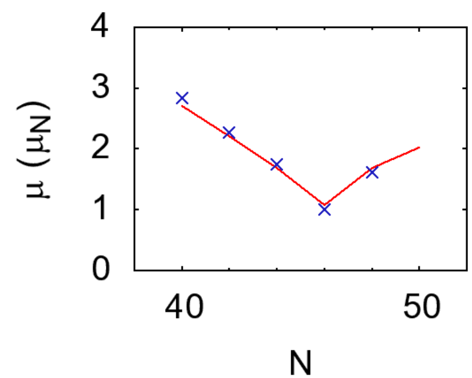




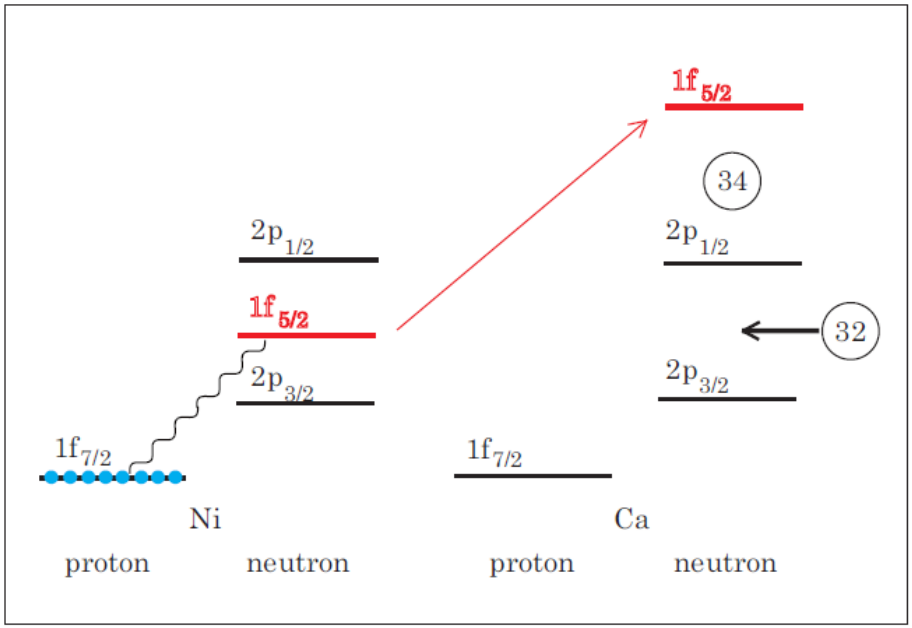


$j_< = l - 1/2$
$j_> = l + 1/2$

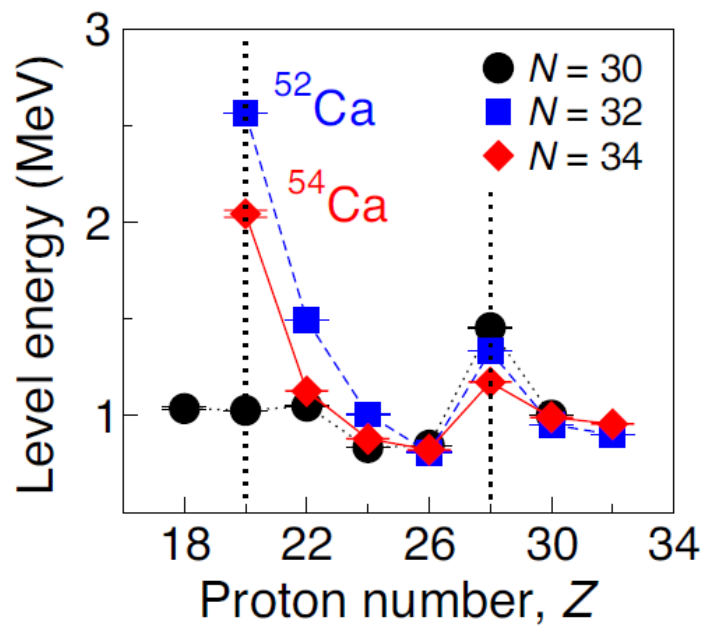
magnetic moments of g.s.



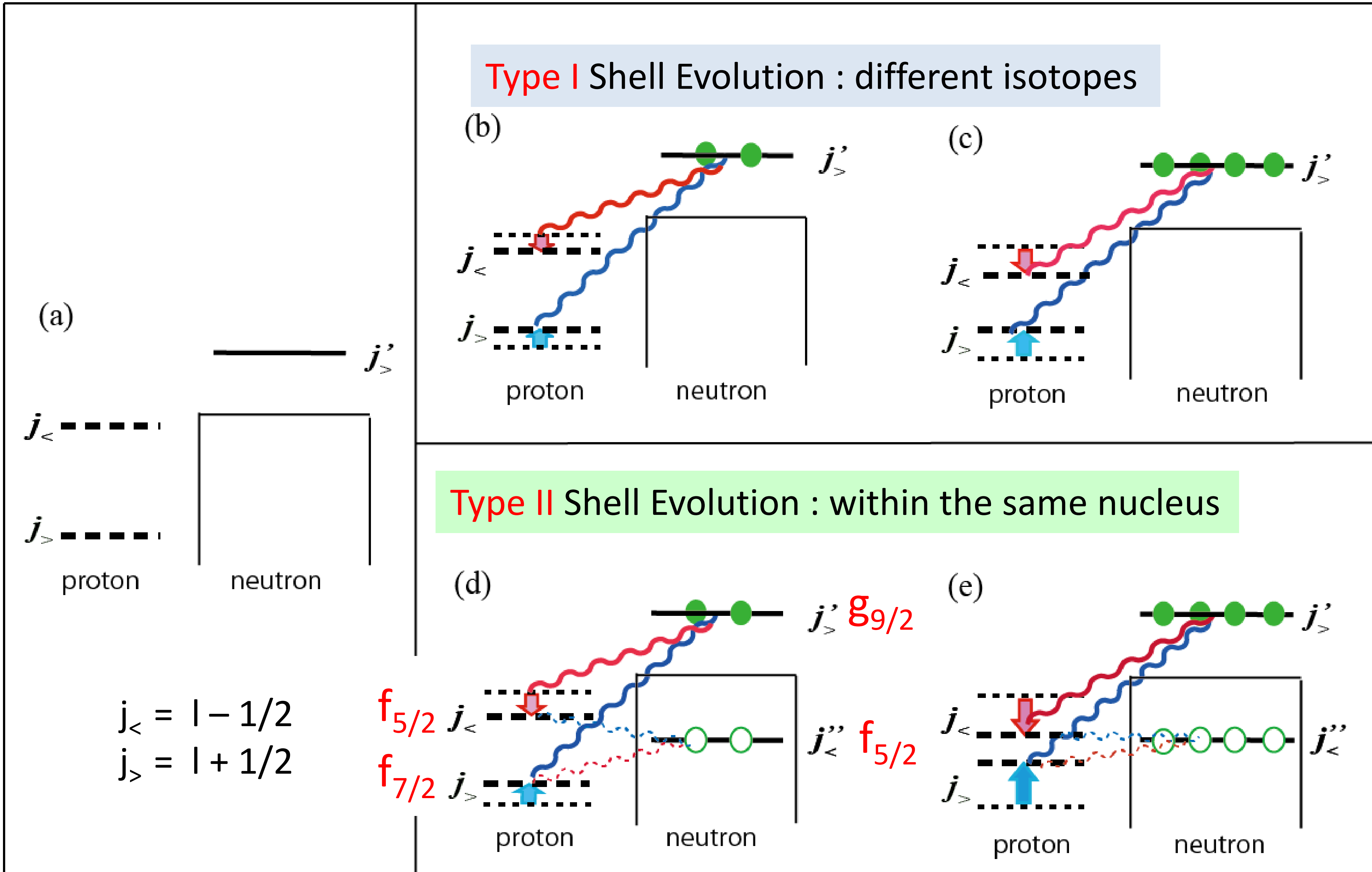
Shell evolution in Ca isotopes



Ex(2+)



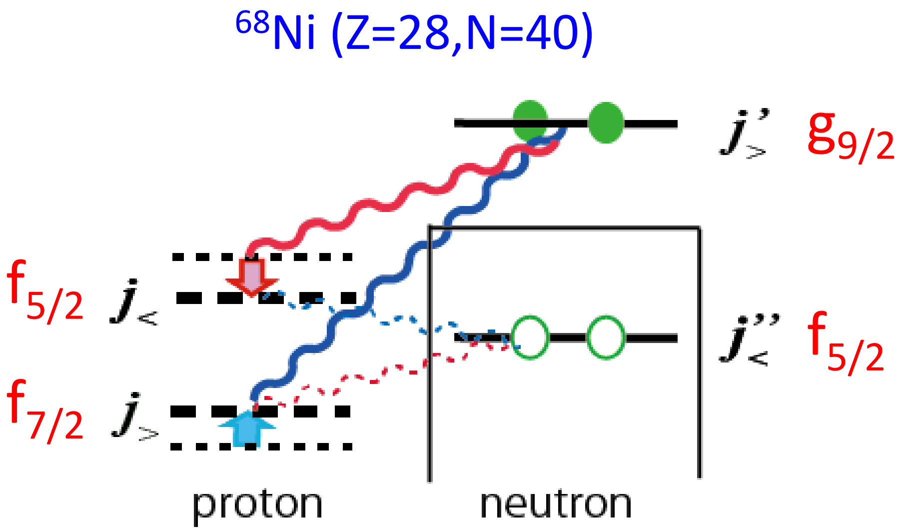
Type I and Type II Shell Evolutions

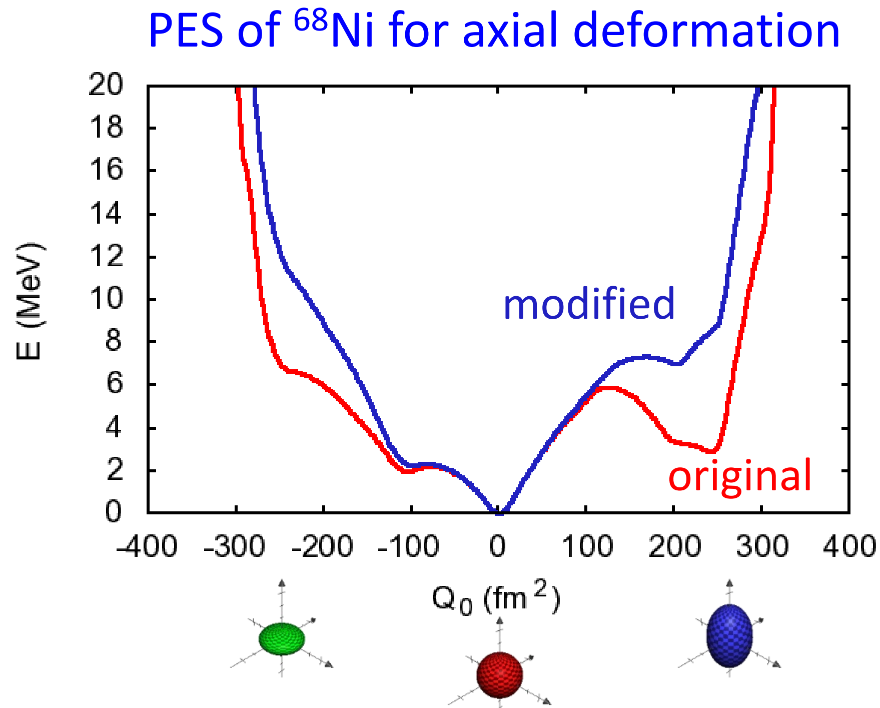


T. Otsuka, YT, J. Phys. G: Nucl. Part. Phys. **43** 024009(2016)

O : holes

Type II Shell Evolution and Shape Coexistence





In original interaction
used for calculations,
type II SE occurs in prolate state.

Many nucleons are excited.

Deformation energy
can be gained easily.

In modified interaction,
monopole interactions are reset
so that Type II SE does not occur.

Prolate state has higher energy.

Shape coexistence is stabilized by type II shell evolution

T. Otsuka, YT, J. Phys. G: Nucl. Part. Phys. **43** 024009(2016)

Monte Carlo shell model (MCSM)

- We want to obtain eigenvalues and eigenstates of a Hamiltonian: $H = \sum_i t_i c_i^\dagger c_i + \sum_{i<j,k<l} v_{ijkl} c_i^\dagger c_j^\dagger c_l c_k$
- Model space (Hilbert space) is finite dimensional but huge (more than 10^{15} in our model spaces)
- Approximated wave function in Monte Carlo shell model (MCSM):

$$\underbrace{|\Psi_N\rangle}_{\text{wave function}} = \sum_{n=1}^{N} \sum_{K=-J}^{J} f_{n,K}^{(N)} \underbrace{P_{MK}^{J\pi}}_{\text{angular-momentum, parity projection}} \underbrace{|\psi_n\rangle}_{\text{Slater determinant}}, \qquad \underbrace{|\psi_n\rangle}_{\text{Slater determinant}} = \prod_k \left(\sum_l D_{lk}^{(n)} \underbrace{c_l^\dagger}_{\text{creation operator}} \right) \underbrace{|-\rangle}_{\text{core}}$$

For efficient angular-momentum projection, see Shimizu and YT, arXiv:2205.04119

Monte Carlo shell model (MCSM)

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

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

Conventional Shell Model
all Slater determinants

Direct diagonalization is infeasible in large model space

about 100

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

Monte Carlo Shell Model
bases important for a specific eigenstate

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

Generated to minimize eigenenergies using quantum MC + variational method

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

eigenstate

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

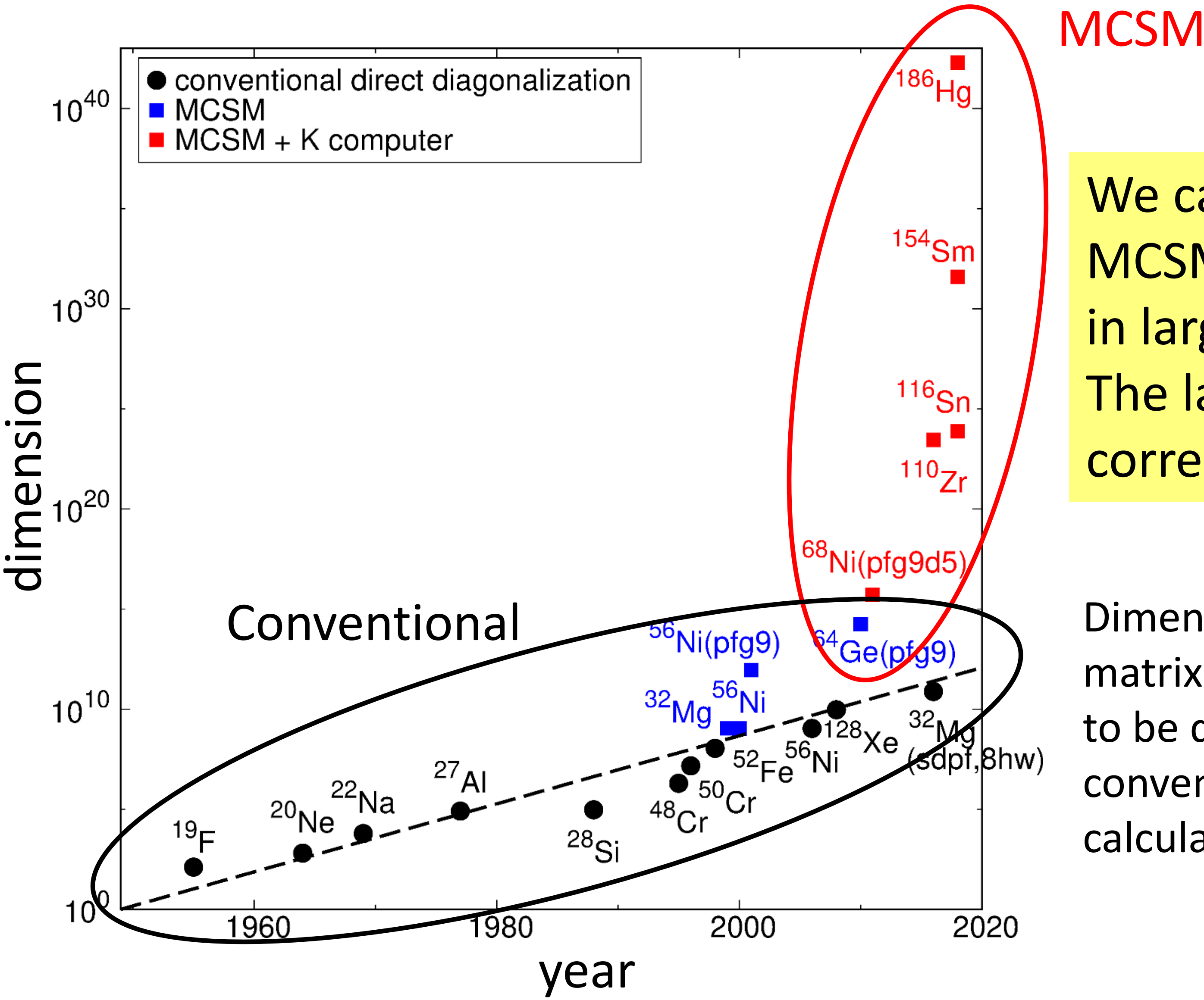
Slater determinant

$$|\psi_n\rangle = \prod_k \left(\sum_l D_{lk}^{(n)} c_l^\dagger \right) |-\rangle$$

angular-momentum, parity projection

We extract information of nuclear shape from MCSM bases

Monte Carlo shell model (MCSM)



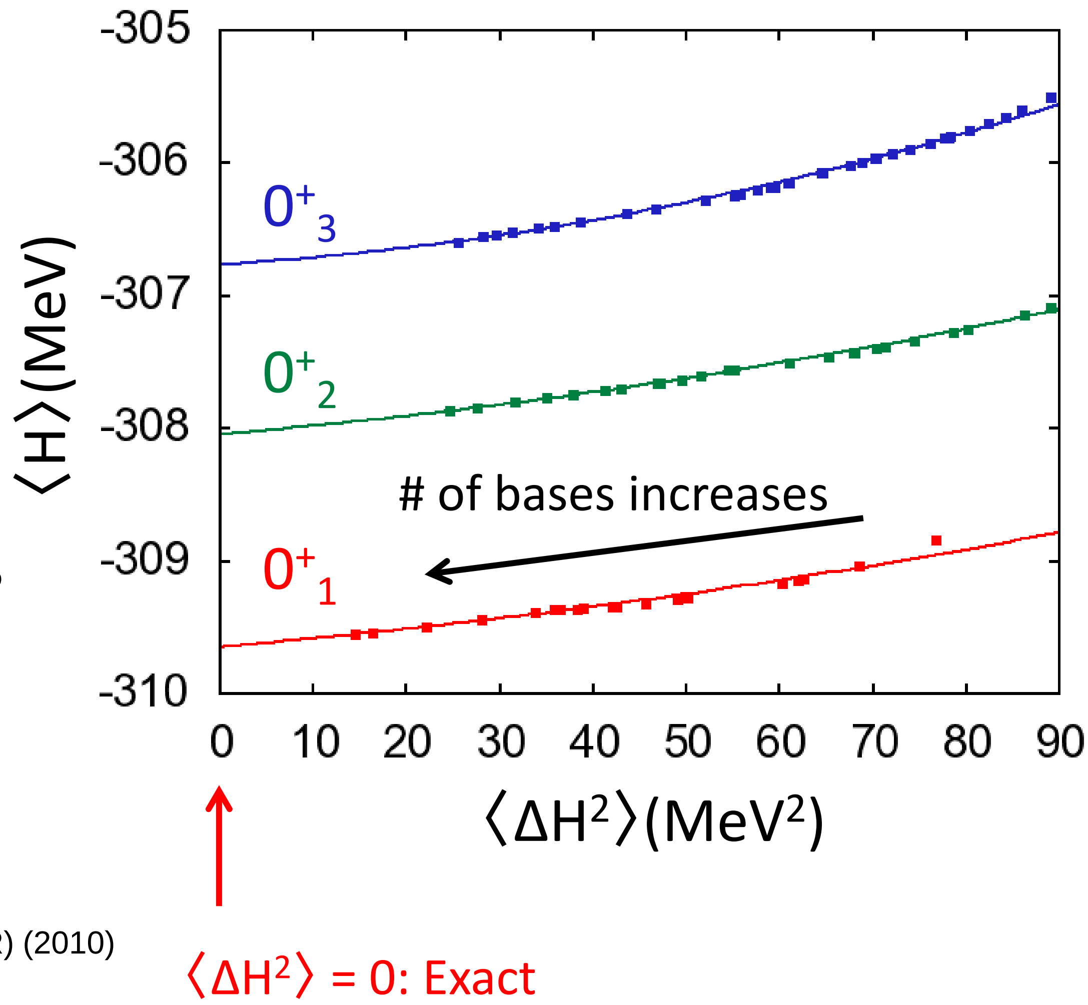
We can perform MCSM calculations in large model spaces. The largest case corresponds to ~10^{42}

Dimension of Hamiltonian matrix for many-body states to be diagonalized in the conventional shell-model calculation

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

Extrapolation of ^{68}Ni 0^+



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

Quadrupole deformation of nuclei

- Quadrupole moments:

$$Q_0 \equiv \sqrt{\frac{16\pi}{5}} r^2 Y_2^0 = 2z^2 - x^2 - y^2,$$

$$Q_2 \equiv \sqrt{\frac{16\pi}{5}} r^2 Y_2^2 = \sqrt{\frac{3}{2}}(x^2 + 2ixy - y^2) = \sqrt{\frac{3}{2}}(x^2 - y^2).$$

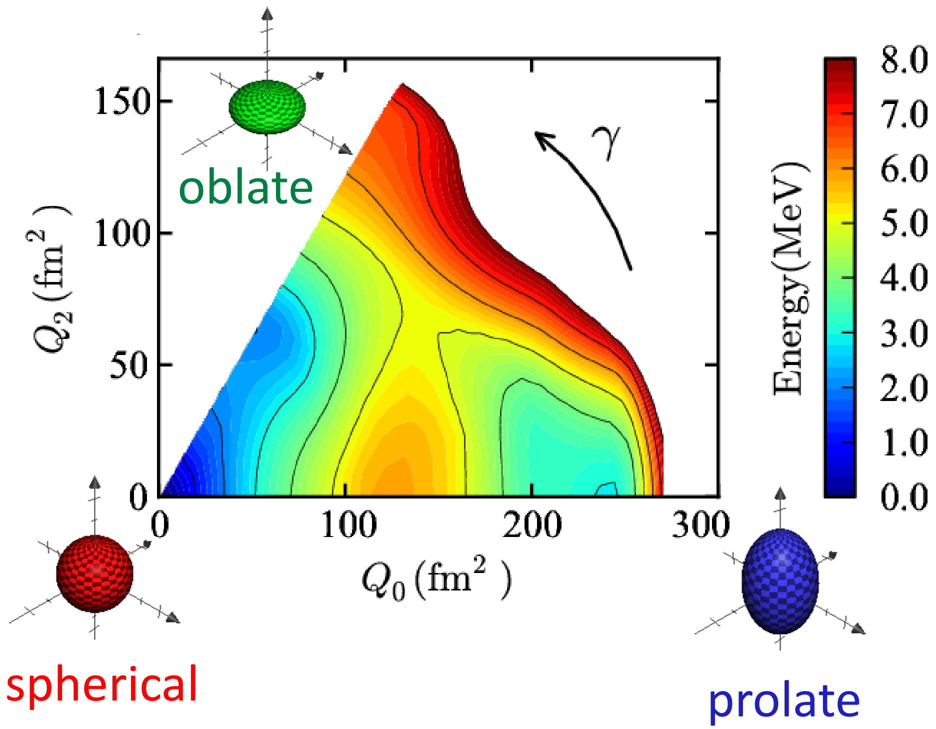
$Q_0 = Q_2 = 0$: spherical

$\gamma = 0^\circ$: prolate

$\gamma = 60^\circ$: oblate

$0^\circ < \gamma < 60^\circ$: triaxial

Potential Energy Surface (PES)



- $\psi(Q_0,Q_2)$ is calculated from Constrained HF
- $E = \langle\psi(Q_0,Q_2)|H|\psi(Q_0,Q_2)\rangle$ is shown in PES

same Hamiltonian of MCSM calculations

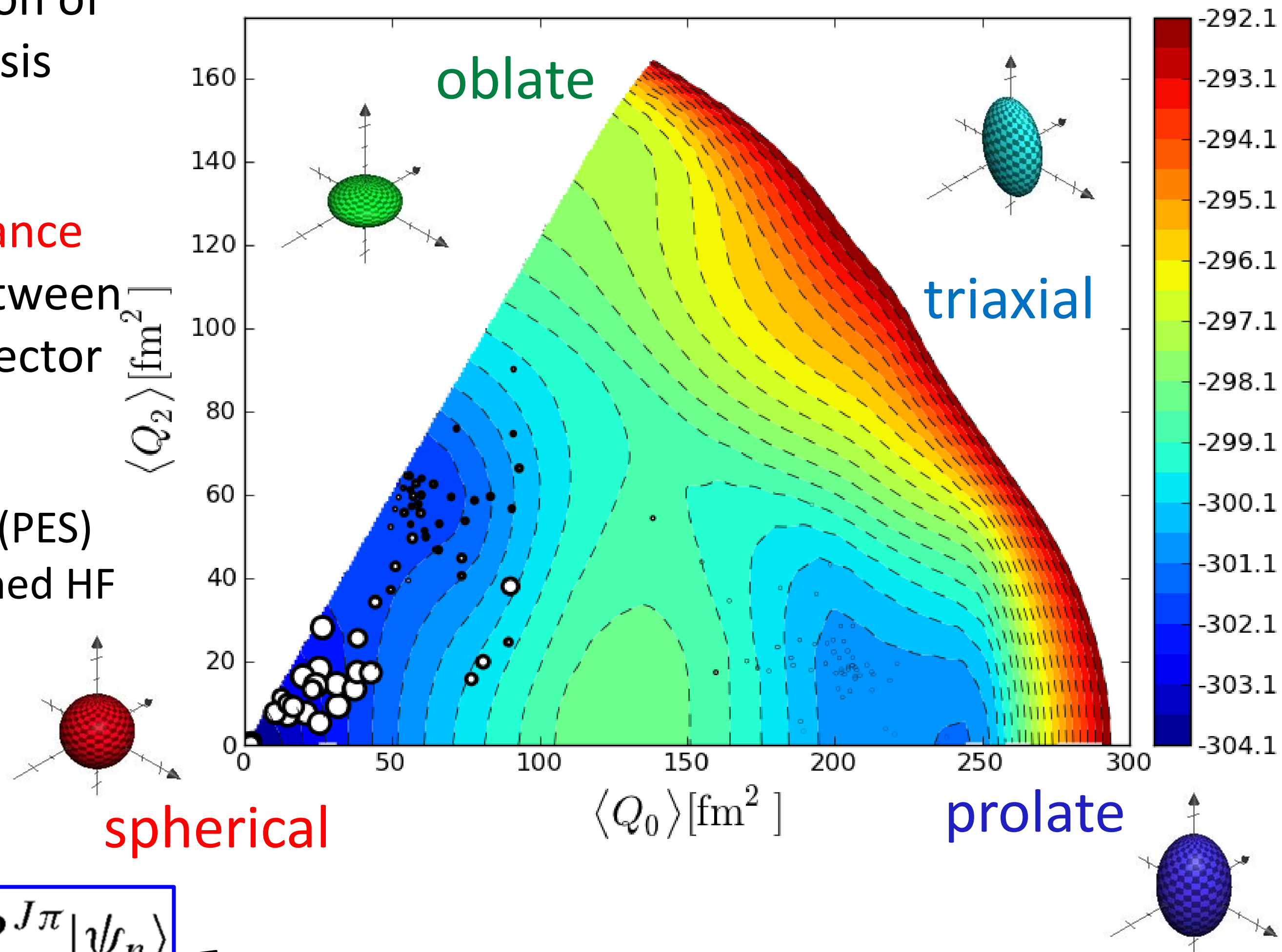
Analysis of nuclear shape in MCSM method (T-plot)

- Location of circle: shape
  quadrupole deformation of unprojected MCSM basis vector

- Area of circle: importance
  overlap probability between each projected basis vector and wave function

- Potential energy surface (PES) is calculated by Constrained HF with same interaction of

‘T-plot’ of 0^+_1 state of ^{68}Ni (Z=28, N=40)



angular-momentum, parity projection

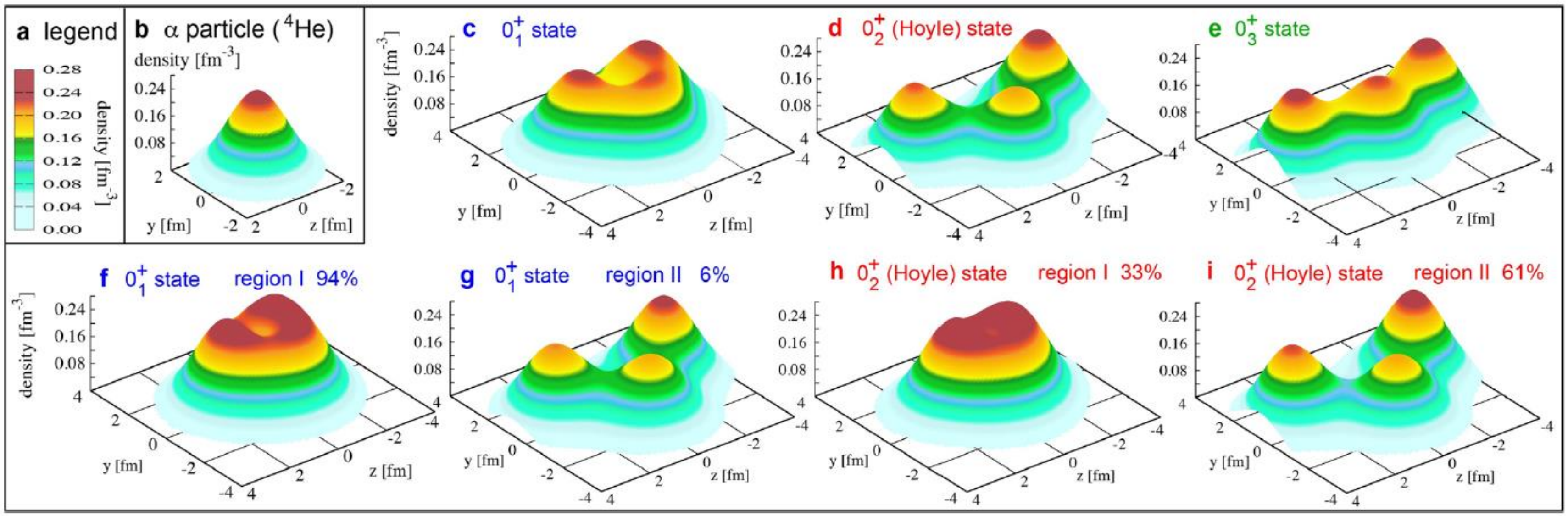
$$\boxed{|\Psi\rangle} = \sum_n f_n \boxed{P^{J\pi}|\psi_n\rangle}$$

Slater determinant

MCSM wave function

MCSM basis vector

Density profile of ^{12}C in no-core MCSM



Otsuka *et al.*, Nat. Commun. **13**, 2234 (2022)

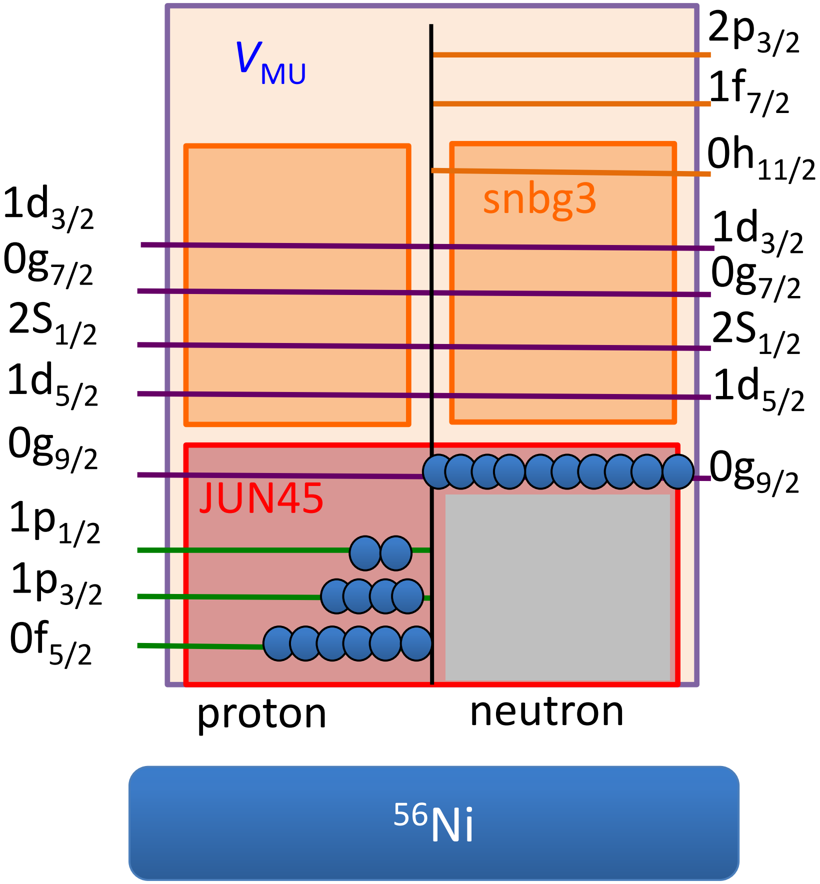
Shapes of Zr isotopes by Monte Carlo Shell Model

- Effective interaction:
  JUN45 + snbg3 + V_{MU}

  known effective interactions

  + minor fit for a part of T=1 TBME's

  Nucleons are excited fully within this model space (no truncation)

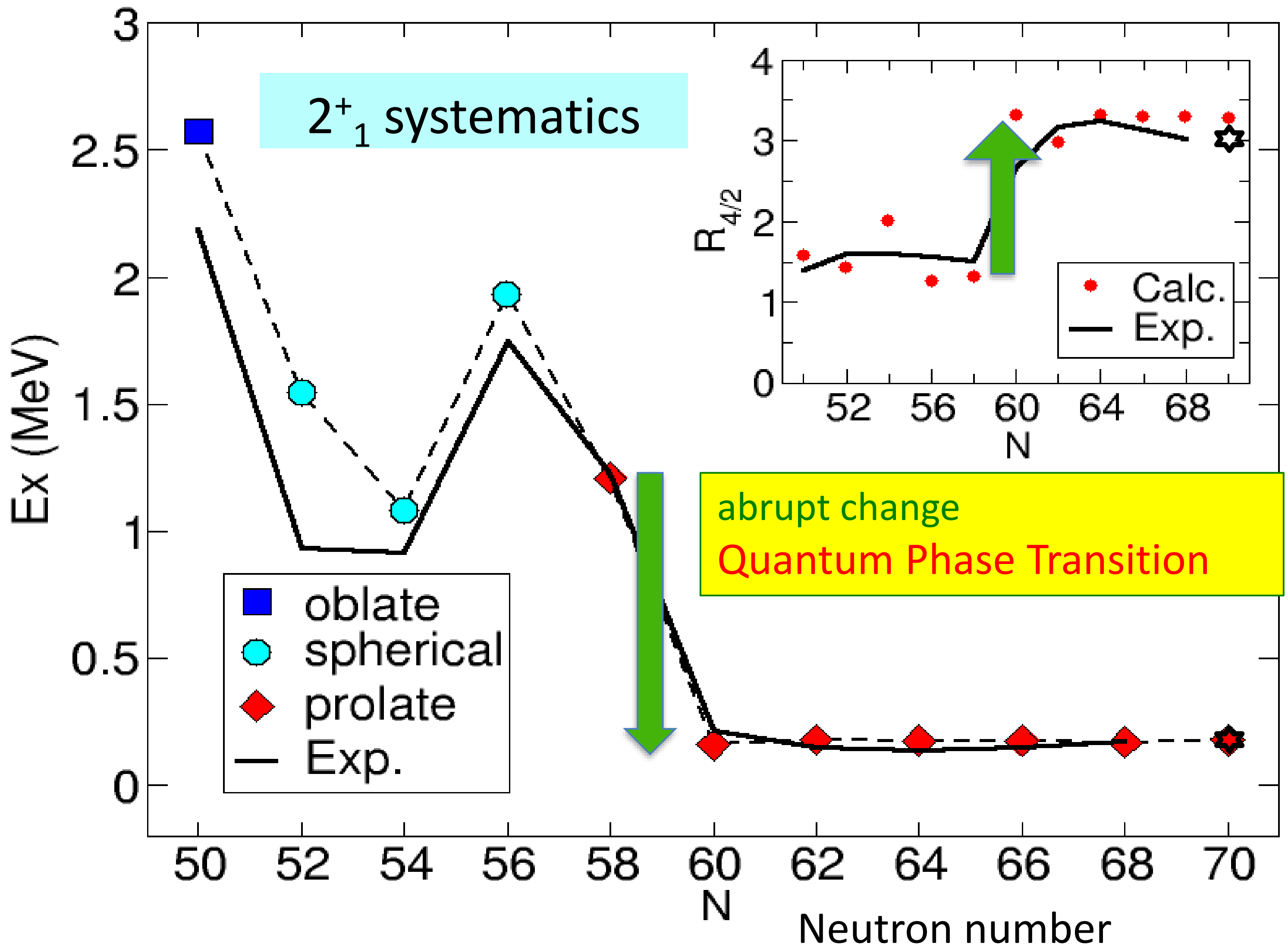


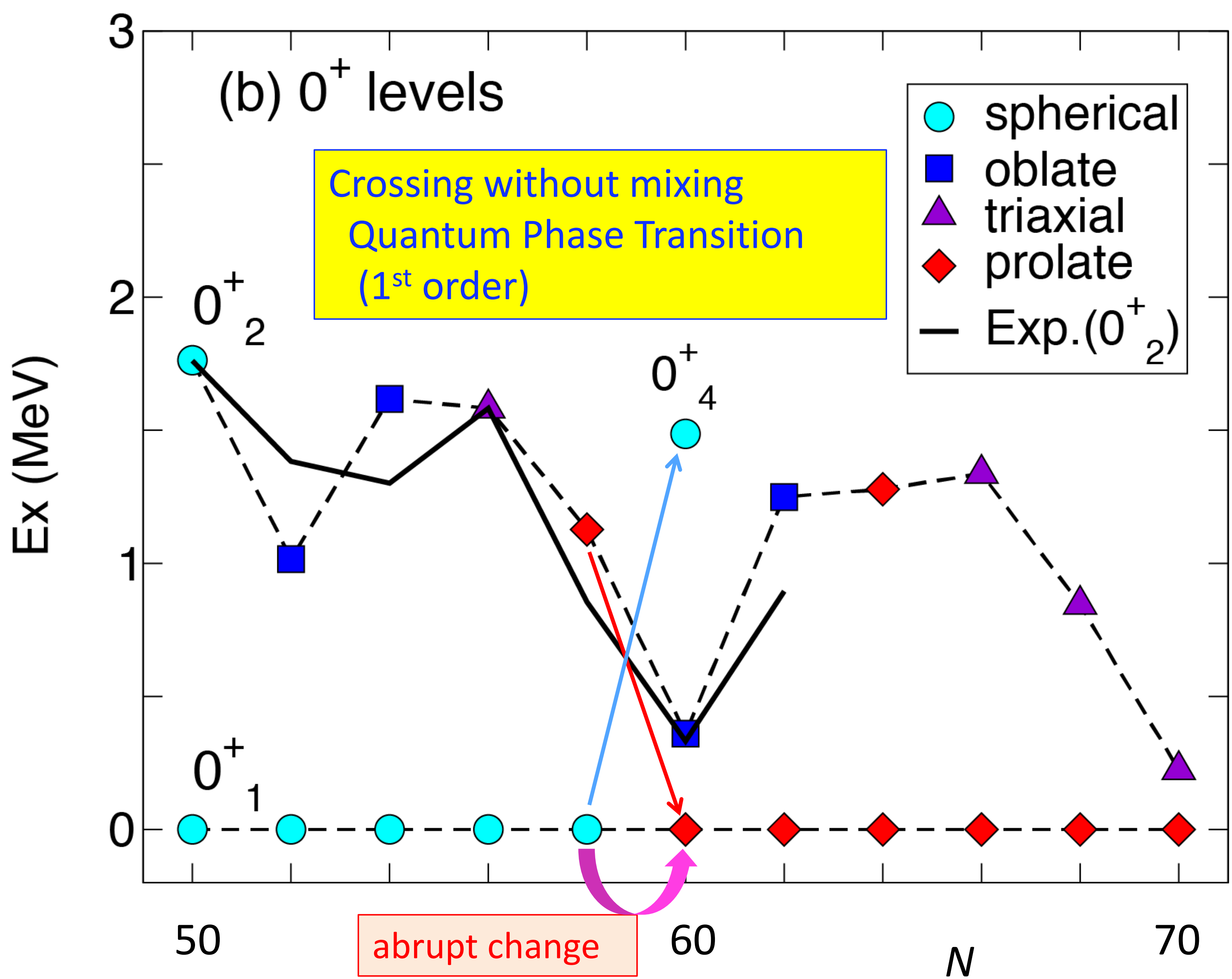
We performed Monte Carlo Shell Model (MCSM) calculations, where the largest case corresponds to the diagonalization of 3.7×10^{23} dimension matrix.

Togashi, YT, Otsuka *et al.*
PRL117, 172502 (2016)

Quantum Phase Transition in the Shape of Zr isotopes

Tomoaki Togashi,[1] Yusuke Tsunoda,[1] Takaharu Otsuka,[1,2,3,4] and Noritaka Shimizu[1]



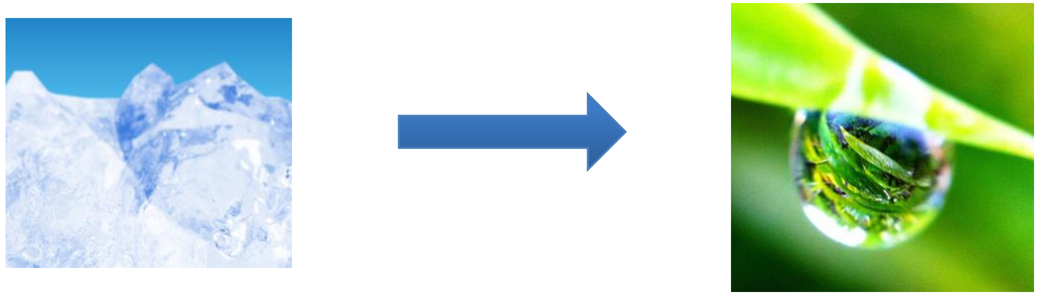

(b) 0+ levels
Crossing without mixing
Quantum Phase Transition
(1st order)
spherical
oblate
triaxial
prolate
Exp.(0+2)
0+2
0+4
0+1
Ex (MeV)
3
2
1
0
50
60
70
N
abrupt change

Can this be a “Phase Transition” ?

Phase Transition :

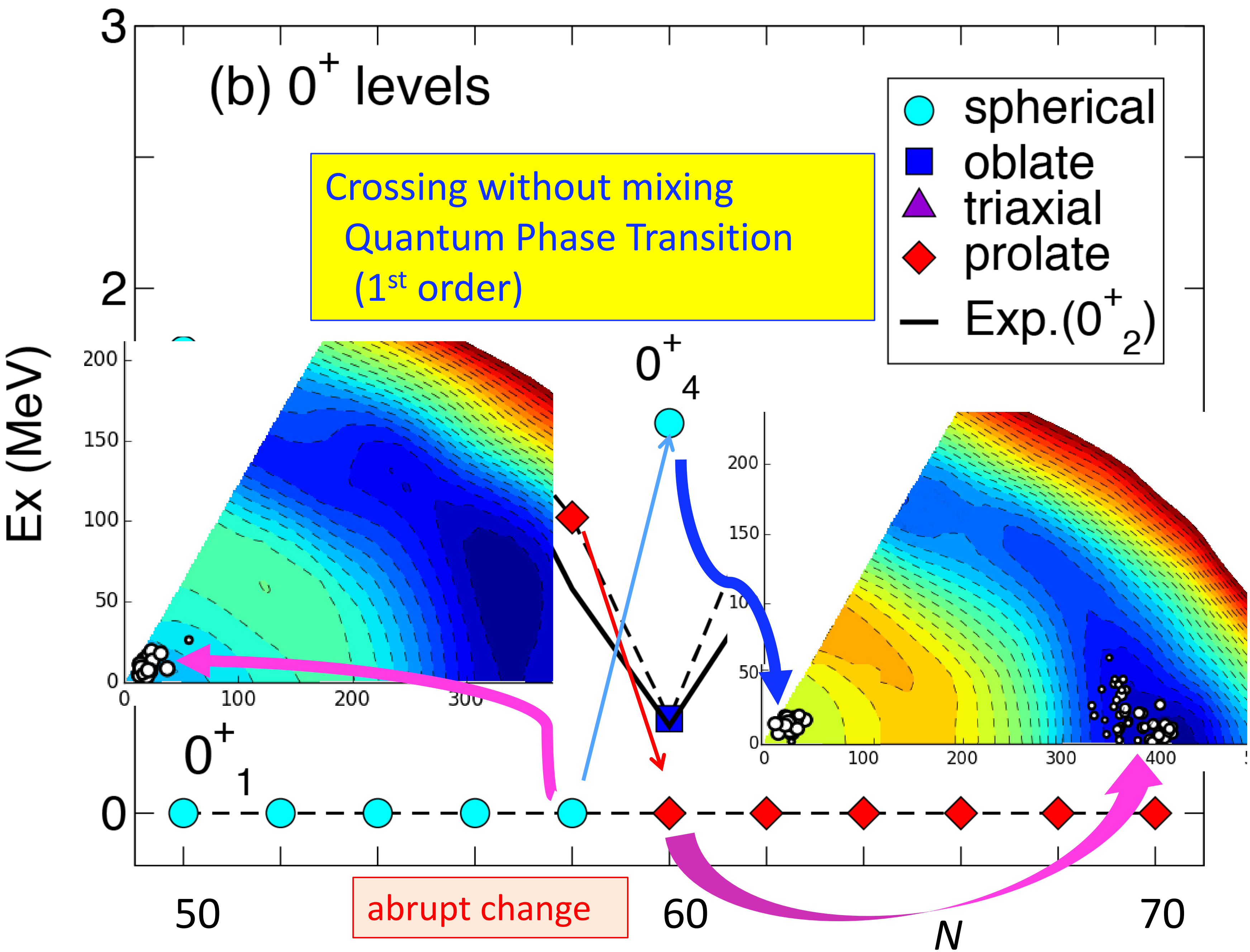
A macroscopic system can change qualitatively from a stable state (*e.g.* ice for H_2O) to another stable state (*e.g.*, water for H_2O) as a function of a certain parameter (*e.g.*, temperature).

The phase transition implies this kind of phenomena of macroscopic systems consisting of almost infinite number of molecules.

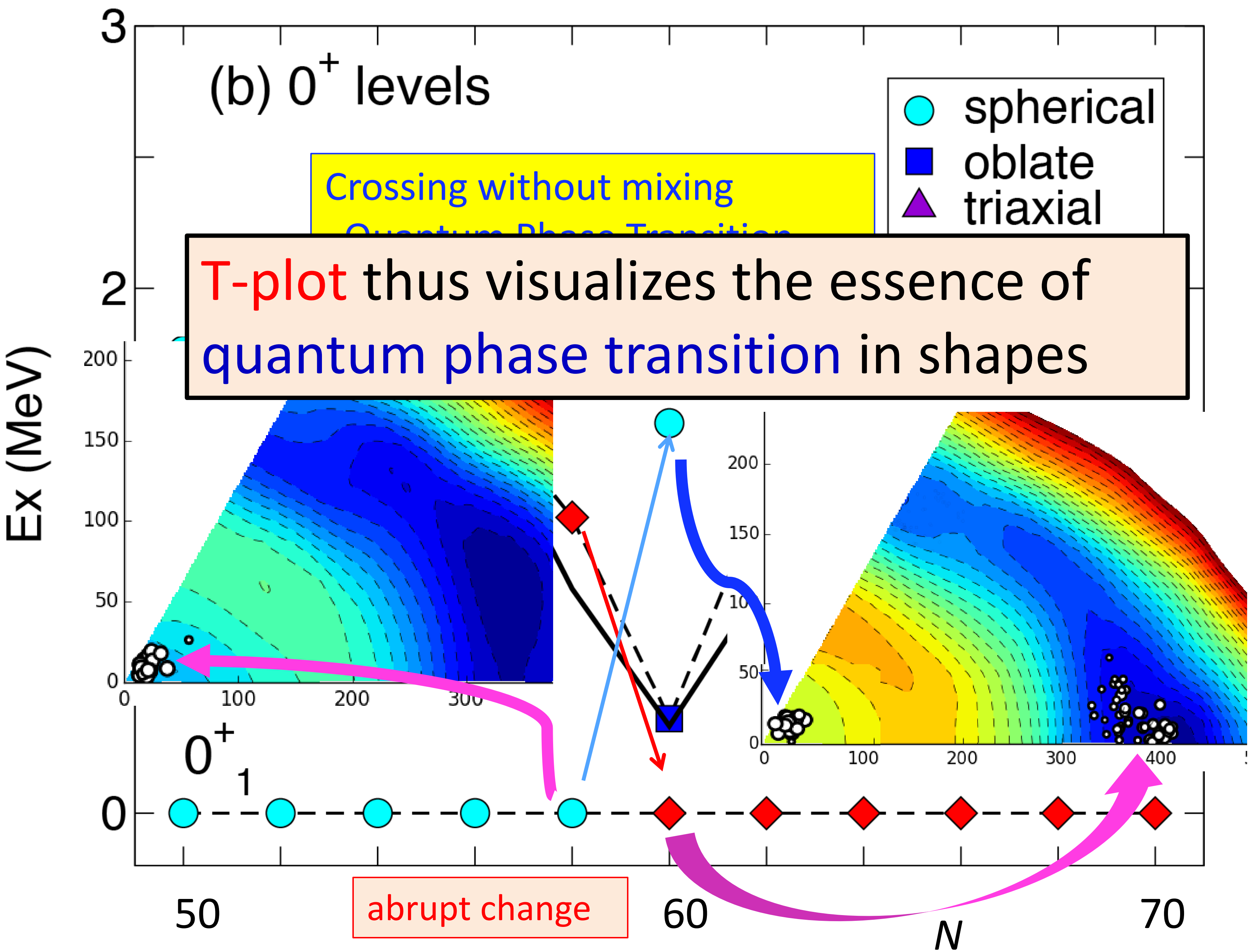


Quantum Phase Transition *(QPT)*

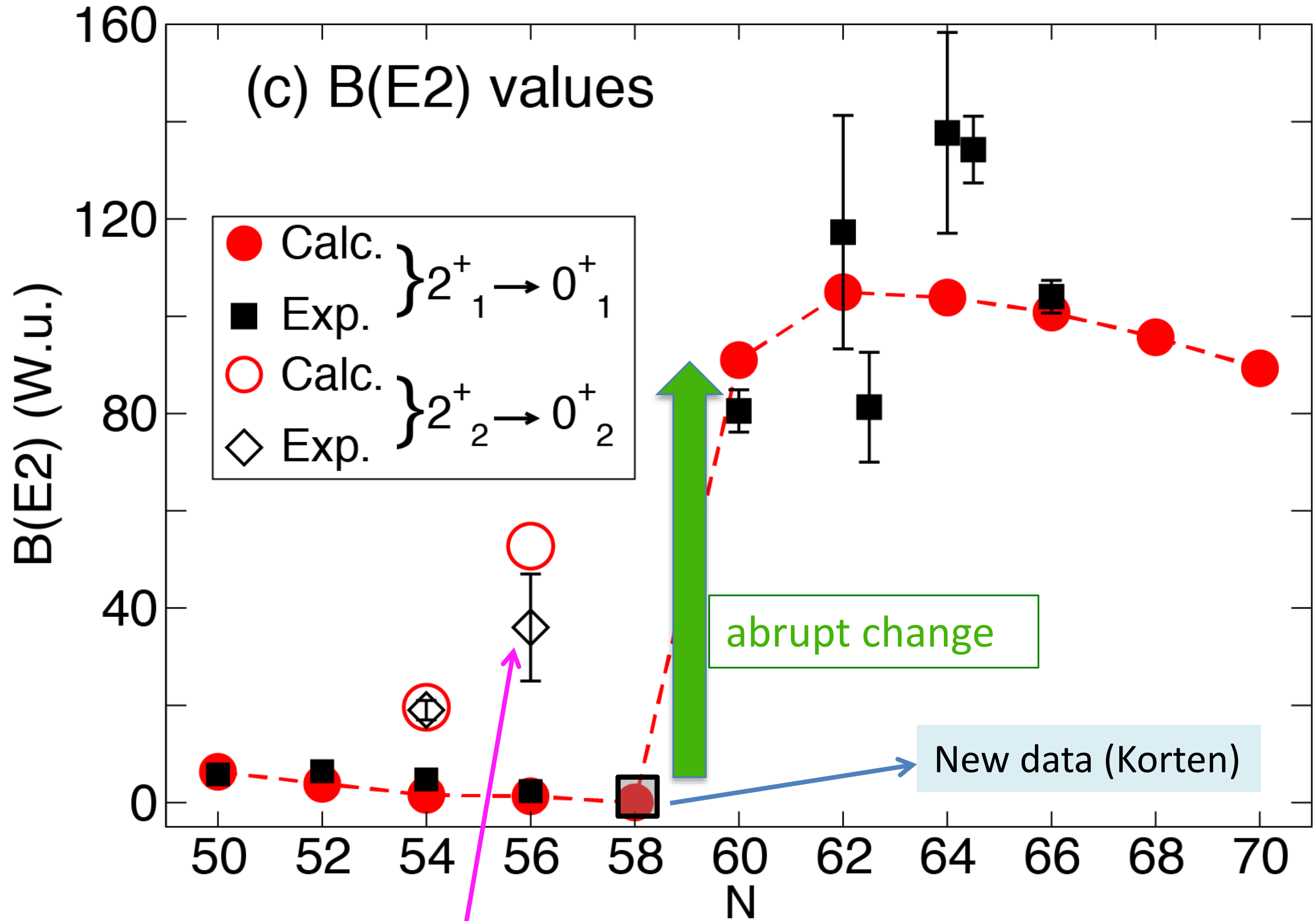
The concept of the phase transition cannot be applied to microscopic systems as it is. The QPT has been introduced as *an abrupt change* (of order parameter) *in the ground state of a many-body system by varying a physical (i.e., control) parameter at zero temperature. (cf., Wikipedia)*



(b) 0+ levels
Crossing without mixing
Quantum Phase Transition
(1st order)
spherical
oblate
triaxial
prolate
Exp.(0+2)
Ex (MeV)
0+4
0+1
abrupt change
N


(b) 0+ levels
spherical
oblate
triaxial
Crossing without mixing
Quantum Phase Transition
T-plot thus visualizes the essence of quantum phase transition in shapes
Ex (MeV)
0+1
abrupt change
N
50
60
70

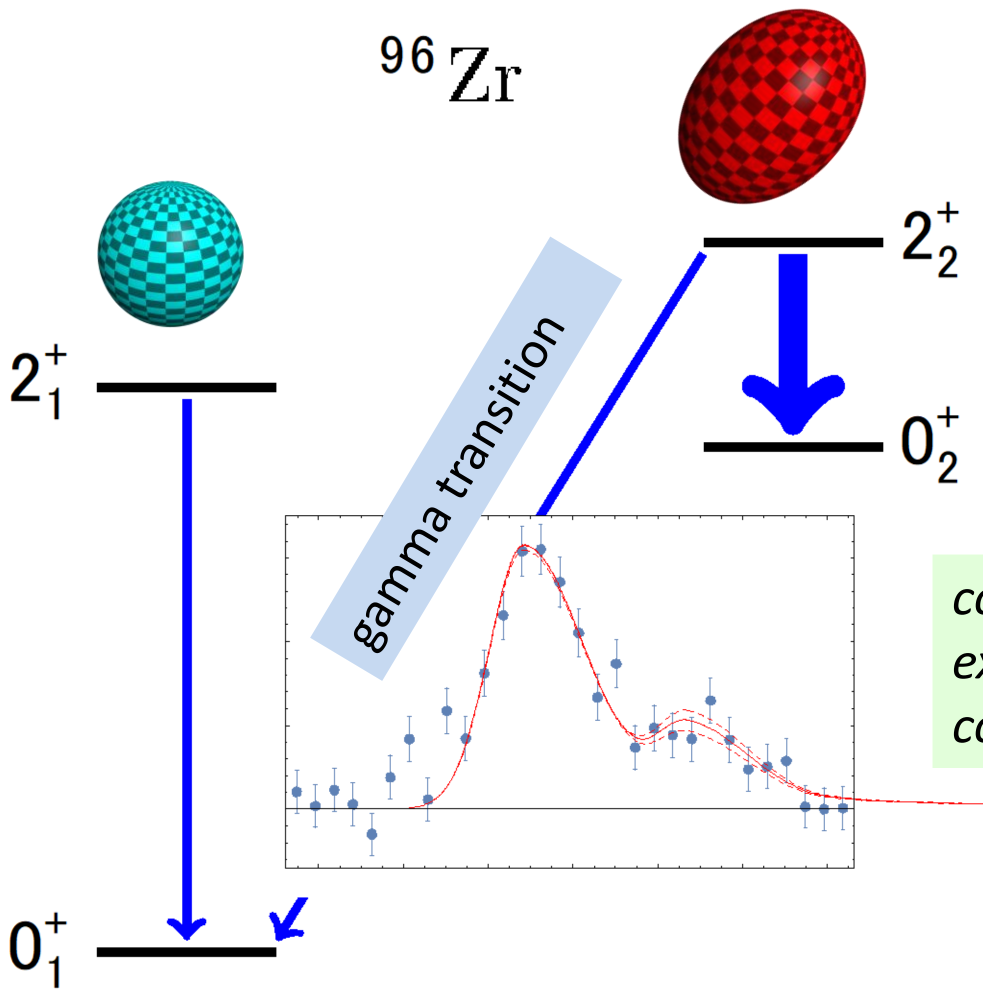
B(E2; 2^+ -> 0^+) systematics

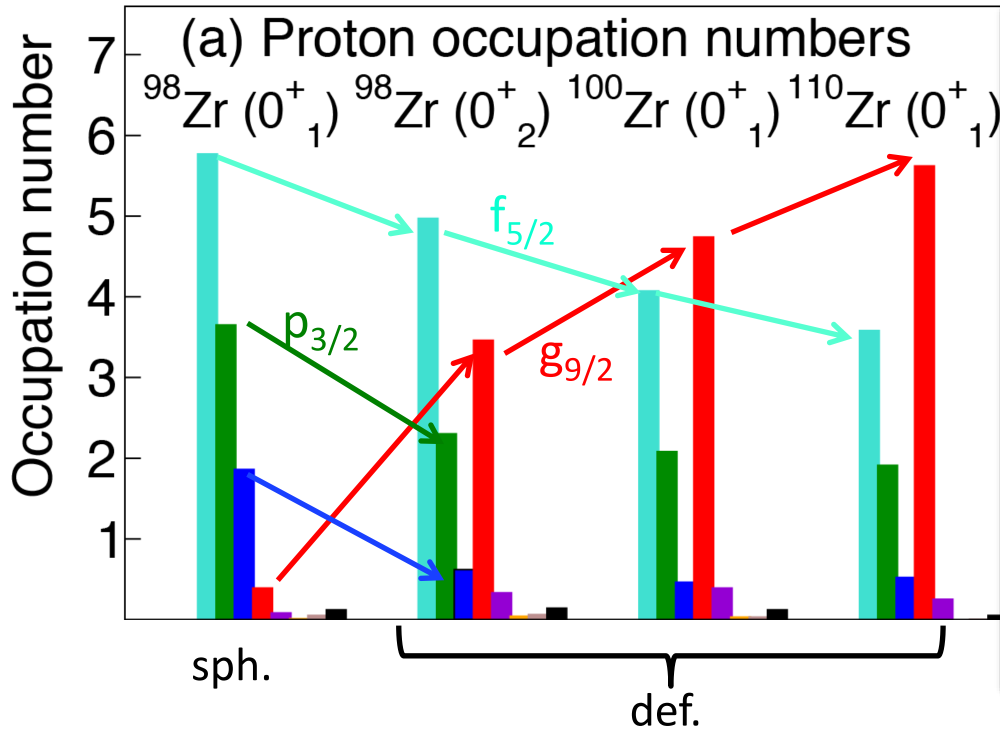


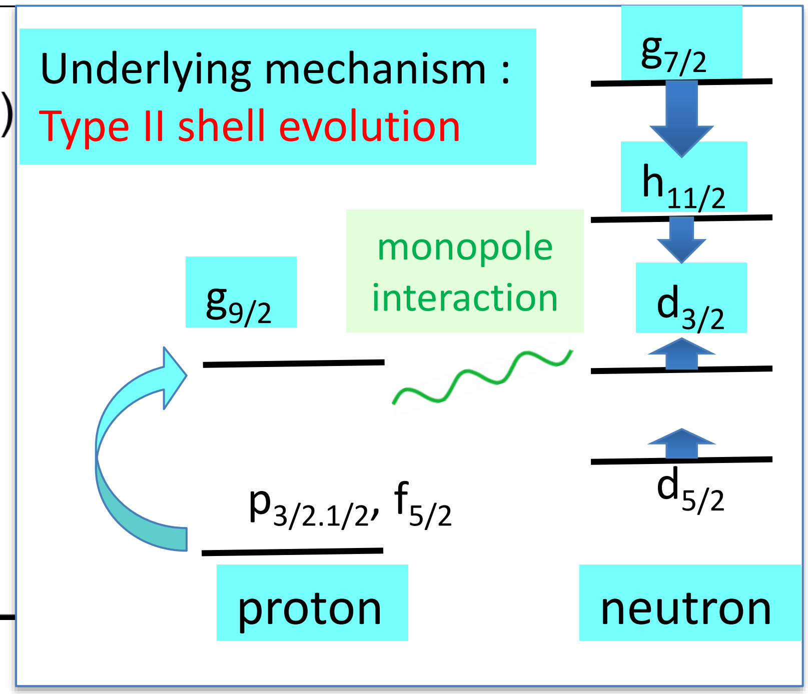
New data from Darmstadt, Kremer *et al*. PRL 117, 172503 (2016)

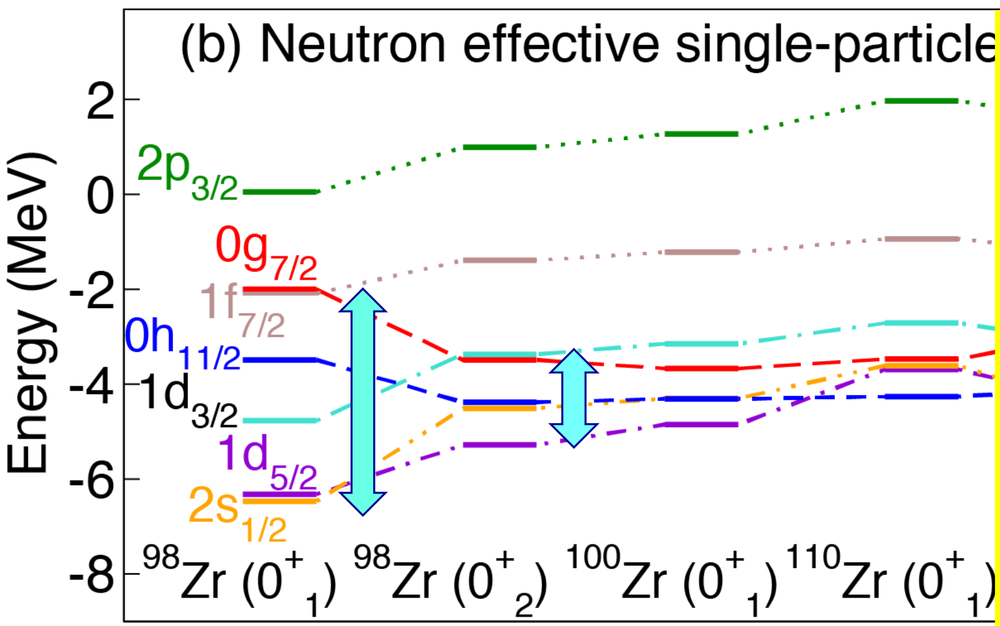
First Measurement of Collectivity of Coexisting Shapes Based on Type II Shell Evolution: The Case of ^{96}Zr

C. Kremer,[1] S. Aslanidou,[1] S. Bassauer,[1] M. Hilcker,[1] A. Krugmann,[1] P. von Neumann-Cosel,[1] T. Otsuka,[2,3,4,5] N. Pietralla,[1] V. Yu. Ponomarev,[1] N. Shimizu,[3] M. Singer,[1] G. Steinhilber,[1] T. Togashi,[3] Y. Tsunoda,[3] V. Werner,[1] and M. Zweidinger[1]









Relevant neutron single-particle levels get closer as a combined effect of nuclear forces (tensor and central) and particular configurations.

The resistance power against deformation is then reduced.

Large difference in ESPEs and configurations ➔ crossing w/o mixing

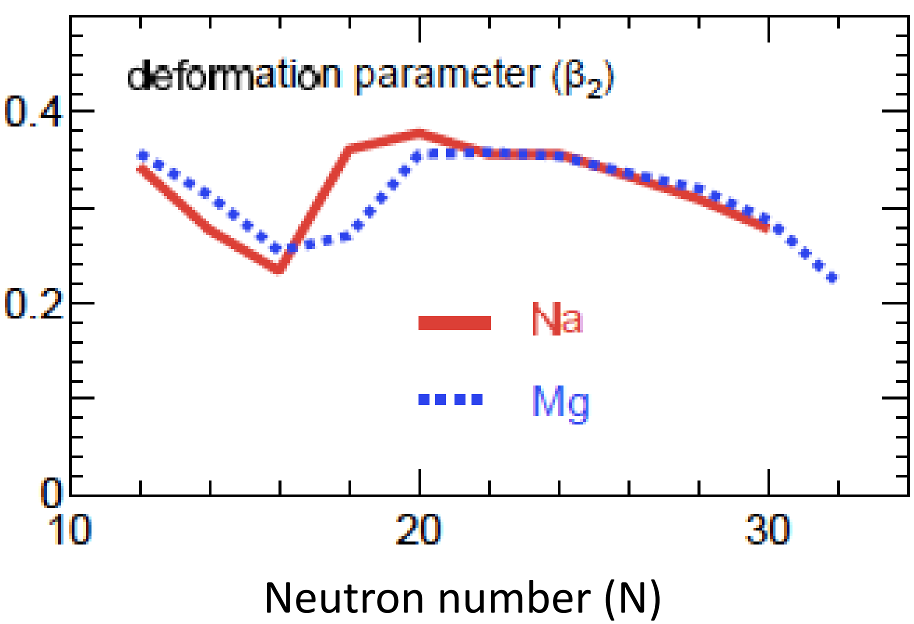
Charge radius is calculated from the usual relation

$$\langle r^2\rangle_{ch} = \langle r^2\rangle_{\mathrm{DM}}\{1 + (5/4\pi)\beta_2^2\}$$

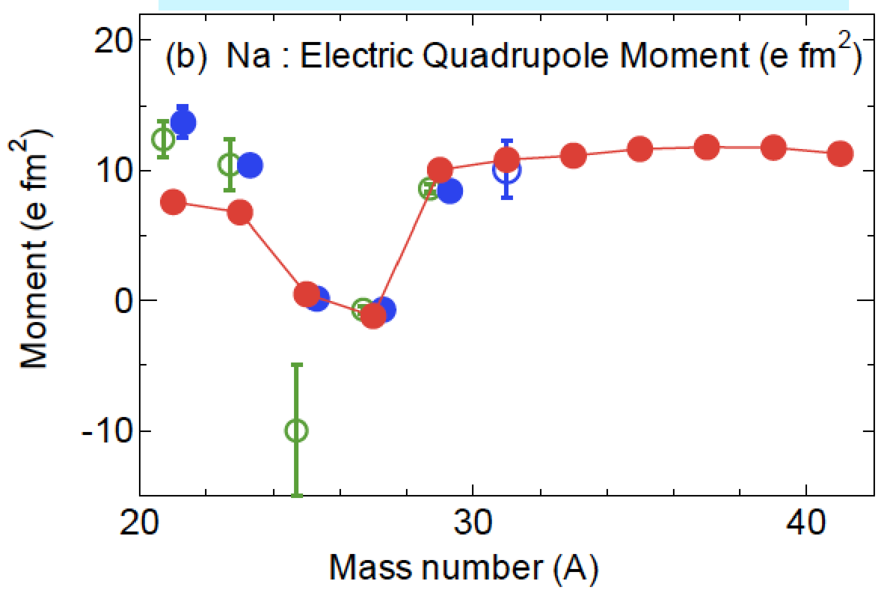
radius from MCSM for Na, Mg:
Otsuka, Shimizu, and YT,
PRC **105**, 014319 (2022)

with a droplet model term,

$$\langle r^2\rangle_{\mathrm{DM}} = (3/5)(R_0A^{1/3})^2 \qquad R_0 = 1.28(\mathrm{fm})$$



The electric quadrupole moments are described well too.



● M. De Rydt, M. Depuydt and G. Neyens, At. Data Nucl. Data Tab. 99, 391 (2013).

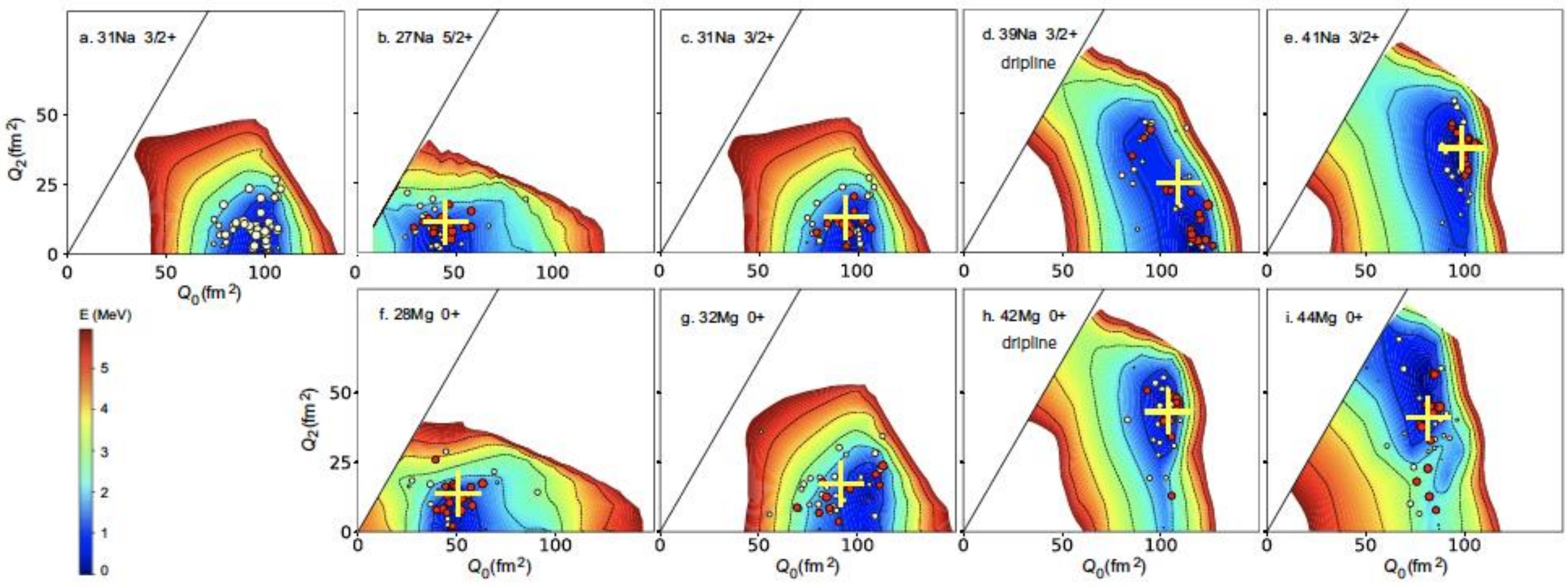
○ M. Keim, in *Proc. of the Int. Conf. on Exotic Nuclei and Atomic Masses (ENAM98)*, edited by B. M. Sherrill, D. J. Morrissey, and C. N. Davis, AIP Conf. Proc. No. **455** (AIP, New York, 1998), p. 50.

○ National Nuclear Data Center. Evaluated Nuclear Structure Data File, https://www.nndc.bnl.gov/ensdf/.

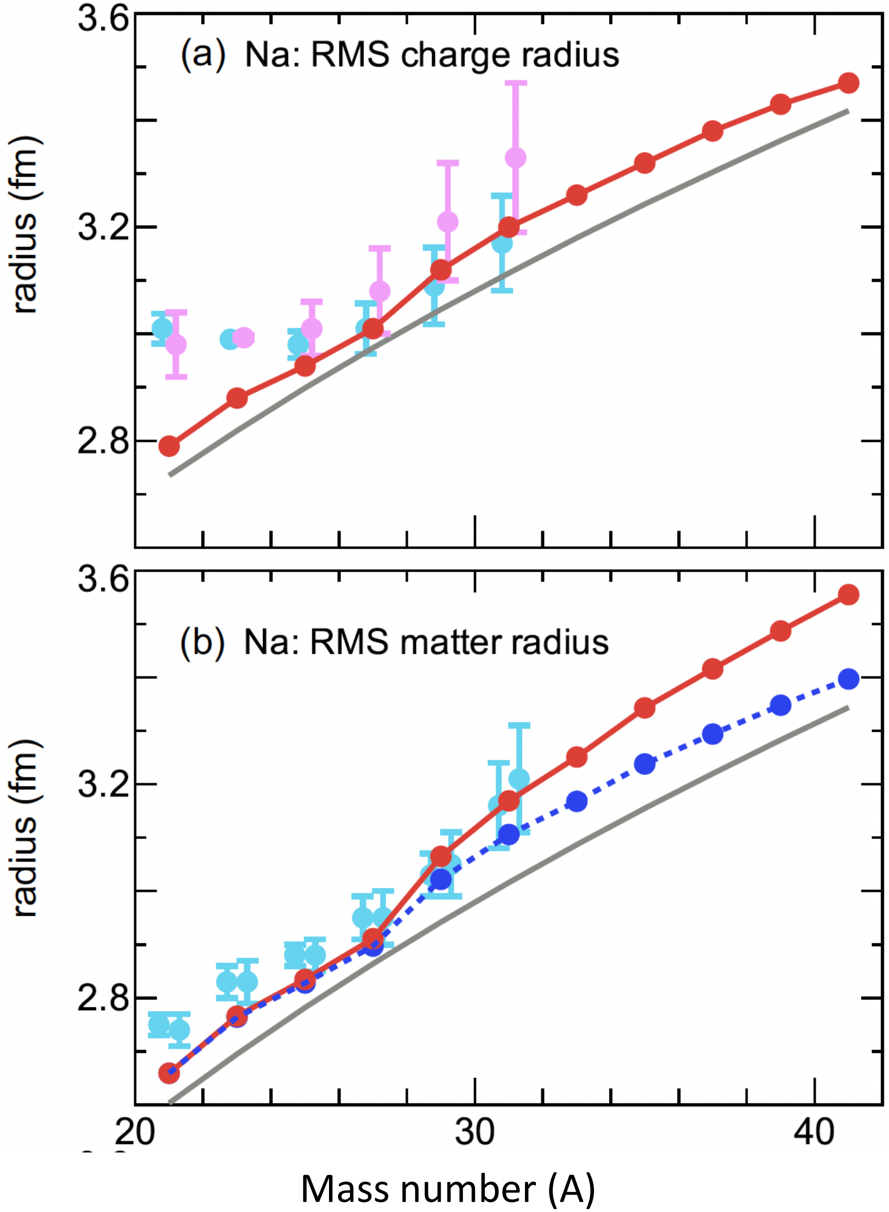
T plots for the ground states of Na isotopes

Crosses indicate the values of Q_0 and Q_2 representing those states

Deformation parameter β_2 is obtained from such Q_0 and Q_2 values



charge and matter radii (fm)



exp

I. Angelo and K. P. Marinova, At. Data Nucl. Data Tab. 99, 69 (2013).
B. Ohayon, R. F. Garcia Ruiz, Z. H. Sun, G. Hagen, T. Papenbrock,4 and B. K. Sahoo, arXiv:2019.10539v1.

present calc.

Droplet model

exp

from the interaction cross section

T. Suzuki *et al.*, Nucl. Phys. A **630**, 661 (1998).

calc. (full)

calc.

Droplet model

Summary

- Introduction of shell model calculation
- Change of shell structure (shell evolution)
  and need for a larger model space
- Monte Carlo shell model (MCSM) can be performed
  in a large model space
- We can analyze nuclear shapes by making use of
  intrinsic structure of MCSM wave functions (T-plot)
- MCSM calculations for quantum phase transition
  in shape of Zr isotopes
- Radius from MCSM for Na, Mg isotopes