RIKEN NISHINA CENTER

東京大学 THE UNIVERSITY OF TOKYO

KU LEUVEN

MICHIGAN STATE UNIVERSITY Founded 1855

TALENT school
ect*
July 11, 2017

Monte Carlo Shell model and related topics

Takaharu Otsuka

This work has been supported by MEXT and JICFuS as a priority issue (Elucidation of the fundamental laws and evolution of the universe) to be tackled by using Post 'K' Computer

After mastering the shell model,
three (possible) pillars combined for future

computation

Monte Carlo Shell Model (MCSM)

(almost) unlimited dimensionality

massive parallel computers

Hamiltonian

pf
pfg9d5 (A3DA) (Ni)
8+8 on ^{56}Ni core (Zr)
8+8 on ^{80}Zr core (Sn)
8+10 on ^{132}Sn core (Sm)
...
island of stability

+

χEFT based (multi-)shell int.

many-body dynamics

Shell evolution (Type I & II)

Quantum Phase Transition

Shape coexistence

Quantum Self-organization

Hamiltonian in shell model calculations

ε_i : Single Particle Energy (SPE)

<j1, j2, J, T | V | j3, j4, J, T >

: Two-Body Matrix Element (TBME)

$$H = \Sigma_i \boxed{\epsilon_i} n_i + \Sigma_{i,j,k,l} \boxed{v_{ij,kl}} a_i^\dagger a_j^\dagger a_l a_k$$

Step 1: Calculate matrix elements

$$< \phi_1 | H | \phi_1 >, \quad < \phi_1 | H | \phi_2 >, \quad < \phi_1 | H | \phi_3 >, \; ....$$

where ϕ_1 , ϕ_2 , ϕ_3 are Slater determinants

In the second quantization,

closed shell

$$\phi_1 = a_\alpha^+ \, a_\beta^+ \, a_\gamma^+ \; ..... \boxed{| 0 >}$$

$$\phi_2 = a_{\alpha'}^+ \, a_{\beta'}^+ \, a_{\gamma'}^+ \; ..... \boxed{| 0 >}$$

$$\phi_3 = ...$$

$$H = \Sigma_i \, \epsilon_i \, n_i + \Sigma_{i,j,k,l} \, v_{ij,kl} \, a_i^\dagger \, a_j^\dagger \, a_l \, a_k$$

Step 2: we solve the eigenvalue problem : $\mathbf{H}\,\Psi = \mathbf{E}\,\Psi$

$$
\begin{pmatrix}
\langle \phi_1 |H| \phi_1 \rangle & \langle \phi_1 |H| \phi_2 \rangle & \cdots \\
\langle \phi_2 |H| \phi_1 \rangle & \langle \phi_2 |H| \phi_2 \rangle & \cdots \\
\langle \phi_3 |H| \phi_1 \rangle & \cdot & \cdots \\
\langle \phi_4 |H| \phi_1 \rangle & \cdot & \cdots \\
\cdot & \cdot & \cdots
\end{pmatrix}
\begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ \cdot \\ \cdot \end{pmatrix}
= E
\begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ \cdot \\ \cdot \end{pmatrix}
$$

$$\Psi = c_1\,\phi_1 + c_2\,\phi_2 + c_3\,\phi_3 + \ldots..$$

c_i probability amplitudes

With Slater determinants ϕ_1, ϕ_2, ϕ_3 ,...,

the eigen wave function is expanded as

$$\Psi = c_1\, \phi_1 + c_2\, \phi_2 + c_3\, \phi_3 + \ldots..$$

c_i **probability amplitudes**

With this, we can calculate various physical quantities.

for instance, E2, M1, ... matrix elements
(transitions and moments)
spectroscopic factors for transfer reactions

$$< \Psi' \,|\, T \,|\, \Psi >$$

Two types of shell-model calculations

dim. <~ 10^{10}

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

Conventional Shell Model

all Slater determinants

Direct diagonalization

For even bigger problem,

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

~100 dim.

Monte Carlo Shell Model

bases important for a specific eigenstate

Selected

important basis vectors

Monte Carlo Shell Model

Auxiliary-Field Monte Carlo (AFMC) method

general method for quantum many-body problems

For nuclear physics, **Shell Model Monte Carlo (SMMC)** calculation has been introduced by **Koonin** et al. Good for finite temperature.

- **minus-sign problem**
- **only ground state, not for excited states in principle.**

Quantum Monte Carlo Diagonalization (QMCD) method

No sign problem. Symmetries can be restored.
Excited states can be obtained.

→ **Monte Carlo Shell Model (MCSM)**

Background of Monte Carlo Shell Model (I)

Two-body interaction can be rewritten as $V = (1/2)\ \Sigma_\alpha\ v_\alpha\, O_\alpha{}^2$

α : index
O_α : one-body operators (rearranged by diagonalization)

Hubberd-Stratonovichi transformation

True eigenstate : $\psi = \Sigma_\sigma\, e^{-\beta h(\sigma)}\ e^{-\beta h(\sigma')}\ \ldots\ \psi_0$

imaginary time (β) evolution by one-body field $h(\sigma)$

One-body operator is introduced as $h(\sigma) = \Sigma_\alpha\ s_\alpha\, \sigma_\alpha\, v_\alpha\, O_\alpha$

σ_α : random number (Gaussian) σ : set of σ_α's
s_α : phase (1 for v_α<0, i for v_α>0)

Background of Monte Carlo Shell Model (II)

True eigenstate : $\psi = \Sigma_{\sigma,\sigma', \dots} e^{-h(\sigma)} e^{-h(\sigma')} \dots \psi_0$

Use $\phi(\sigma,\sigma',\dots) = e^{-\beta h(\sigma)} e^{-\beta h(\sigma')} \dots \psi_0$
as a basis for shell-model diagonalization

$\phi(\sigma,\sigma',\dots)$ are selected and refined :

(i) Random sampling -> only those lowering energy are kept
(ii) Polished by varying **$\sigma,\sigma',\dots$** gradually (random noise reduced)
(iii) Symmetry restoration (Angular momentum, parity)

Slater determinants (or Cooper-pair type wave functions) are used

Usually, 20~50 bases are kept (many more thrown away)

Advanced Monte Carlo Shell Model (currently used)

N_B : number of basis vectors (dimension)

N_p : number of (active) particles

N_{sp} : number of single-particle states

$$\left|\Psi(D)\right\rangle = \sum_{n=1}^{N_B} c_i P^{J,\Pi} \left|\phi(D^{(n)})\right\rangle$$

amplitude

Projection op.

$$\left|\phi(D^{(n)})\right\rangle = \prod_{\alpha=1}^{N_p} \underbrace{\left(\sum_{i=1}^{N_{sp}} a_i^{\dagger} D_{i\alpha}^{(n)}\right)}_{\text{Deformed single-particle state}} \left|-\right\rangle$$

n-th basis vector (Slater determinant)

$$E(D) = \left\langle \Psi(D) \middle| H \middle| \Psi(D) \right\rangle$$

Minimize $E(D)$ as a function of D utilizing qMC and conjugate gradient methods

Step 1 : stochastic generation of candidates of the n-th MCSM basis vector

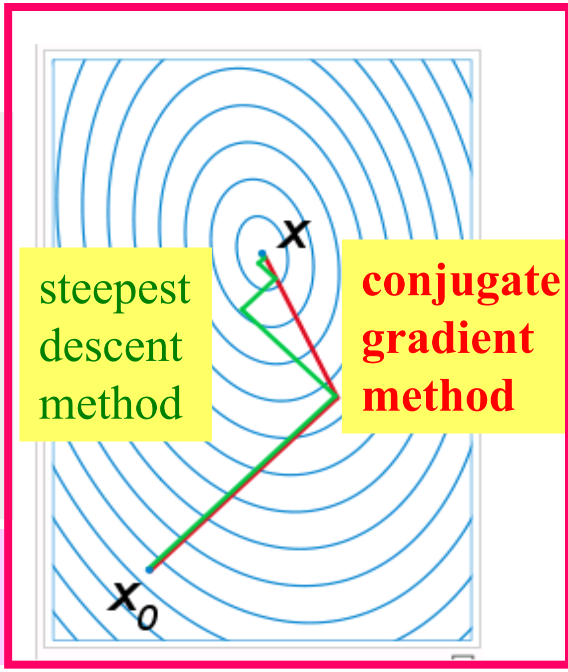
$$\cancel{\left|\phi(\sigma)\right\rangle = \prod e^{-\Delta\beta h(\sigma)}} \cdot \left|\phi^{(0)}\right\rangle$$ *only theoretical background*

Shift randomly matrix elements of the matrix D.

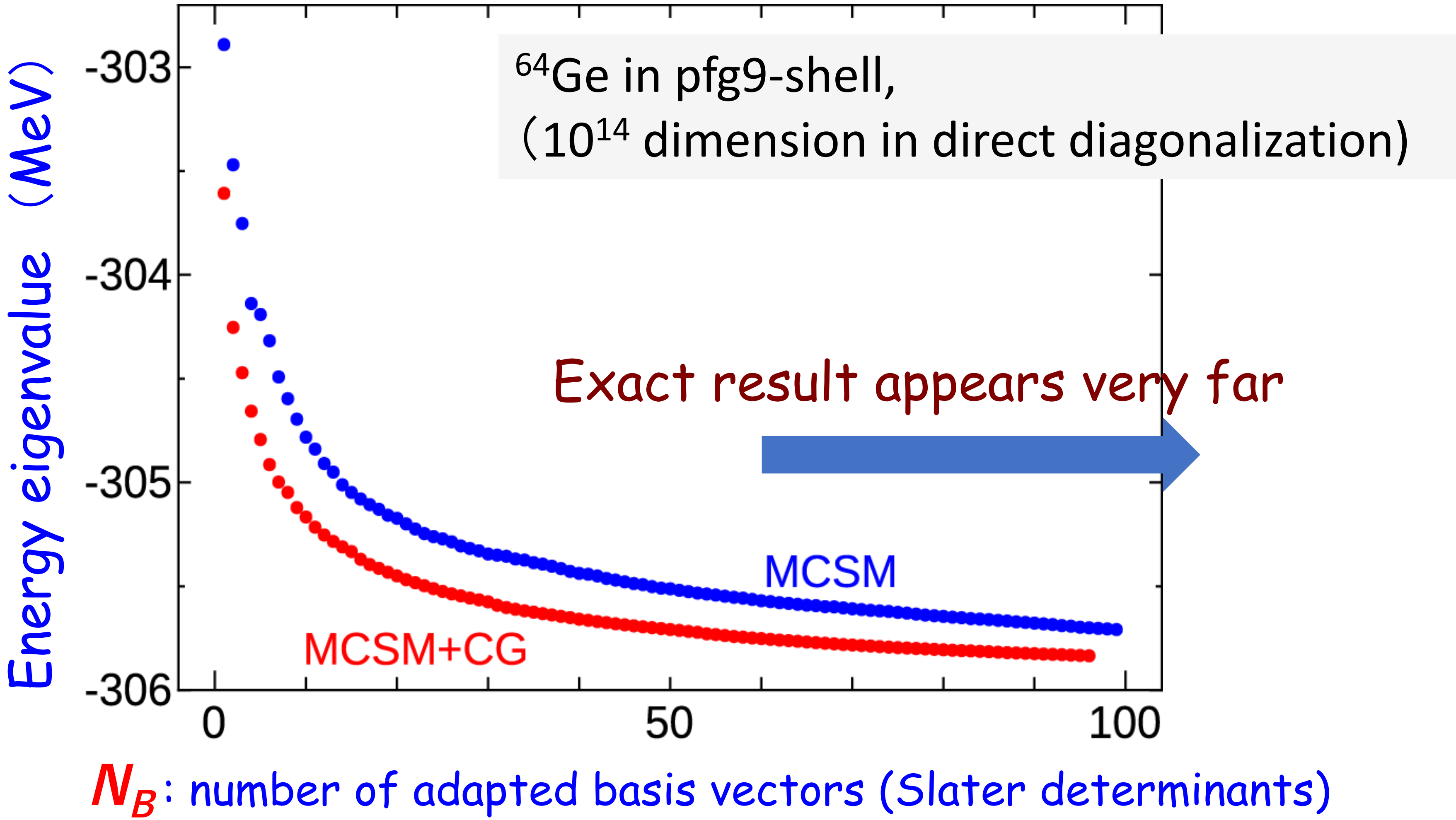
(The very initial one can be a Hartree-Fock state.)

Select the one producing the lowest *E(D)* (rate < 0.1 %)

Step 2 : polish *D* by means of the conjugate gradient (CG) method "variationally".



Example of MCSM calculation



Numerous MC trials and CG optimization for each basis vector

Advanced Monte Carlo Shell Model (currently used)

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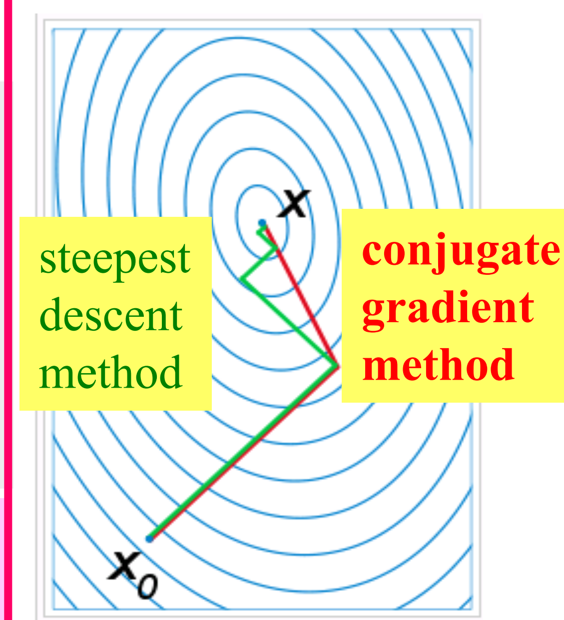
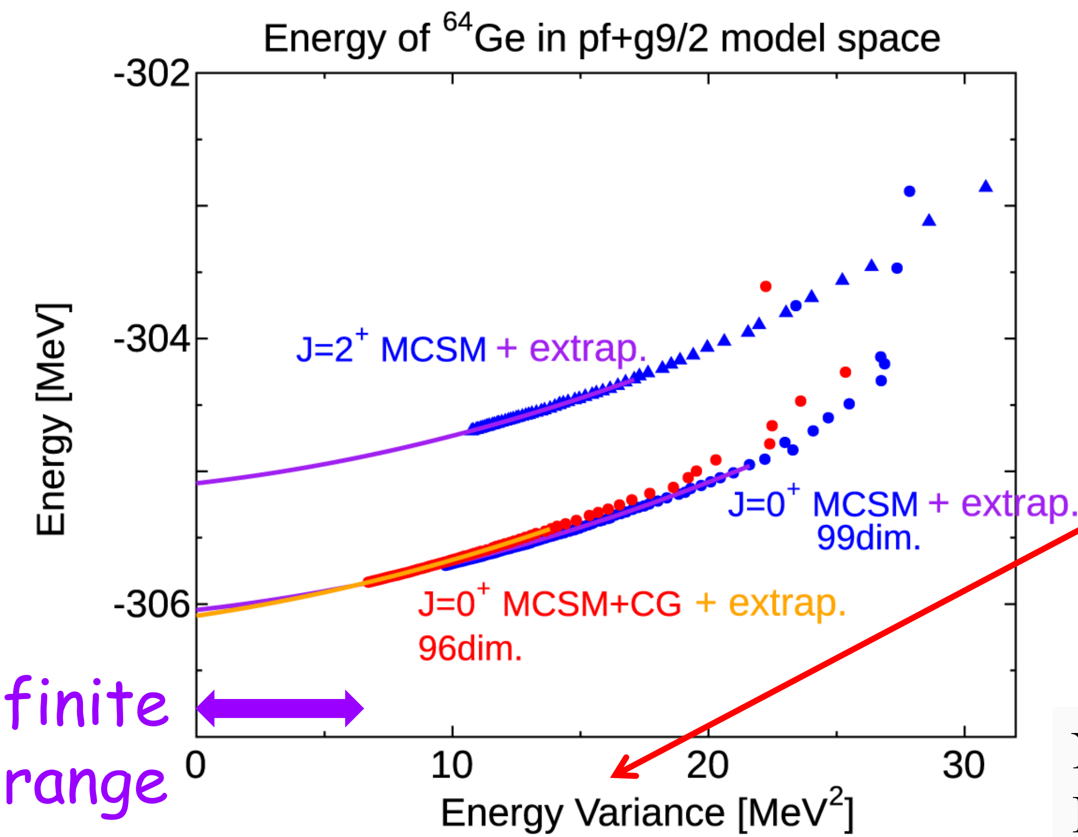
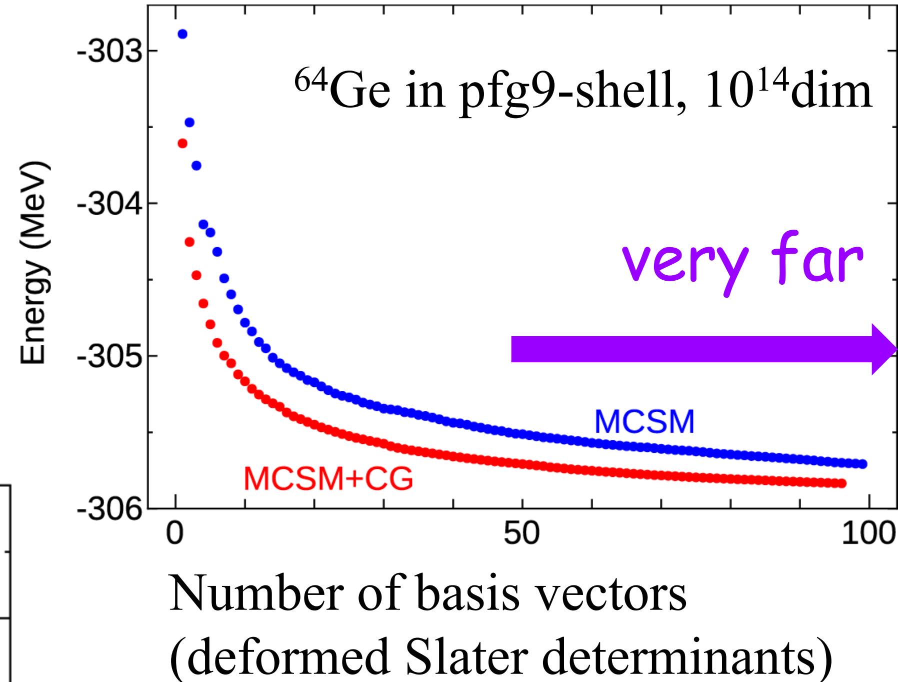


Extrapolation by Energy Variance





Variance : $\langle \Delta H^2 \rangle = \langle H^2 \rangle - \langle H \rangle^2$

$$\langle H \rangle = E_0 + a\langle \Delta H^2 \rangle + b\langle \Delta H^2 \rangle^2 + \dots$$

N. Shimizu, et al.,
Phys. Rev. C **82,** 061305(R) (2010).

MCSM (Monte Carlo Shell Model *-Advanced version-*)

1. Selection of important many-body basis vectors
   by quantum Monte-Carlo + diagonalization methods
   basis vectors : about 100 selected Slater determinants
   composed of "deformed" single-particle states
2. Variational refinement of basis vectors
   conjugate gradient method
3. Variance extrapolation method -> exact eigenvalues

+ innovations in algorithm and code (=> now moving to GPU)

K computer (in Kobe) 10 peta flops machine

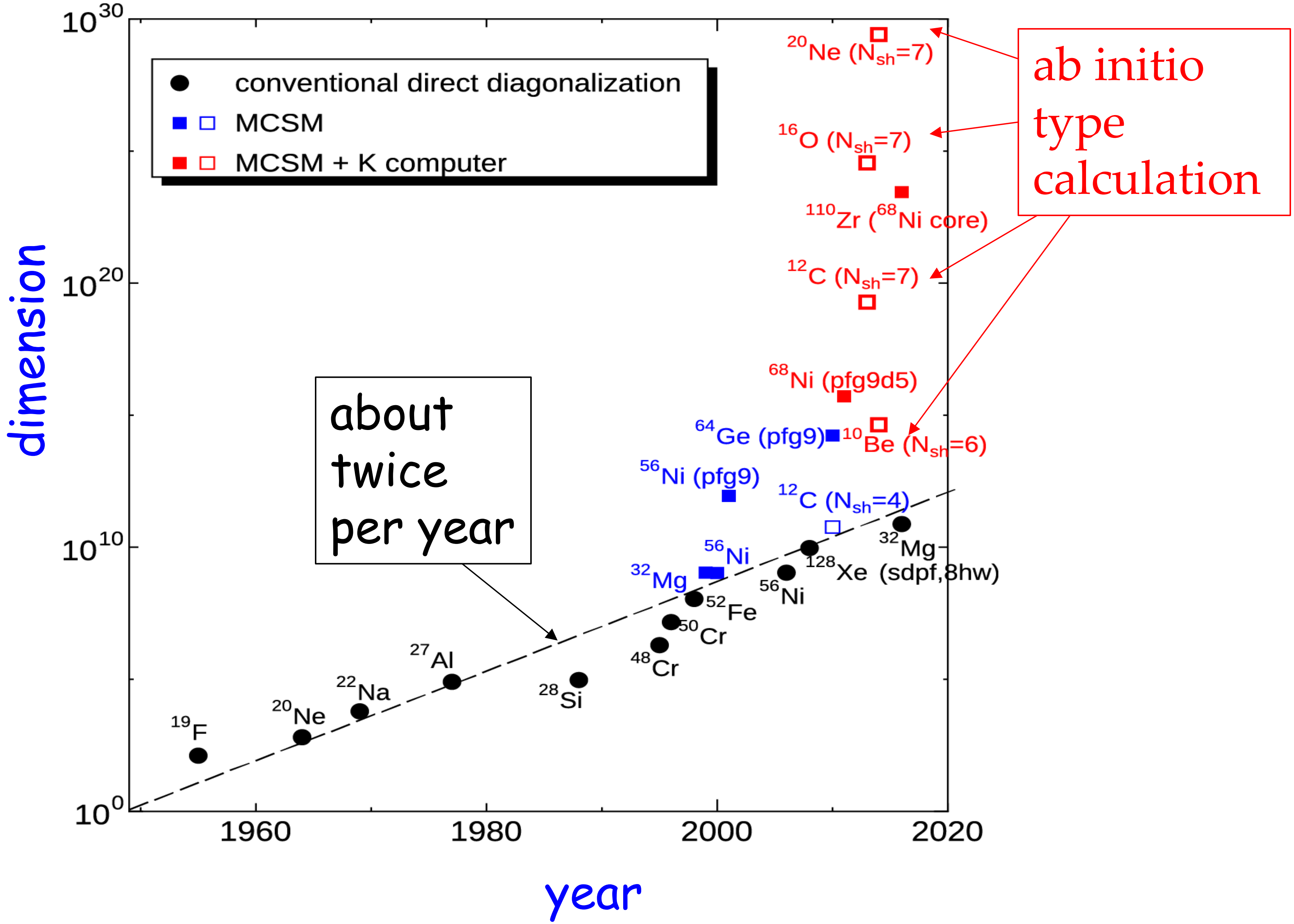
$\Rightarrow$ *Projection of basis vectors*

Rotation with three Euler angles

with about 50,000 mesh points

Example : 8^+ ^{68}Ni 7680 core x 14 h

Dimension of the shell-model many-body Hilbert space



MCSM basis vectors on Potential Energy Surface

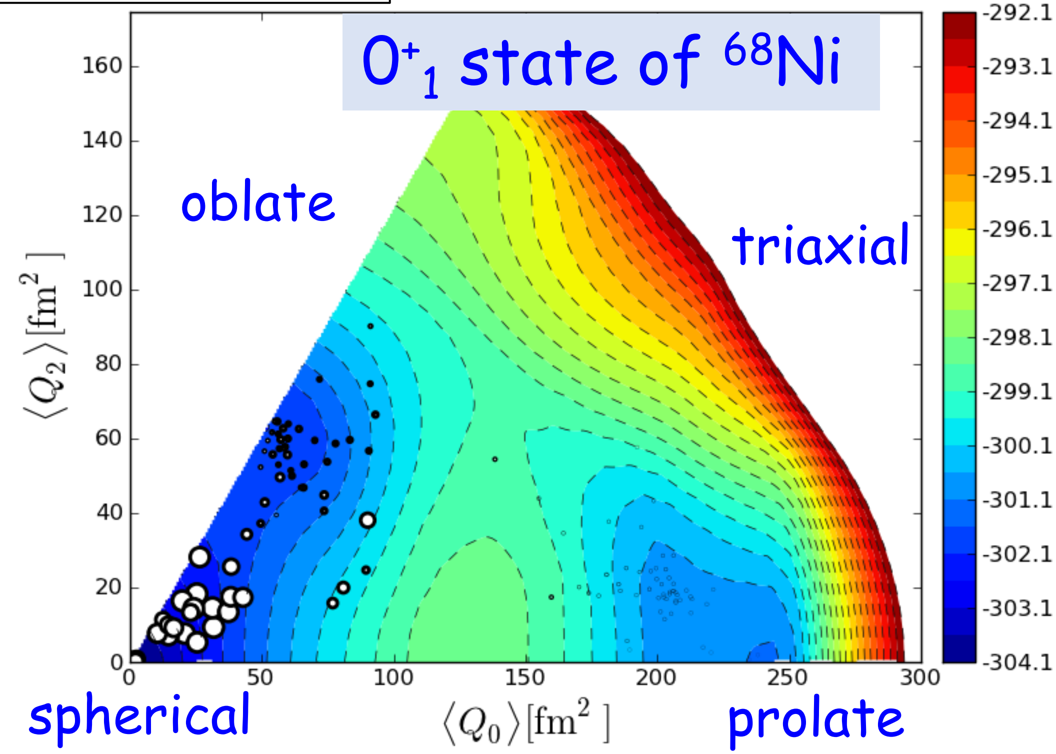
eigenstate $\Psi = \sum_i c_i P[J^\pi] \Phi_i$

amplitude

projection onto J^π

Slater determinant of deformed s. p. states → intrinsic shape

- PES is calculated by CHF for the shell-model Hamiltonian
- Location of circle : quadrupole deformation of unprojected MCSM basis vectors
- Area of circle : overlap probability between each projected basis and eigen wave function



Called ***T*-plot** in reference to

Y. Tsunoda, *et al.*

PRC 89, 031301 (R) (2014)

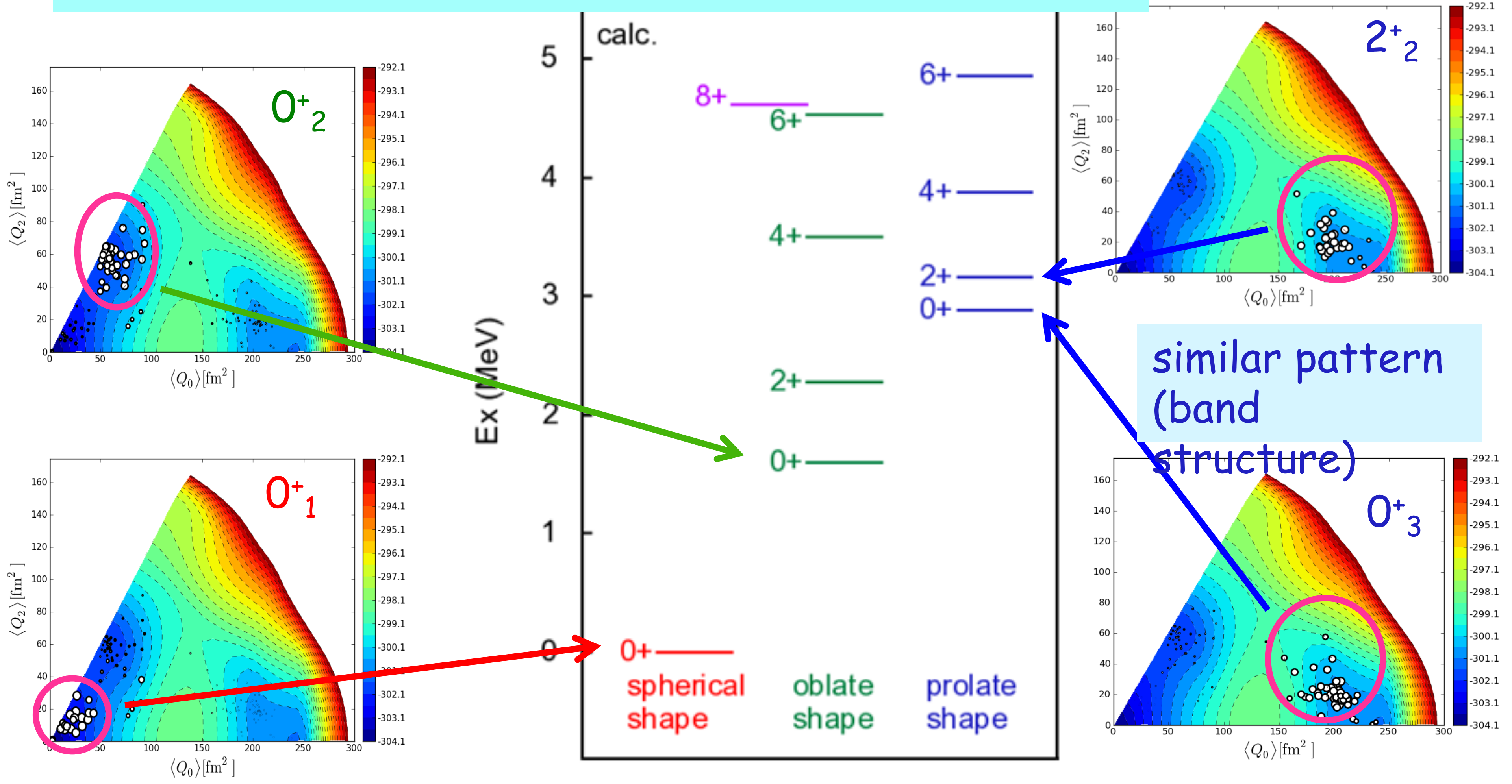
General properties of T-plot :

Certain number of large circles in a small region of PES

⇔ pairing correlations

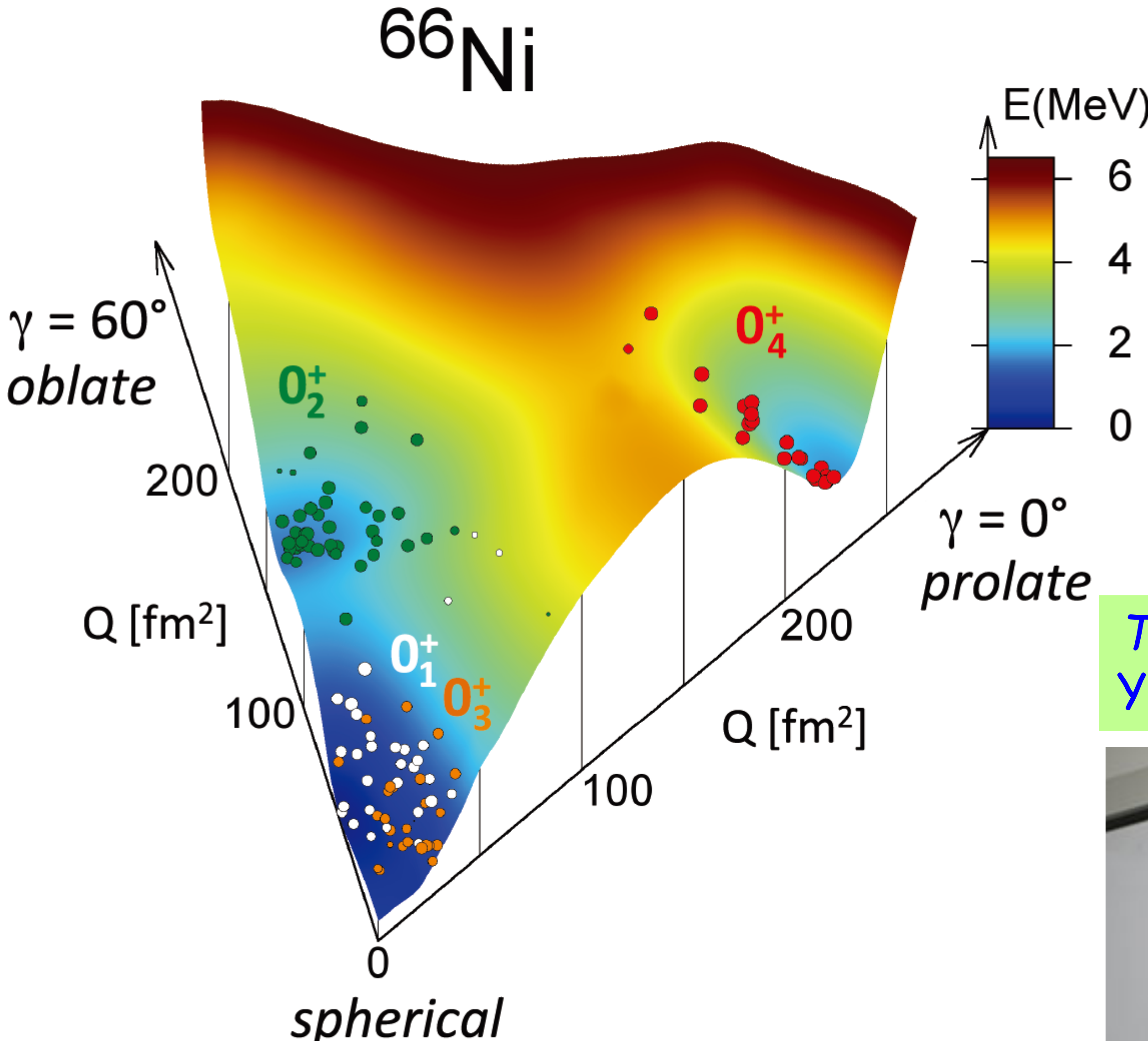
Spreading beyond this can be due to shape fluctuation

Example : shape assignment to various 0^+ states of ^{68}Ni



3-dimensional T-plot

~ Alpine villages



T-plot invented by Yusuke Tsunoda

Three pillars combined for future

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island of stability
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χEFT based multi-shell int.

many-body dynamics

Shell evolution (Type I & II)

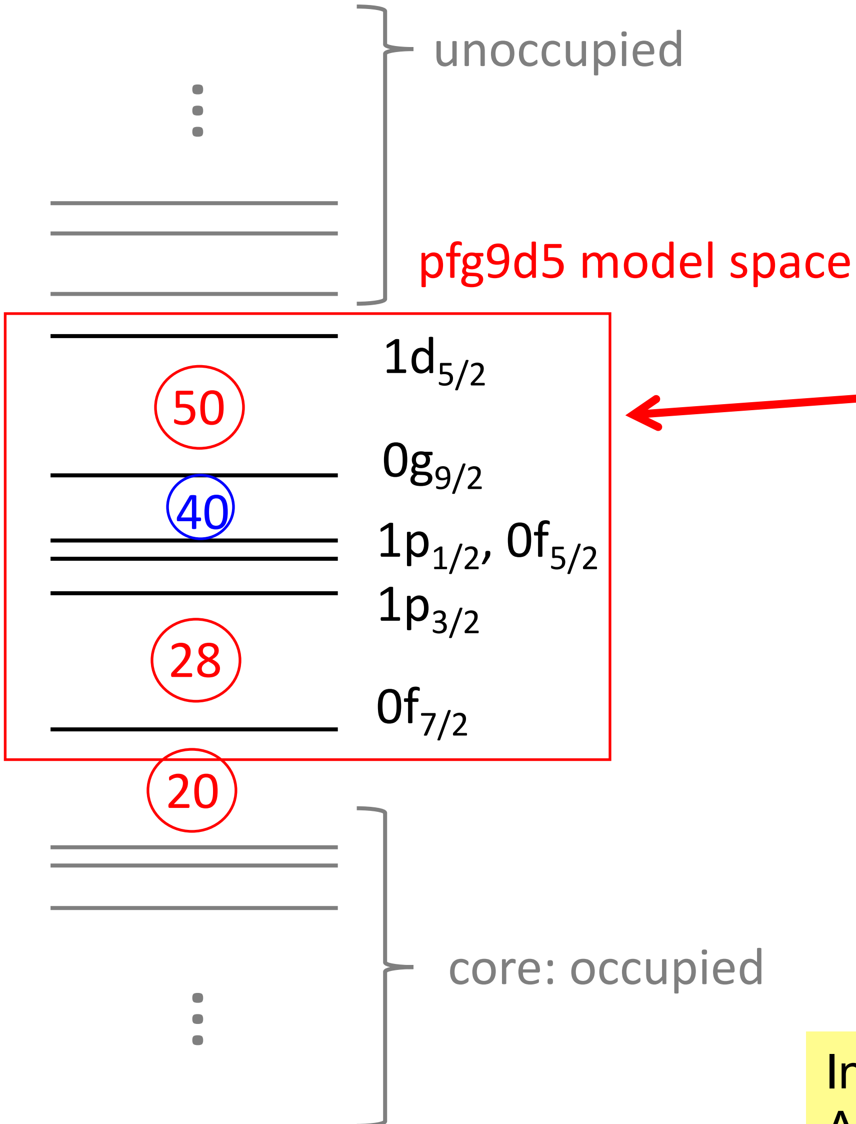
Quantum Phase Transition

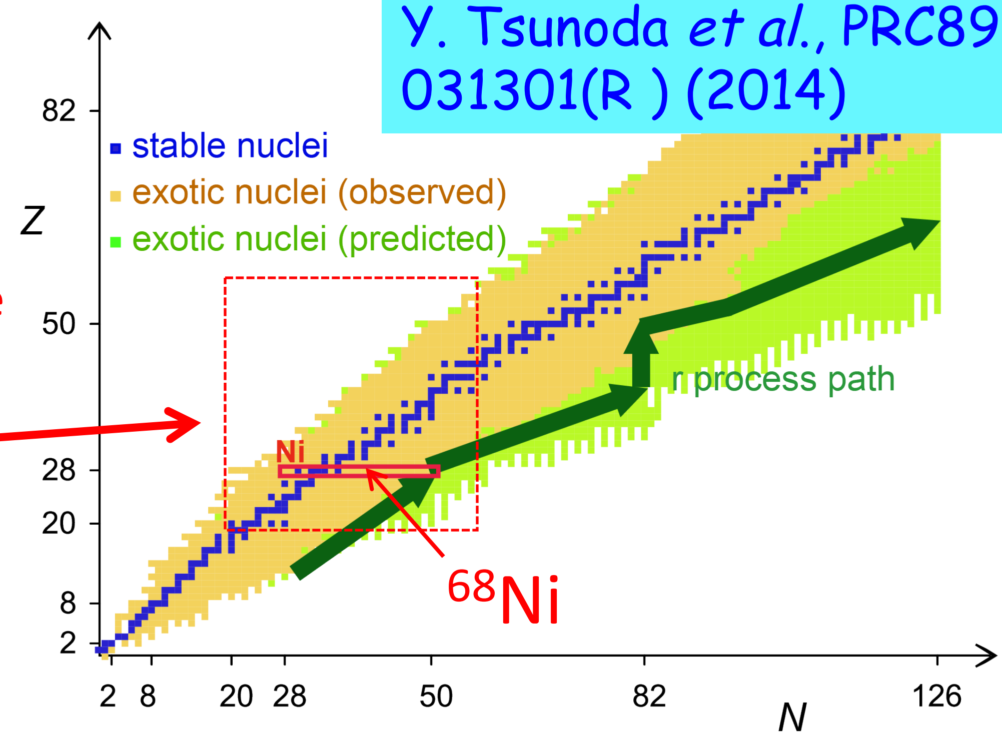
Shape coexistence

Quantum Self-organization

Monte Carlo Shell Model (MCSM) calculation on Ni isotopes

Y. Tsunoda *et al.*, PRC89, 031301(R) (2014)





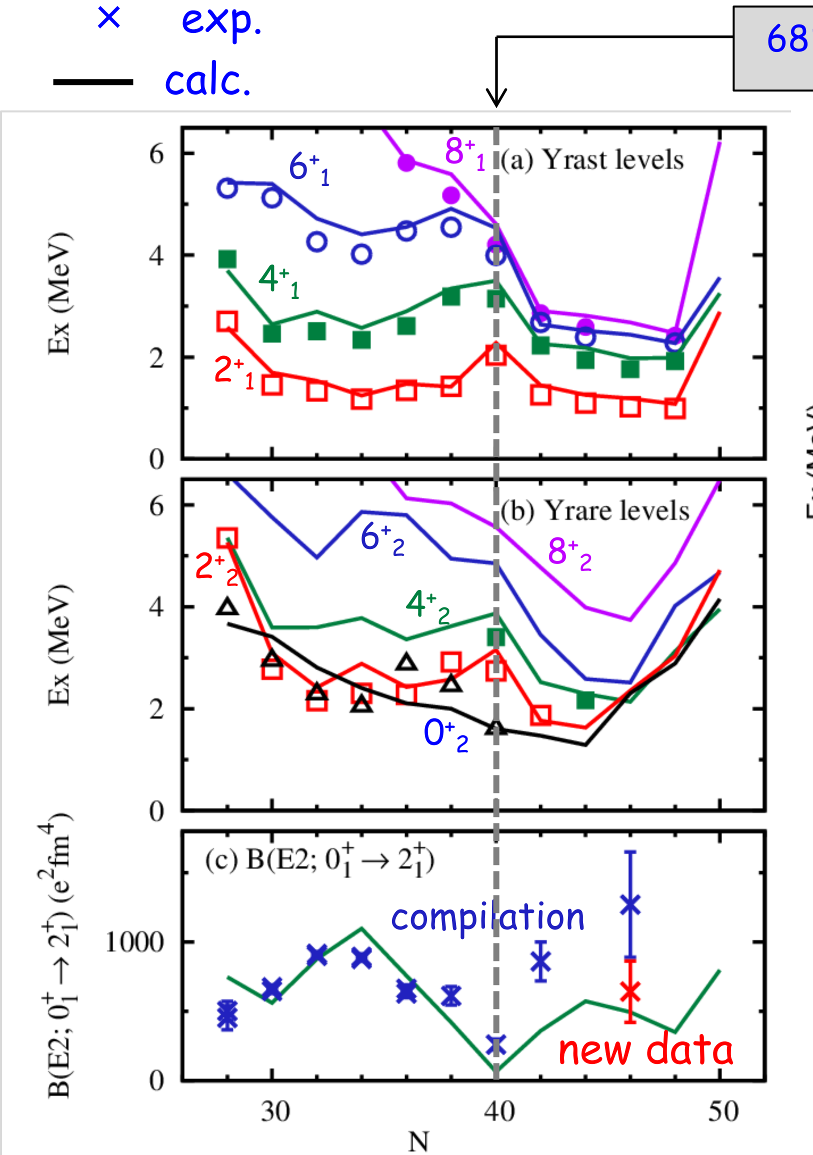
This model space is wide enough to discuss how magic numbers 28, 50 and semi-magic number 40 are visible or smeared out.

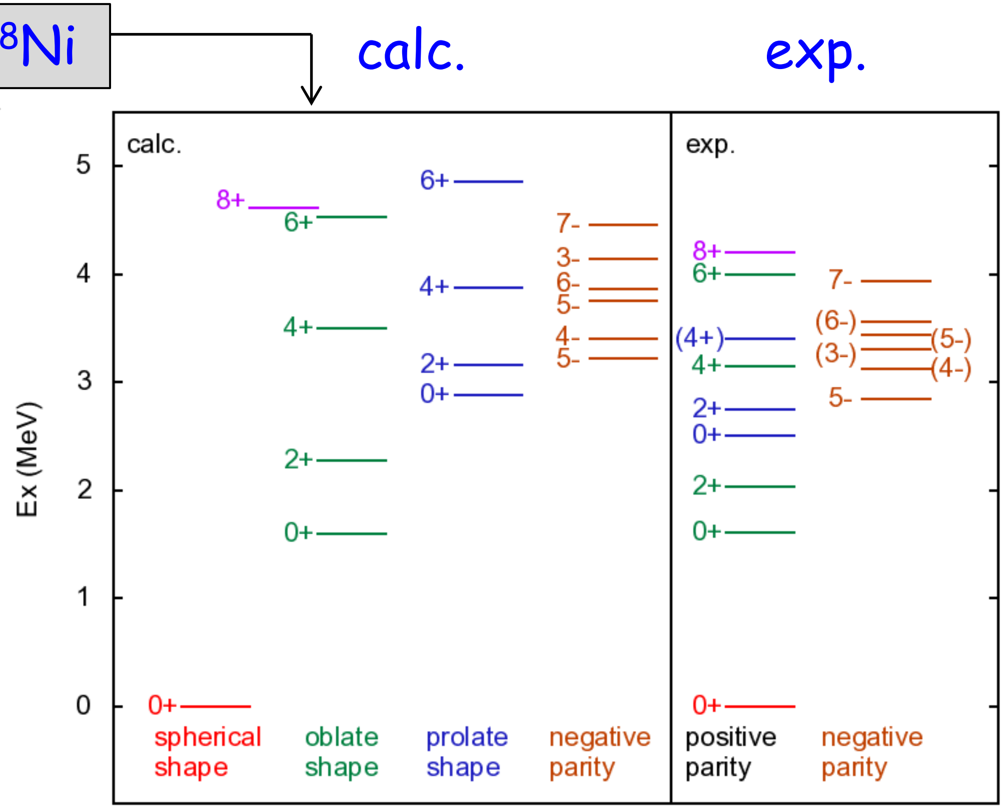
Interaction:
A3DA interaction is used with minor corrections

Energy levels and B(E2) values of Ni isotopes

Description by the same Hamiltonian

Shape coexistence in ^{68}Ni





Y. Tsunoda, TO, Shimizu, Honma and Utsuno, PRC 89, 031301 (R) (2014)

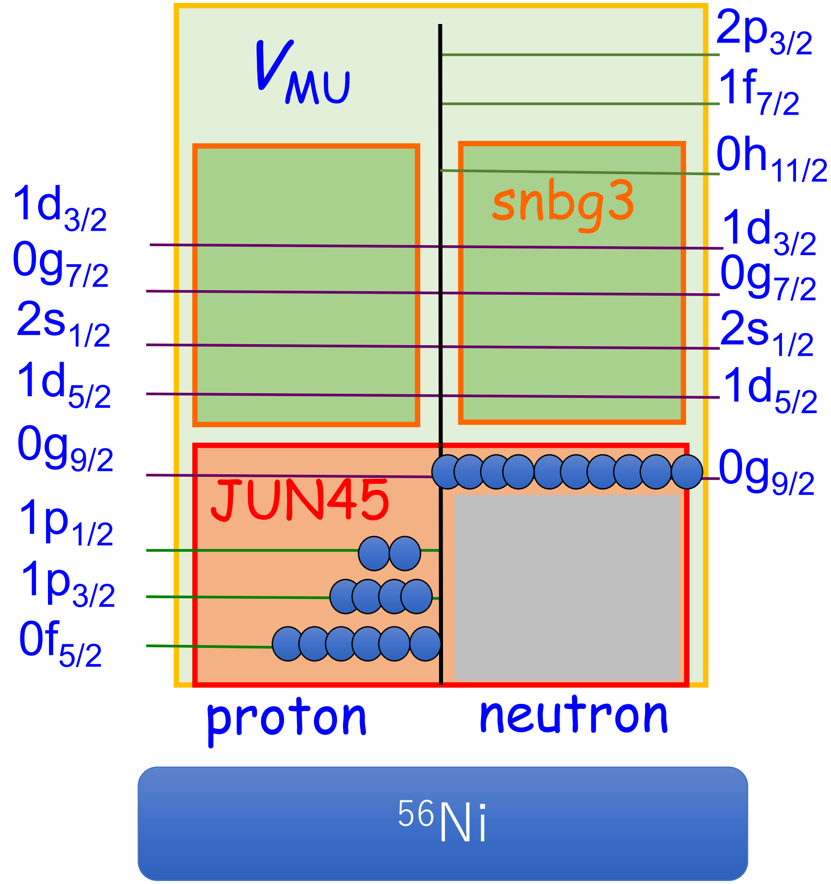
An example : shapes of Zr isotopes by Monte Carlo Shell Model

- 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, Tsunoda, TO *et al.* PRL 117, 172502 (2016)

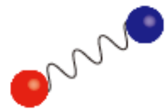
Part I : shell model powered by modern nuclear forces

QCD

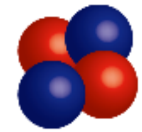
Lattice QCD

Effective Field Theory

Nuclear force

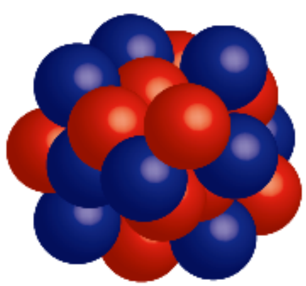


Light nuclei ~A≒10-20



Few body techniques
No core shell model
and many others…

Medium mass nuclei~A≒20-100



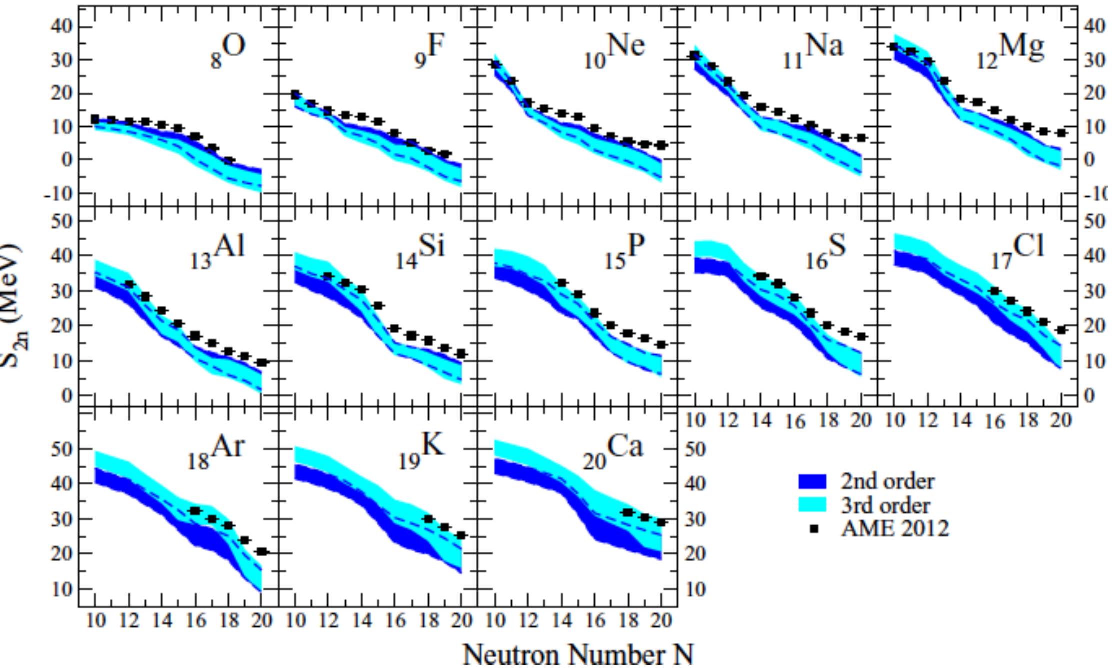
shell model with core
via the **effective interaction**
derived from **nuclear force**

Courtesy from N. Tsunoda

Examples of structure calculations starting from chiral EFT forces

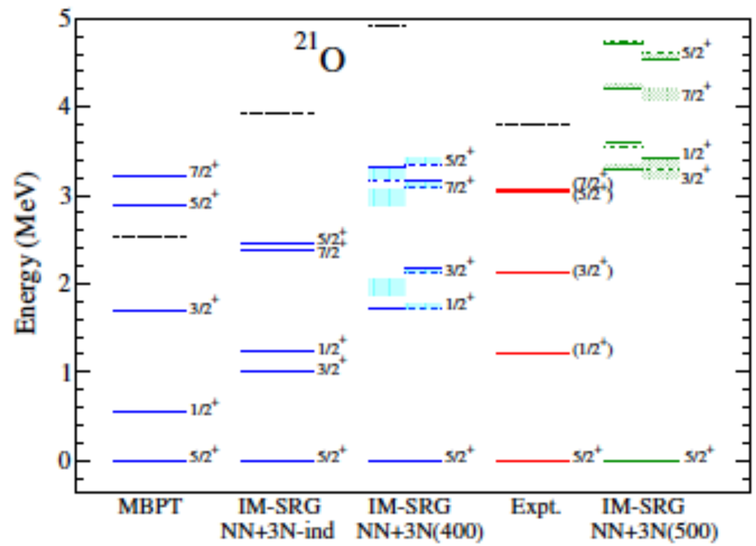
NN force: N3LO + 3N force: N2LO
-> valence shell interaction

MBPT
(Many-body Perturbation Theory)
applicable to one major shell



Simonis et al. PRC 93, 011302(R) (2016)

IM-SRG
(In-Medium Similarity Renormalization Group)

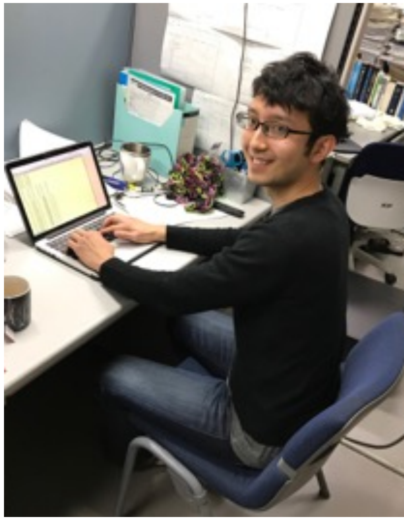


Bogner et al. PRL 113, 142501 (2014)

+ Coupled Cluster calculation + N2LOsat potential + ...

A recent development starting from ***chiral EFT + 3NF***

EKK method to handle consistently
two (or more) major shells
-> Effective shell-model interaction
(i) without fit of two-body m. e.,
(ii) applicable to broken magicity,
or fusion of two shells,
both are crucial for exotic nuclei.



PHYSICAL REVIEW C 95, 021304(R) (2017)

Exotic neutron-rich medium-mass nuclei with realistic nuclear forces

Naofumi Tsunoda,[1] Takaharu Otsuka,[1,2,3,4] Noritaka Shimizu,[1] Morten Hjorth-Jensen,[5,6]
Kazuo Takayanagi,[7] and Toshio Suzuki[8]

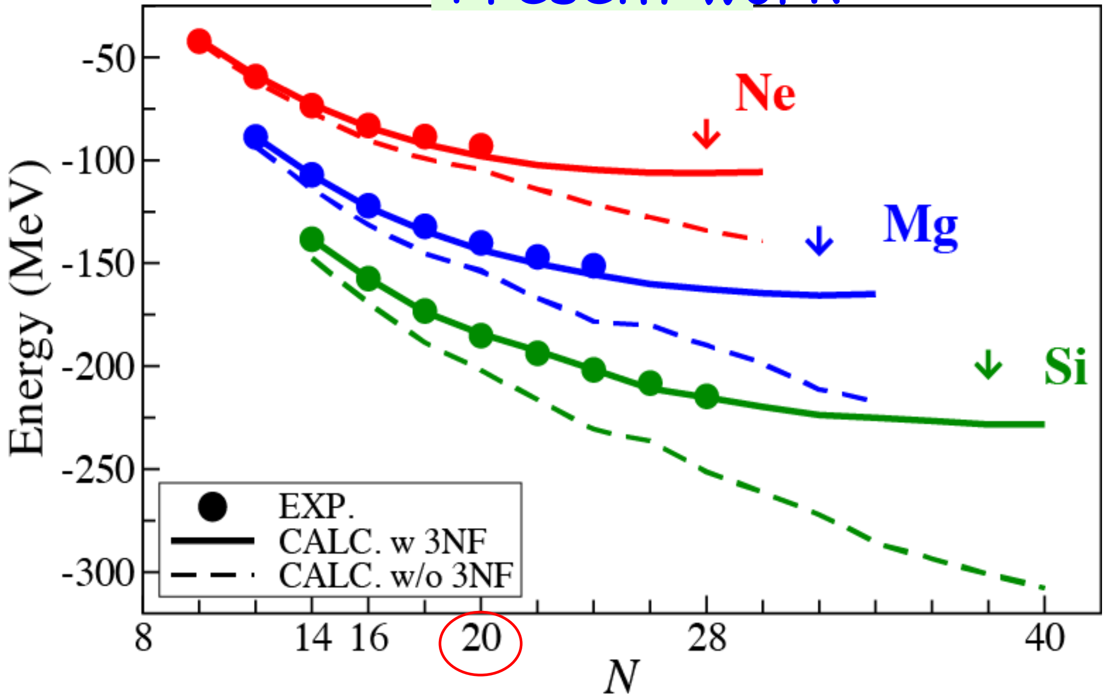
*E. M. Krenciglowa and T. T. S. Kuo, Nucl. Phys. A 235, 171 (1974).

Re-visit to the "Island of Inversion" with ab initio TBMEs

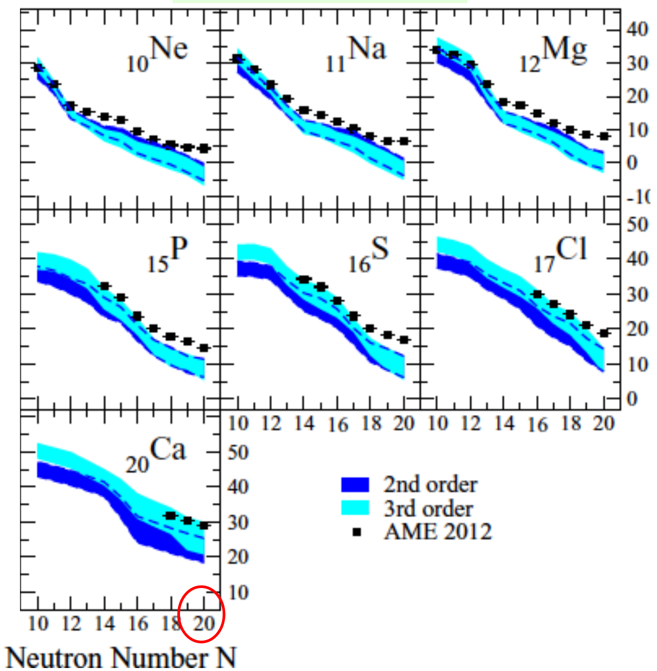
Calculations *with full sd + pf* shell

ground-state energies

Present work



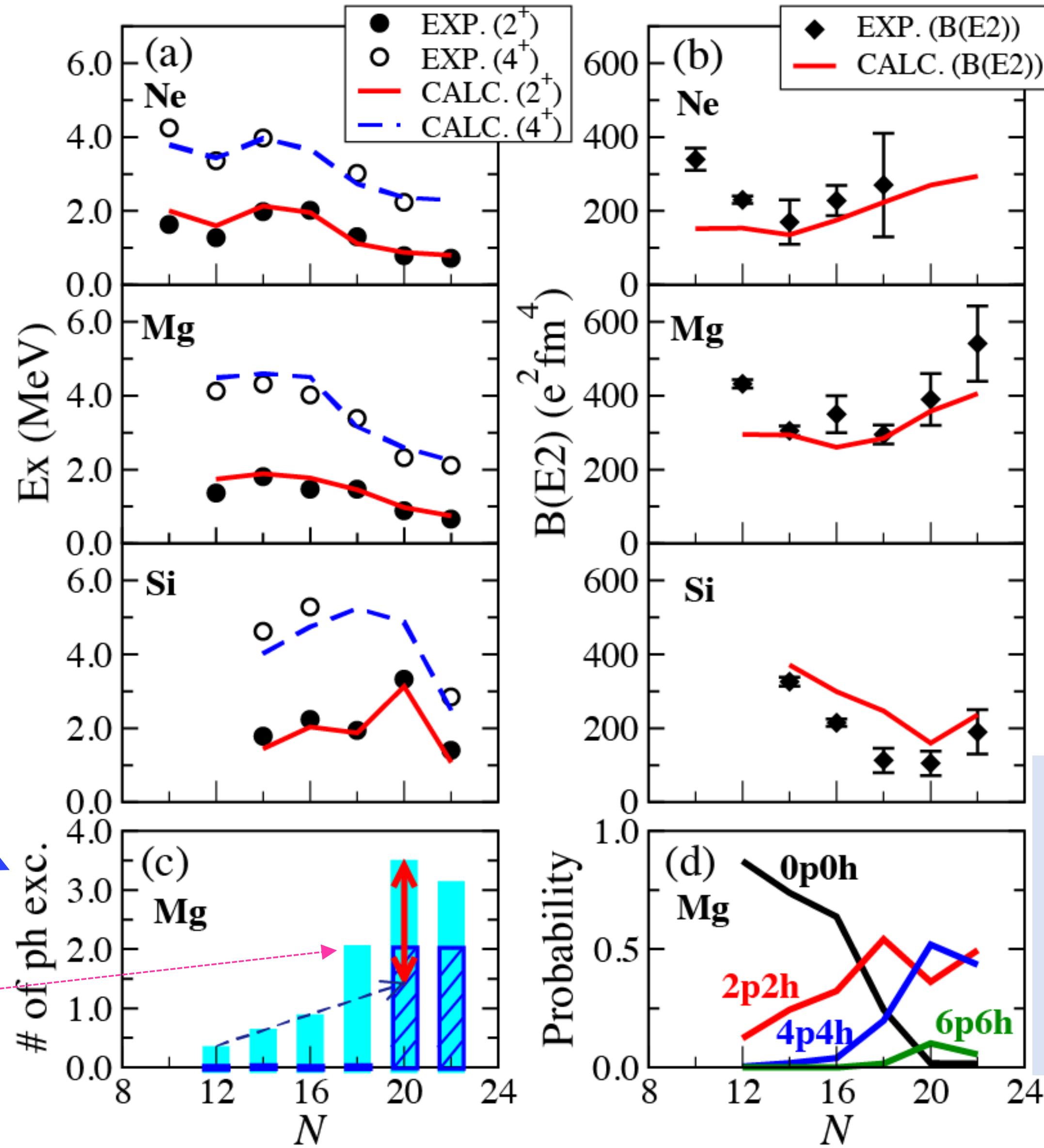
Earlier work



Simonis et al. PRC 93, 011302(R) (2016)

Ne-Mg-Si

2^+ & 4^+ levels and B(E2) values

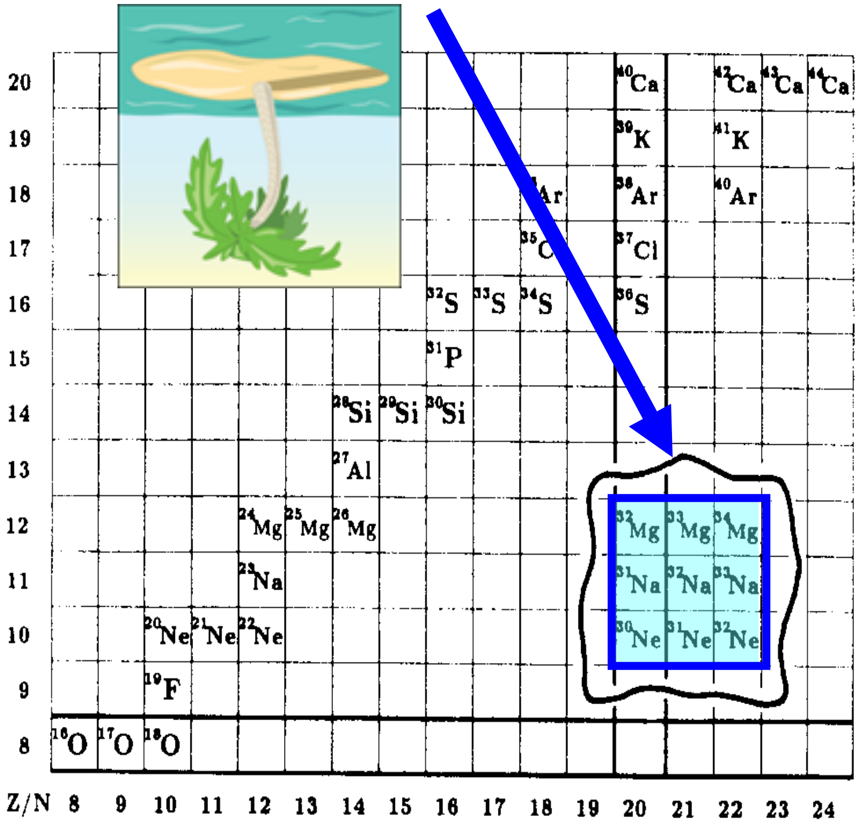


# of particle-hole excitations across N=20 gap :
(modest) steady increase
+
abrupt increase after N=18

ground states of Mg isotopes

Early idea of the Island of Inversion (WBB)
0p-0h or 2p-2h (discrete)

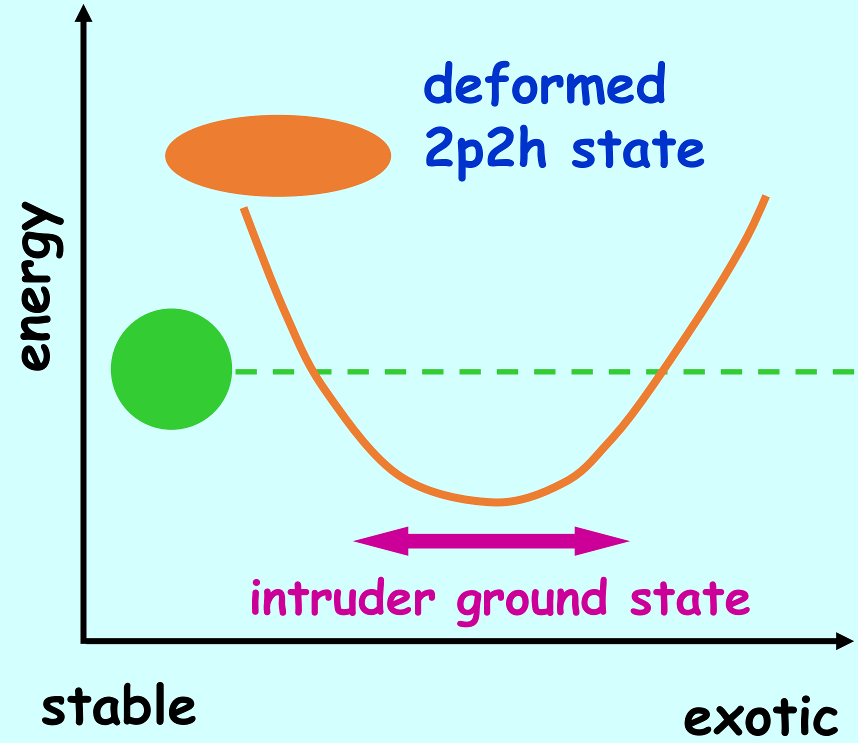
Island of Inversion

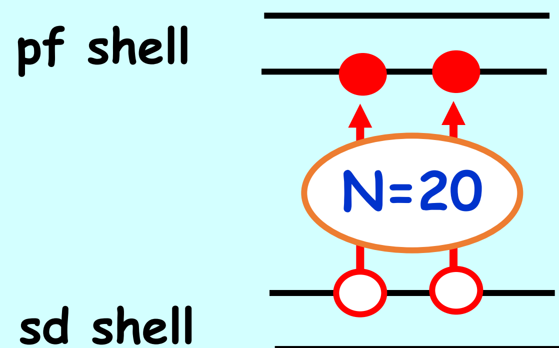


9 nuclei:
Ne, Na, Mg with N=20-22

Phys. Rev. C 41, 1147 (1990), Warburton, Becker and Brown

Basic picture was





gap ~ constant

$^{31}_{12}Mg_{19}$: *very difficult to fit* by the shell model

N3LO + 3NF by EKK

conventional interactions

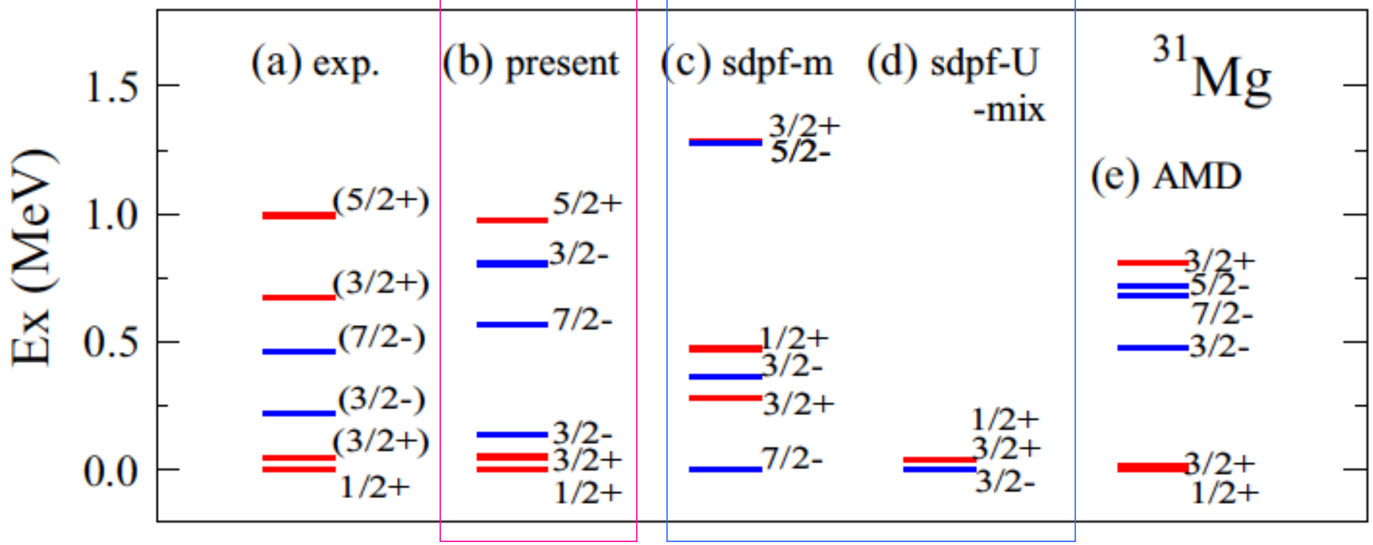


FIG. 4. Energy levels of ^{31}Mg. (a) experimental values, (b) present work, (c) sdpf-m [16], (d) sdpf-U-mix [17], and (e) AMD+GCM calculation [52].

exp. : Phys. Rev. Lett. 94, 022501 (2005), G. Neyens, *et al.*

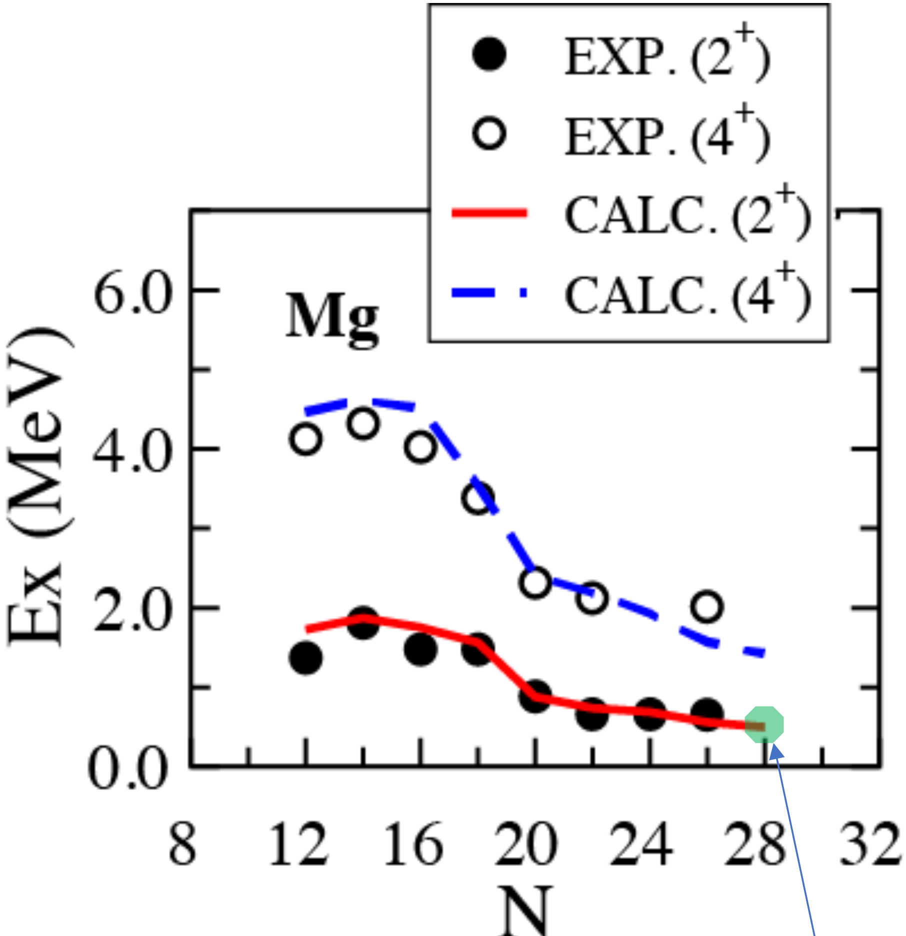
Mixing between sd and pf shells is crucial
Fit of relevant TBME's is infeasible : too many TBME's but too few data

[16] Y. Utsuno, T. Otsuka, T. Mizusaki, and M. Honma, Phys. Rev. C 60, 054315 (1999).

[17] E. Caurier, F. Nowacki, and A. Poves, Phys. Rev. C 90, 014302 (2014).

[52] M. Kimura, Phys. Rev. C 75, 041302 (2007).

Mg up to N=28   2⁺ & 4⁺ levels

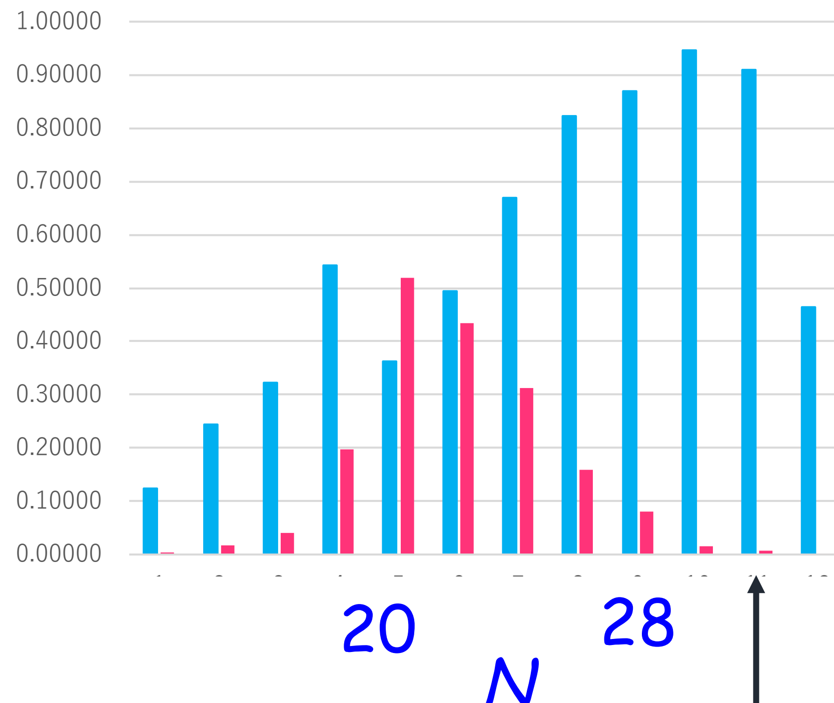


Recent data
Crawford *et al.*
(ARIS 2017 + priv. com.)

Probability of ph configurations over Z=N=20 (ground state)

2 ph excitations over N=20

4 ph excitations over N=20



our
drip line

We also found ….

χEFT based effective interaction seems to produce more particle-hole excitations than conventional phenomenological effective interactions.

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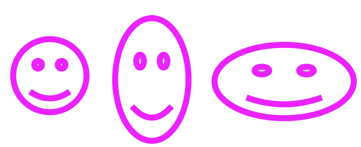
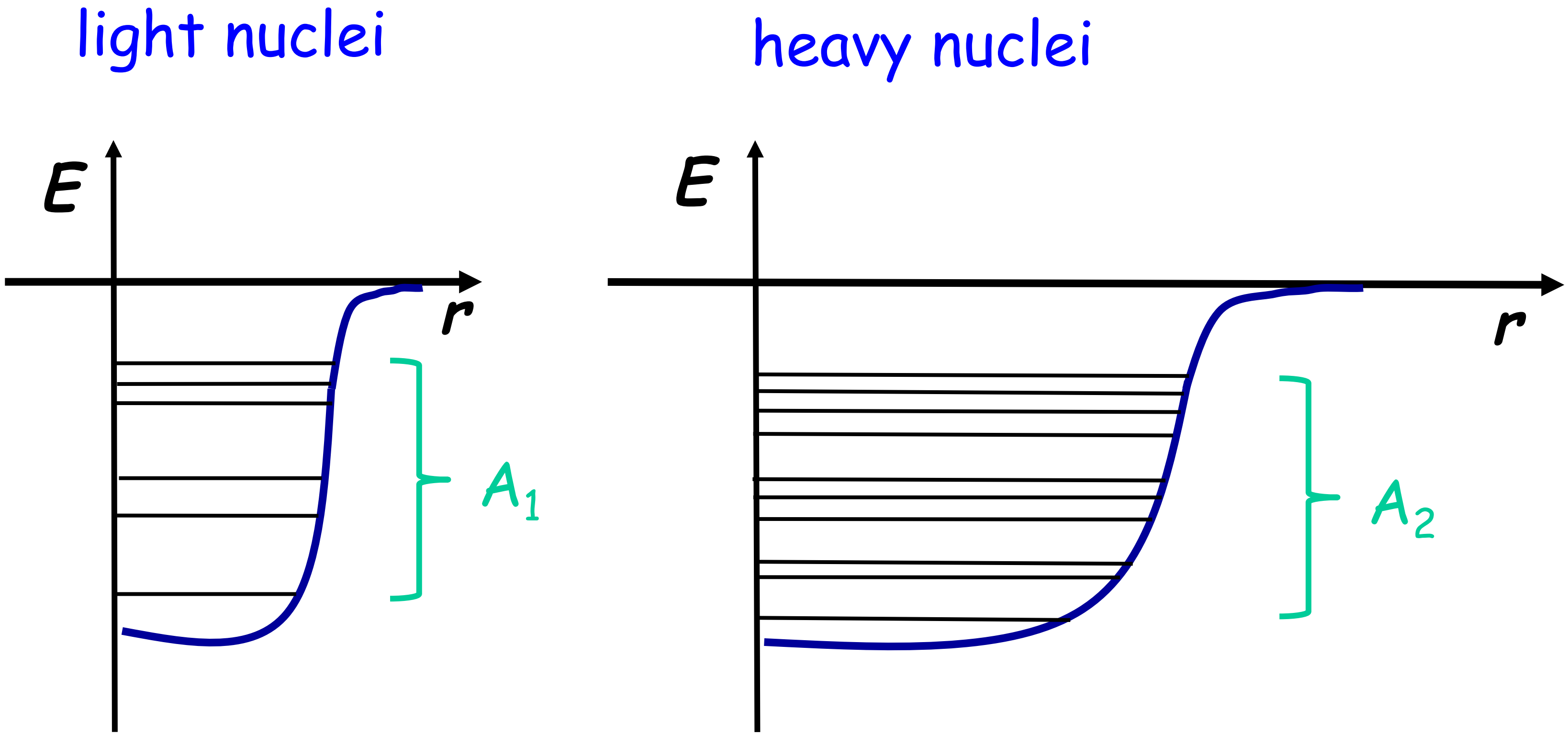
Difference between stable and exotic nuclei

	stable nuclei	exotic nuclei
life time	infinite or long	short
number	~300	7000 ~ 10000
properties density	constant inside (density saturation)	low-density surface (halo, skin)
shell	same magic numbers (2,8,20,28, … *(1949)*)	?
shape	shape transition 	

Single-particle states - starting point -

Mean potential becomes wider so as to cast A nucleons with the same separation energy.

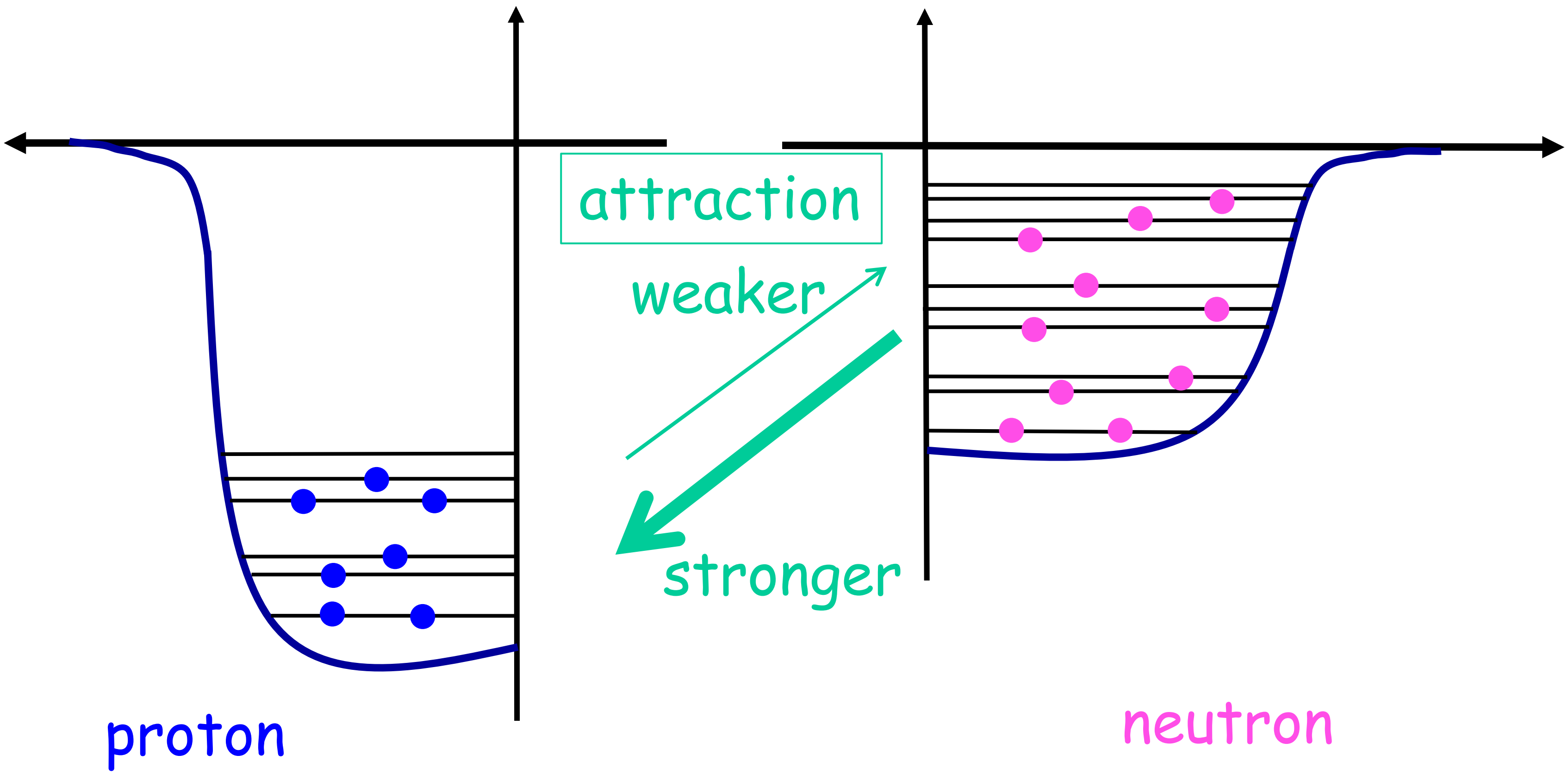


But, this is a story for stable nuclei.

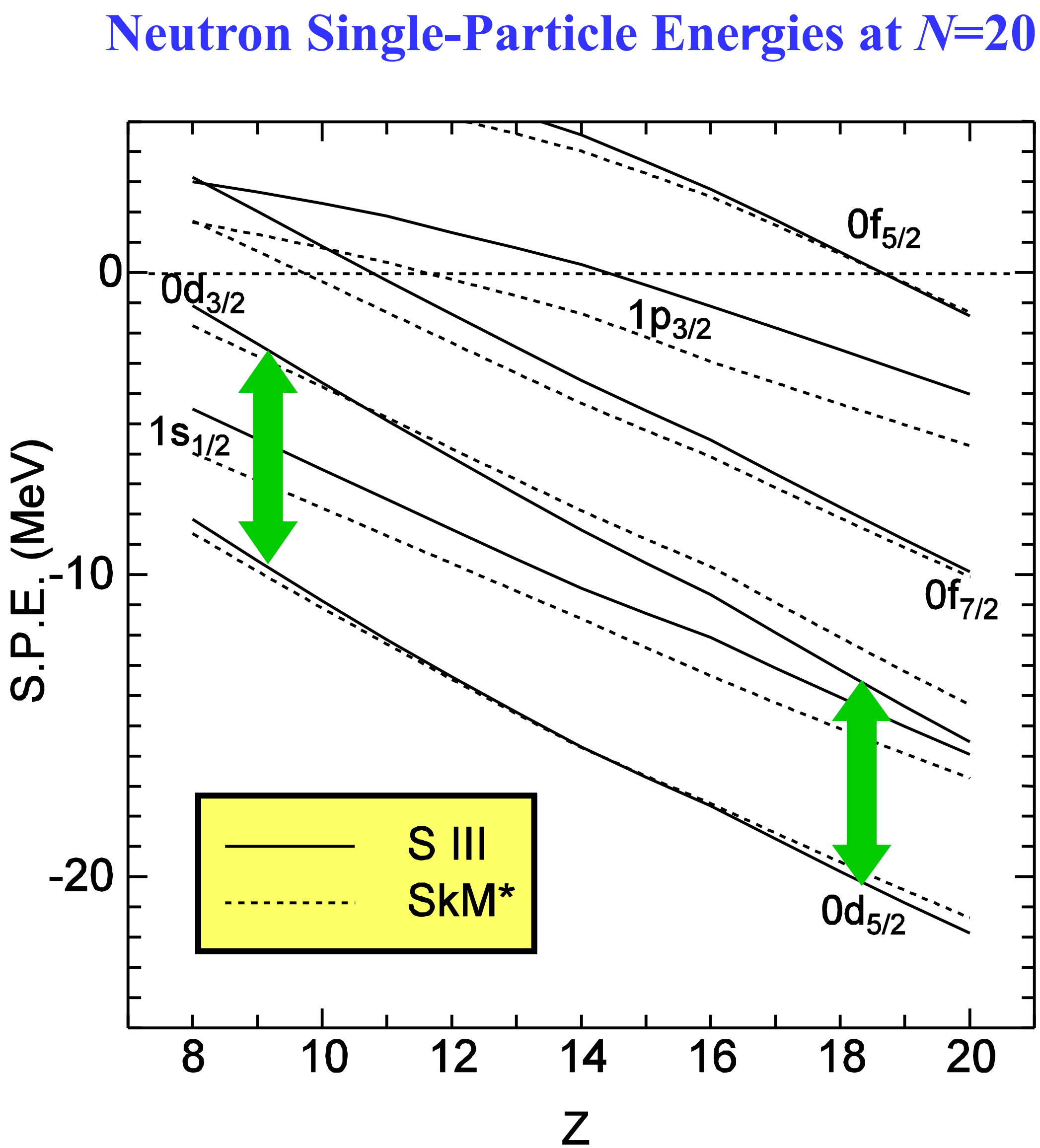
proton-neutron interaction
>> proton-proton or neutron-neutron

If Z << N, protons are more bound.

Relative relations are preserved, because only the depth changes.



Realization in Hartree-Fock energies by Skyrme model



The shell structure remain rather unchanged

-- orbitals shifting together

-- change of potential depth

~ Woods-Saxon.

From simple but general properties as,

density saturation
+ short-range *NN* interaction
+ spin-orbit splitting

→ **Mayer-Jensen's magic number with rather constant gaps**
(except for gradual A dependence)

robust feature -> no way out ???

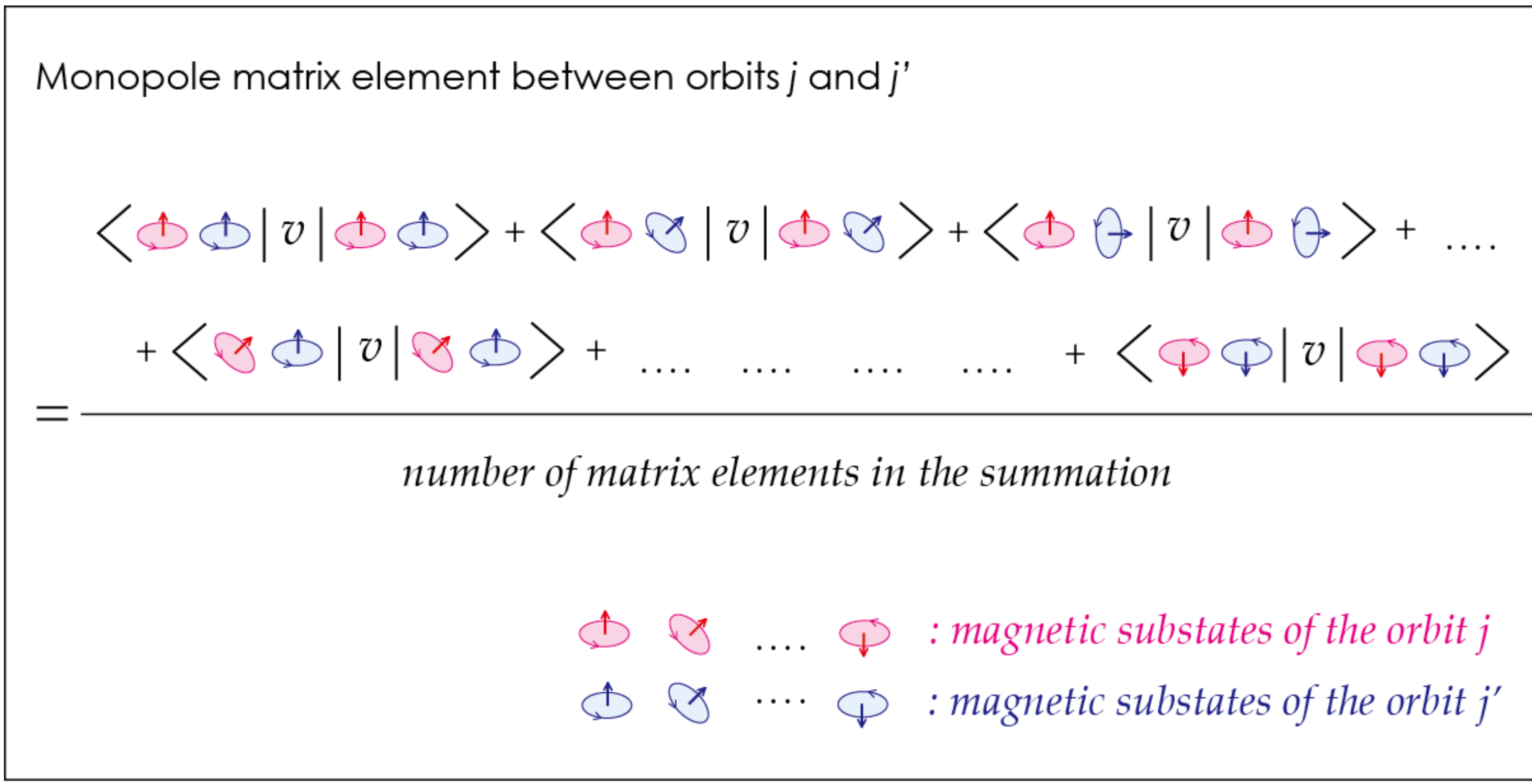
This has been one of the major objectives of nuclear structure physics in recent years.

Let's see what occurs
in the shell structure
of exotic nuclei.

Monopole matrix element between orbits *j* and *j'*

$$V^{m}_{nn}(j,j') = \frac{\sum_{(m,m')} \langle j,m\,;\,j',m' | \hat{v}_{nn} | j,m\,;\,j',m' \rangle}{\sum_{(m,m')} 1},$$

v_{nn} is interaction; *m*, *m'* are magnetic substates



Monopole matrix elements can be written equivalently by usual TBMEs as

$$V_T^m(j,j') = \frac{\sum_J (2J+1)\langle j,j';J,T|\hat{v}|j,j';J,T\rangle}{\sum_J (2J+1)}.$$

$$\text{for } T = 0 \text{ and } 1,$$

Monopole interaction for n-n (or p-p) interaction is defined as

$$\hat{v}_{nn}^m(j,j') = \left\{ \boxed{\begin{array}{ll} V_{nn}^m(j,j)\,\frac{1}{2}\,\hat{n}_j\,(\hat{n}_j - 1) & \text{for } j = j' \\ \\ V_{nn}^m(j,j')\,\hat{n}_j\,\hat{n}_{j'} & \text{for } j \neq j' \end{array}} \right.$$

T=1 part of the p-n monopole interaction is given as

$$\hat{v}_{pn,mono,T=1} = \sum_{j,j'} V^m_{T=1}(j,j')\,\frac{1}{2}\,\hat{n}^p_j\,\hat{n}^n_{j'}$$
$$+\sum_{j<j'} V^m_{T=1}(j,j')\,\frac{1}{2}\left\{\hat{\tau}^+_j\hat{\tau}^-_{j'} + \hat{\tau}^-_j\hat{\tau}^+_{j'}\right\}$$
$$+\sum_{j} V^m_{T=1}(j,j)\,\frac{1}{2} : \hat{\tau}^+_j\hat{\tau}^-_j : .$$

Finally, we get the full expression for the p-n interaction

$$\hat{v}_{pn,mono} = \sum_{j,j'} \frac{1}{2}\left\{V^m_{T=0}(j,j') + V^m_{T=1}(j,j')\right\} \boxed{\hat{n}^p_j\,\hat{n}^n_{j'}}$$
$$-\sum_{j<j'} \frac{1}{2}\left\{V^m_{T=0}(j,j') - V^m_{T=1}(j,j')\right\}$$
$$\left\{\hat{\tau}^+_j\hat{\tau}^-_{j'} + \hat{\tau}^-_j\hat{\tau}^+_{j'}\right\}$$
$$-\sum_{j} \frac{1}{2}\left\{V^m_{T=0}(j,j) - V^m_{T=1}(j,j)\right\} : \hat{\tau}^+_j\hat{\tau}^-_j : .$$

This is consistent with the final form of the monopole interaction of Poves and Zuker (Phys. Rep. 70, 235 (1981)) besides different formulation.

$$
\begin{aligned}
\hat{v}_{pn,mono} = & \sum_{j,j'} \frac{1}{2}\left\{V^{m}_{T=0}(j,j') + V^{m}_{T=1}(j,j')\right\} \hat{n}^{p}_{j}\,\hat{n}^{n}_{j'} \\
& - \sum_{j<j'} \frac{1}{2}\left\{V^{m}_{T=0}(j,j') - V^{m}_{T=1}(j,j')\right\} \\
& \qquad \left\{\hat{\tau}^{+}_{j}\hat{\tau}^{-}_{j'} + \hat{\tau}^{-}_{j}\hat{\tau}^{+}_{j'}\right\} \\
& - \sum_{j} \frac{1}{2}\left\{V^{m}_{T=0}(j,j) - V^{m}_{T=1}(j,j)\right\} :\hat{\tau}^{+}_{j}\hat{\tau}^{-}_{j}:
\end{aligned}
$$

The second and third terms can be visualized as shown in the figure.

They are still monopole, but proton and neutron must exchange their states !

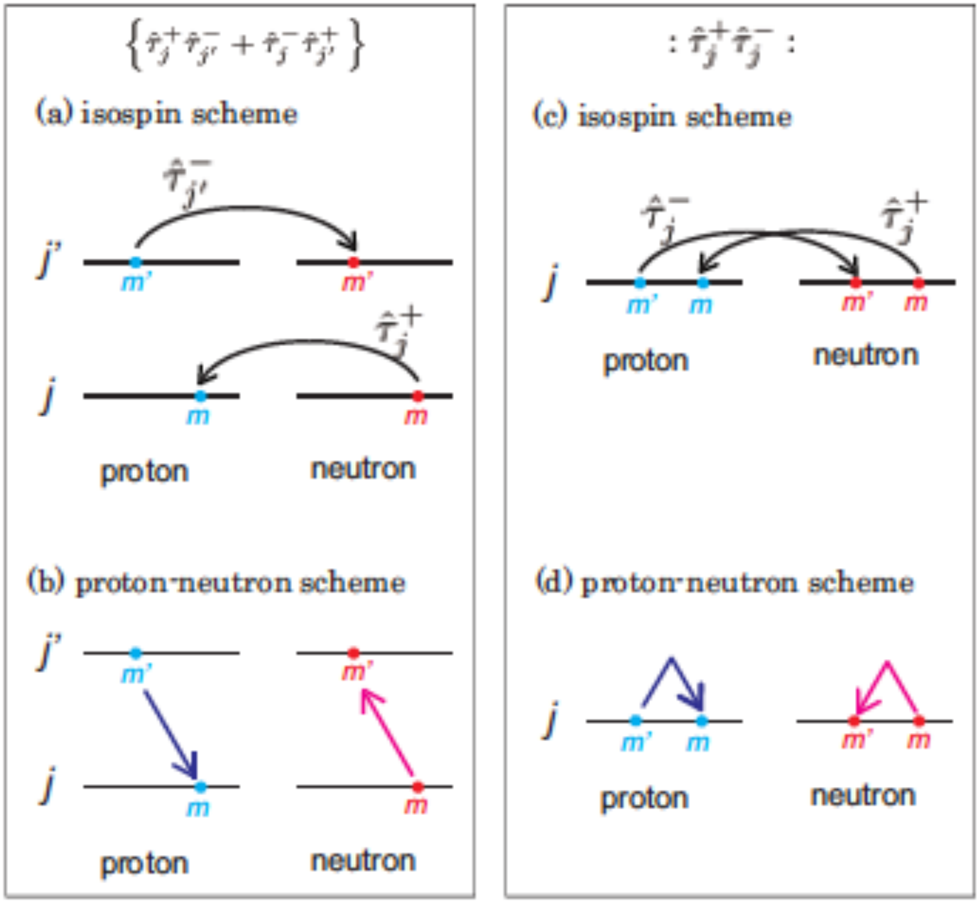


Figure 16 Implication of $\hat{\tau}^{+}_{j}\hat{\tau}^{-}_{j'}$ terms. Panels (a) and (c) are for the $\{\hat{\tau}^{+}_{j}\hat{\tau}^{-}_{j'} + \hat{\tau}^{-}_{j}\hat{\tau}^{+}_{j'}\}$ and $:\hat{\tau}^{+}_{j}\hat{\tau}^{-}_{j}:$ cases in the isospin scheme, respectively. Panels (b) and (d) are similar to (a) and (c), respectively, in the proton-neutron scheme. The magnetic substates are indicated by m and m'.

Effective single-particle energy (ESPE)

$$\epsilon_j = \epsilon_j^0 + \hat{\epsilon}_j \ .$$

Contribution from valence nucleons through the monopole interaction

contribution from the inert core (closed shell) ; constant within a given nucleus

ESPEs are given for protons and neutrons as

$$\hat{\epsilon}_j^p = \sum_{j'} V_{T=1}^m(j,j')\,\hat{n}_{j'}^p + \sum_{j'} \boxed{V_{pn}^m}(j,j')\,\hat{n}_{j'}^n$$

$$\hat{\epsilon}_j^n = \sum_{j'} V_{T=1}^m(j,j')\,\hat{n}_{j'}^n + \sum_{j'} \boxed{V_{pn}^m}(j',j)\,\hat{n}_{j'}^p .$$

where $\boxed{V_{pn}^m}(j,j') = \frac{1}{2}\left\{\tilde{V}_{T=0}^m(j,j') + \boxed{\tilde{V}_{T=1}^m}(j,j')\right\}$ and

$$\boxed{\tilde{V}_{T=0,1}^m}(j,j') = V_{T=0,1}^m(j,j') \quad \text{for} \quad j \neq j' ,$$

$$\boxed{\tilde{V}_{T=0}^m}(j,j) = V_{T=0}^m(j,j)\,\frac{2j+2}{2j+1} ,$$

and

$$\boxed{\tilde{V}_{T=1}^m}(j,j) = V_{T=1}^m(j,j)\,\frac{2j}{2j+1} .$$

with approximation $\quad - :\hat{\tau}_j^+\hat{\tau}_j^- : \sim \dfrac{\hat{n}_j^p\hat{n}_j^n}{2j+1}$

Usually ESPEs are discussed for their differences.

The differences of ESPEs are given
for protons

$$\Delta \hat{\epsilon}_j^p = \sum_{j'} V_{T=1}^m(j,j')\,\Delta \hat{n}_{j'}^p + \sum_{j'} V_{pn}^m(j,j')\,\Delta \hat{n}_{j'}^n \ ,$$

for neutrons

$$\Delta \hat{\epsilon}_j^n = \sum_{j'} V_{T=1}^m(j,j')\,\Delta \hat{n}_{j'}^n + \sum_{j'} V_{pn}^m(j',j)\,\Delta \hat{n}_{j'}^p$$

For a chain of isotopes, $\Delta \hat{n}_{j'}^n$ is the change of the neutron number.

Shell evolution

Monopole matrix element of the central force with a gaussian dependence on the distance.

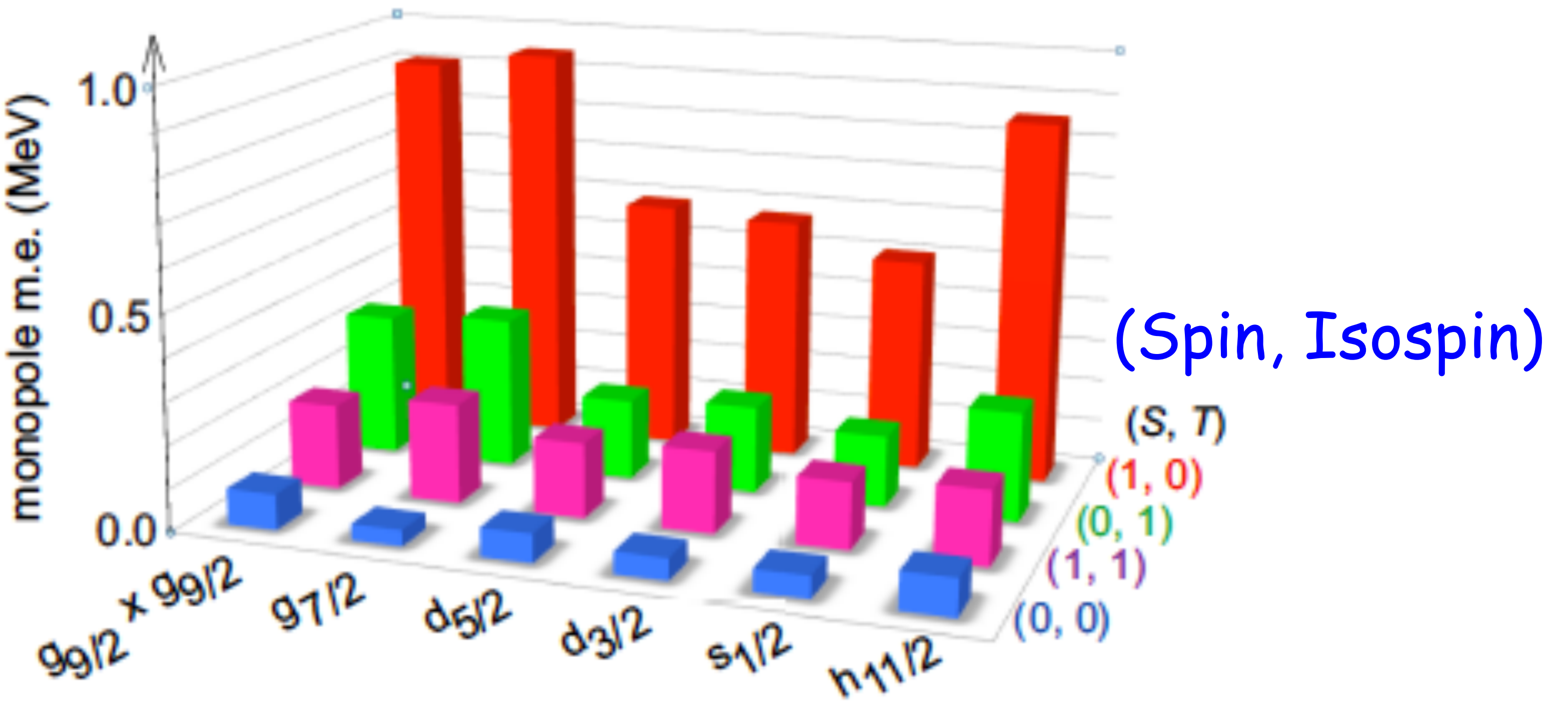


Figure 24 Monopole matrix elements of central gaussian interactions for (S,T) channels with an equal strength parameter (see the text). One of the orbit is $1g_{9/2}$, and the other is shown.

Monopole interaction from a central force : A=100

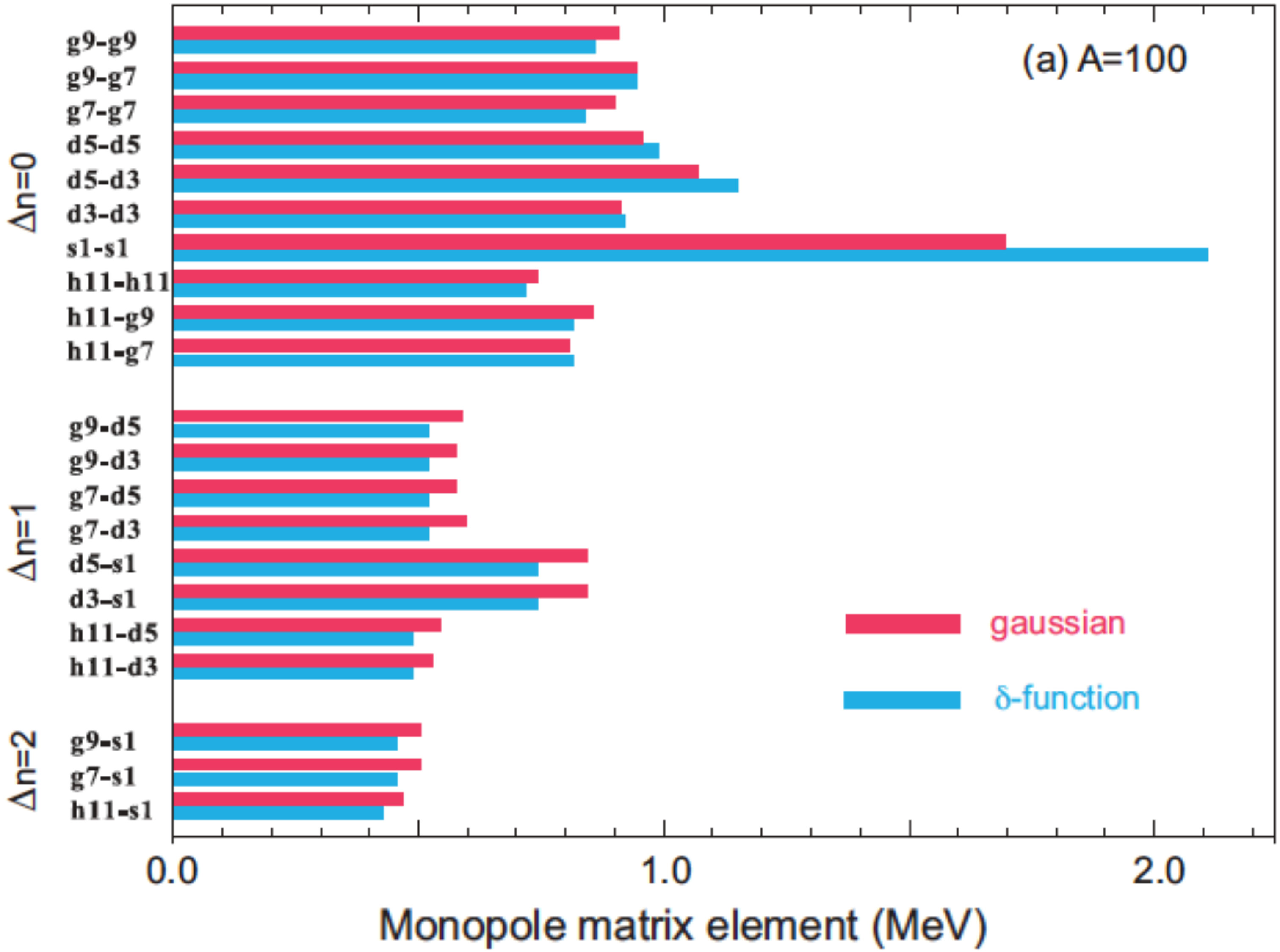


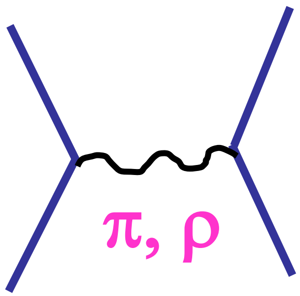
Figure 26 Monopole matrix elements of central gaussian and delta interactions for $(S = 1, T = 0)$ channel. The orbit labeling is abbreviated like g9 for $1g_{9/2}$, *etc.* The orbits are from valence shell for (a) $A = 100$ and (b) $A = 70$.

Besides central corce,
another important contribution
comes from the tensor force

Tensor Force

π meson : primary source

ρ meson (~ π+π) : minor (~1/4) cancellation



Ref: Osterfeld, Rev. Mod. Phys. 64, 491 (92)

Multiple pion exchanges
→ strong effective central forces in *NN* interaction
(as represented by σ meson, *etc*.)
→ nuclear binding

Presently : First-order tensor-force effect
(at medium and long ranges)

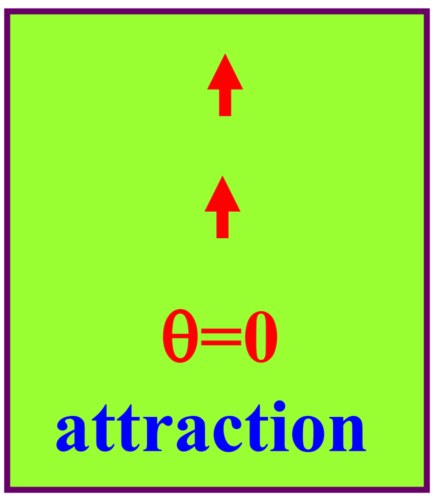
One pion exchange → Tensor force

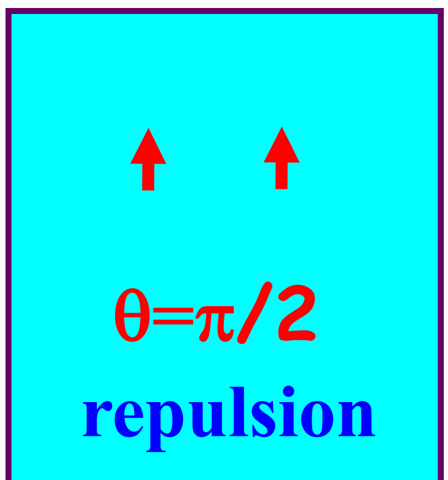
How does the tensor force work ?

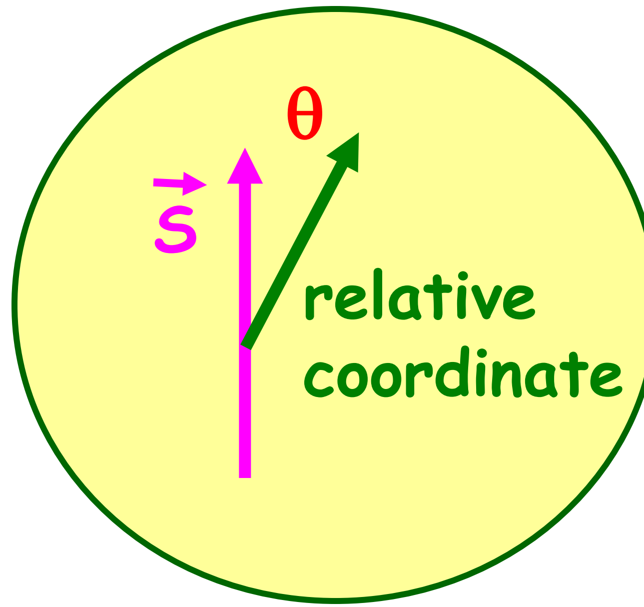
Spin of each nucleon ↑ is parallel, because the total spin must be S=1

The potential has the following dependence on the angle θ with respect to the total spin $\vec{S}$.

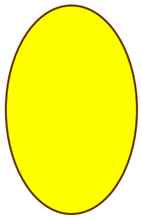
$$V \sim Y_{2,0} \sim 1 - 3\cos^2\theta$$







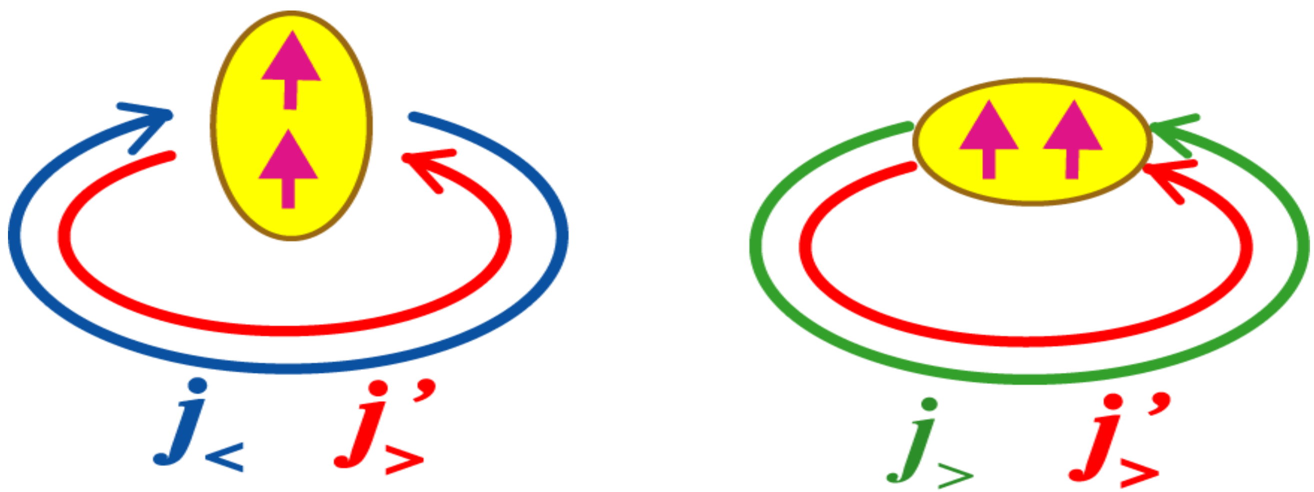
Monopole effects due to the tensor force



wave function of relative motion

spin of nucleon

large relative momentum　　　small relative momentum



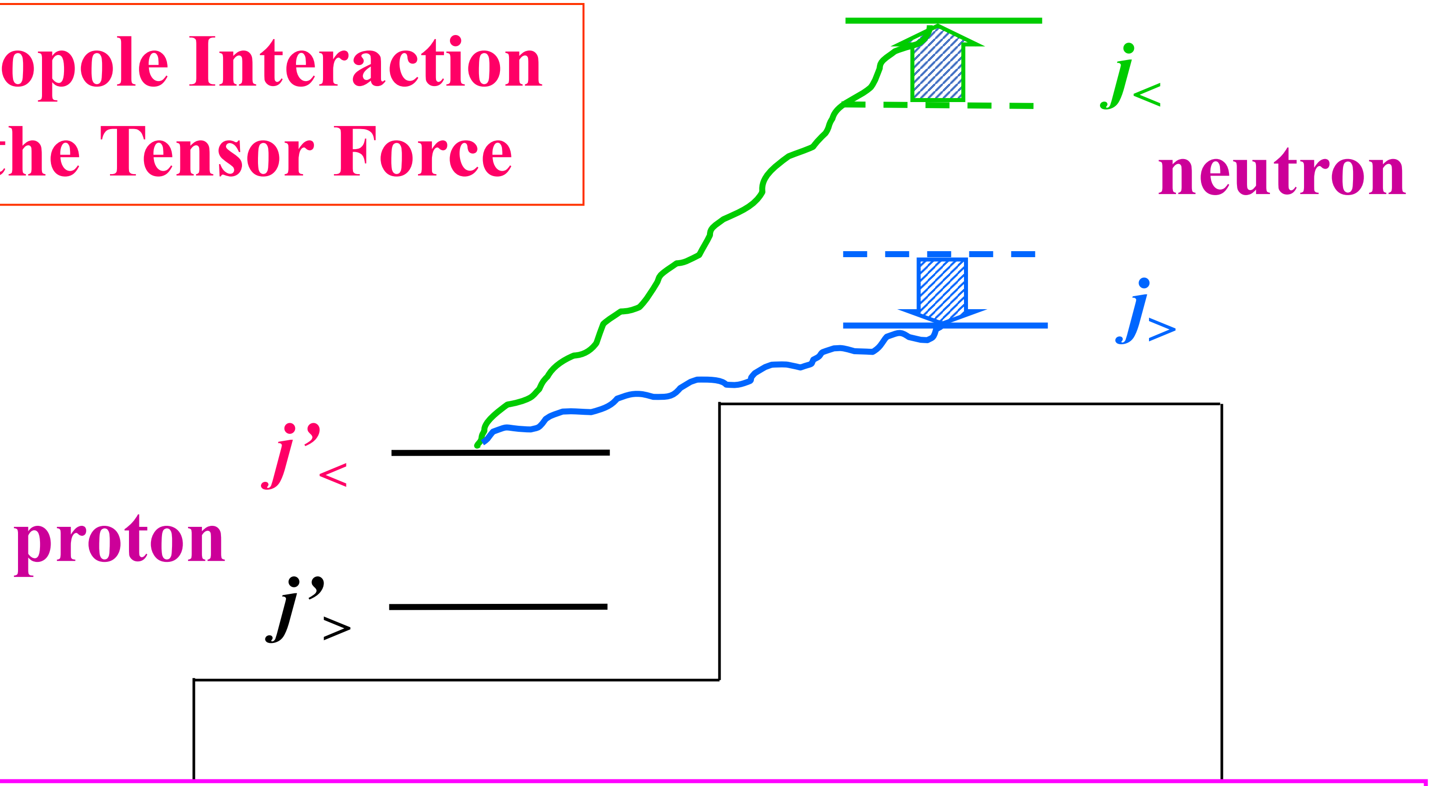
attractive　　　**repulsive**

$j_> = l + \frac{1}{2}$, $j_< = l - \frac{1}{2}$

TO *et al.*, Phys. Rev. Lett. 95, 232502 (2005)

T. Otsuka et al., Phys. Rev. Lett. 95, 232502 (2005)

Monopole Interaction of the Tensor Force



Identity for tensor monopole interaction

$$(2j_> + 1)\ v_{m,T}^{(j'j_>)} + (2j_< + 1)\ v_{m,T}^{(j'j_<)} = 0$$

$v_{m,T}$: monopole strength for isospin T

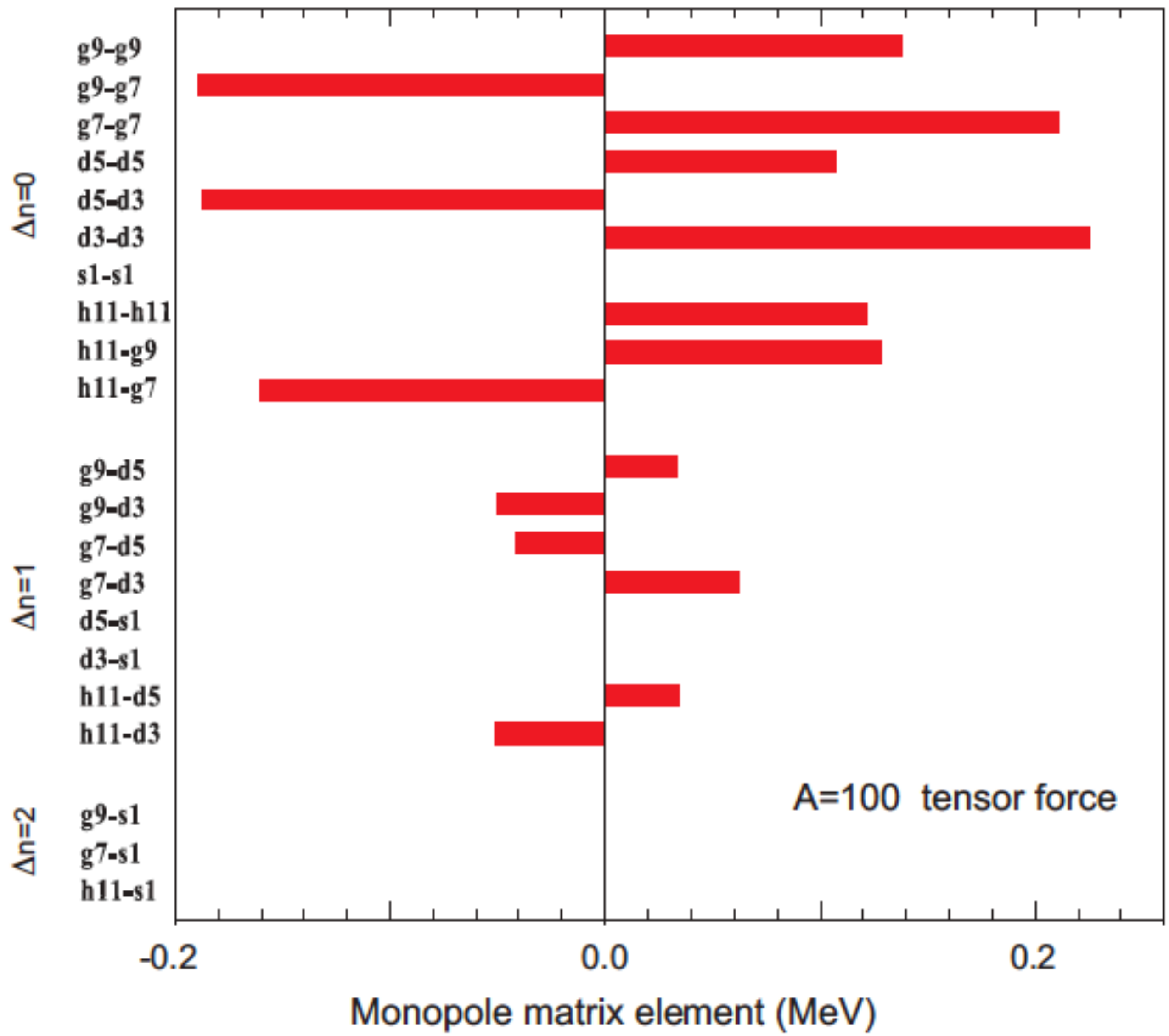
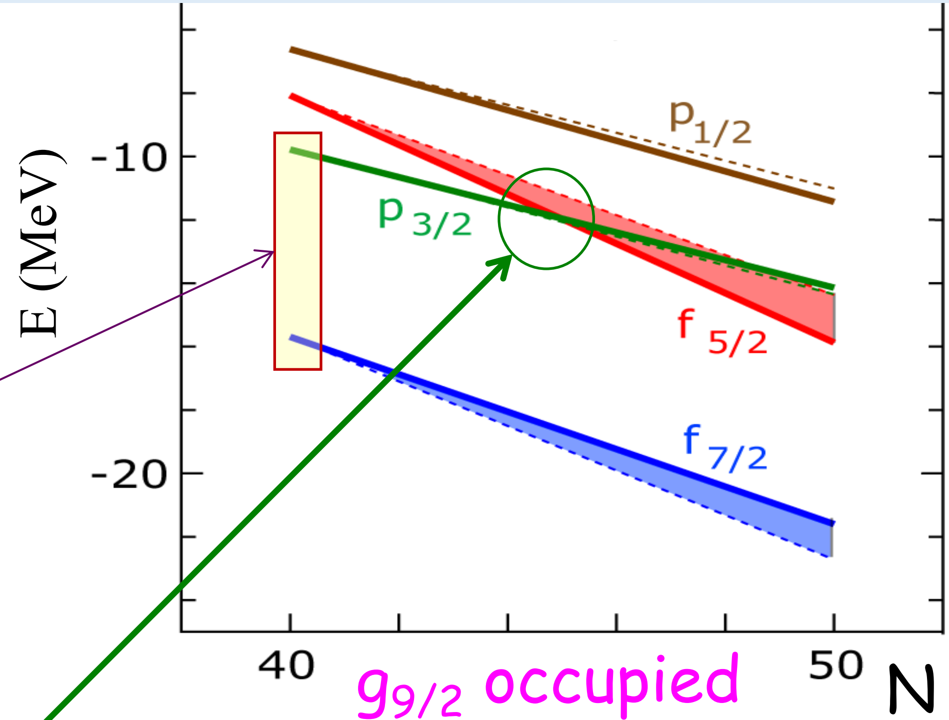


Figure 33 Monopole matrix elements of the tensor force in the T=0 channel. The orbit labeling is abbreviated like g9 for $1g_{9/2}$, *etc.* The orbits are from valence shell for A = 100.

Proton single-particles levels of Ni isotopes



$g_{9/2}$ occupied

Central Gaussian + Tensor

solid line: full effect

dotted line: central only

shaded area : effect of tensor force

From Grawe, EPJA25, 357

Crossing here is consistent with exp. on Cu isotopes

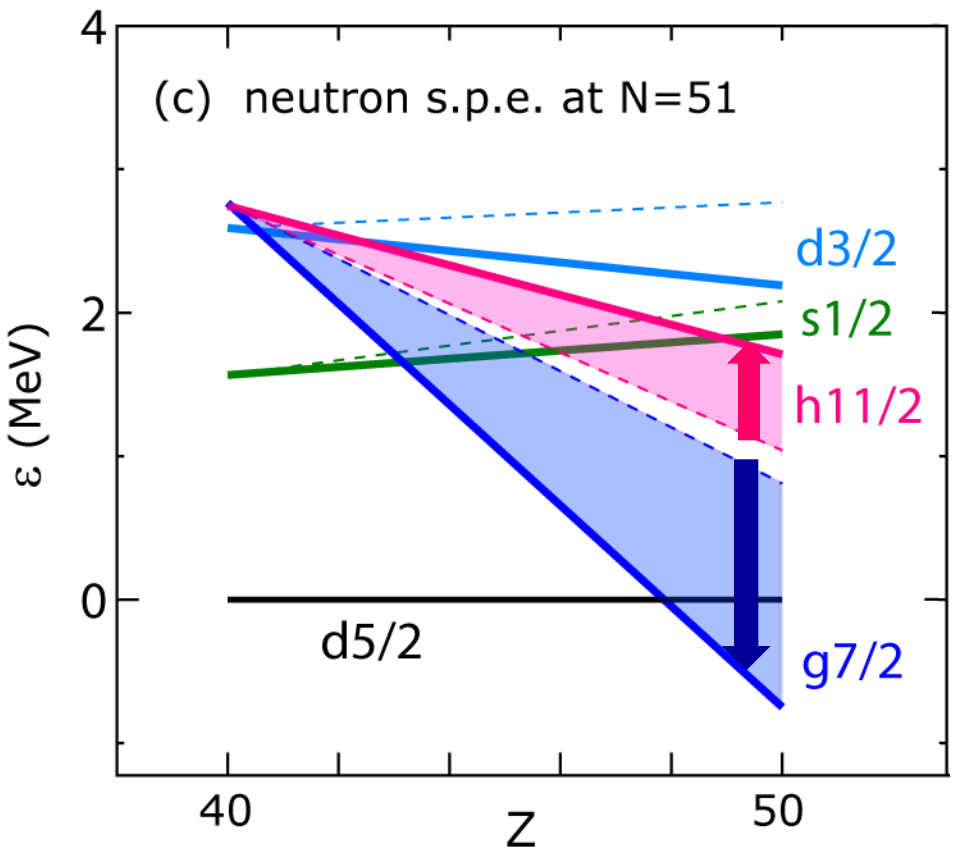
PRL 103, 142501 (2009) PHYSICAL REVIEW LETTERS week ending 2 OCTOBER 2009

Nuclear Spins and Magnetic Moments of ^{71,73,75}Cu: Inversion of $\pi 2p_{3/2}$ and $\pi 1f_{5/2}$ Levels in ^{75}Cu

K. T. Flanagan,[1,2] P. Vingerhoets,[1] M. Avgoulea,[1] J. Billowes,[3] M. L. Bissell,[1] K. Blaum,[4] B. Cheal,[3] M. De Rydt,[1] V. N. Fedosseev,[5] D. H. Forest,[6] Ch. Geppert,[7,8] U. Köster,[10] M. Kowalska,[11] J. Krämer,[9] K. L. Kratz,[9] A. Krieger,[9] E. Mané,[3] B. A. Marsh,[5] T. Materna,[10] L. Mathieu,[12] P. L. Molkanov,[13] R. Neugart,[9] G. Neyens,[1] W. Nörtershäuser,[9,7] M. D. Seliverstov,[13,16] O. Serot,[12] M. Schug,[4] M. A. Sjoedin,[17] J. R. Stone,[14,15] N. J. Stone,[14,15] H. H. Stroke,[18] G. Tungate,[6] D. T. Yordanov,[4] and Yu. M. Volkov[13]

[1]*Instituut voor Kern- en Stralingsfysica, Katholieke Universiteit Leuven, B-3001 Leuven, Belgium*

Shell structure of a key nucleus ^{100}Sn



solid line : full
(central + tensor)

dashed line : central only

Fedderman-Pittel (1977)

shaded area :
effect of tensor force

Exp. d5/2 and g7/2 should be close
Seweryniak et al.
Phys. Rev. Lett. 99, 022504 (2007)
Gryzywacz et al.

New magic number ?

Eigenvalues of HO potential

Magic numbers Mayer and Jensen (1949)

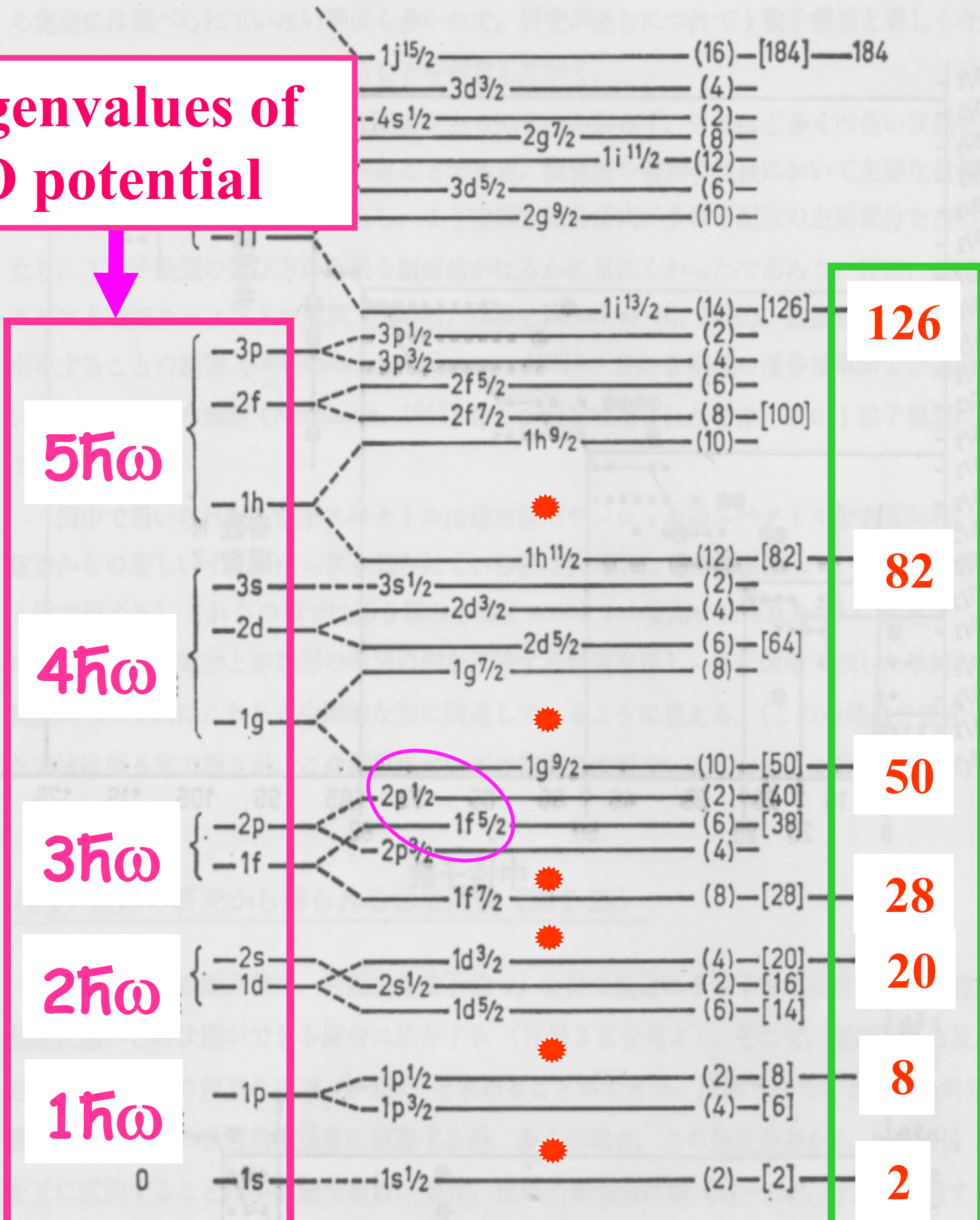
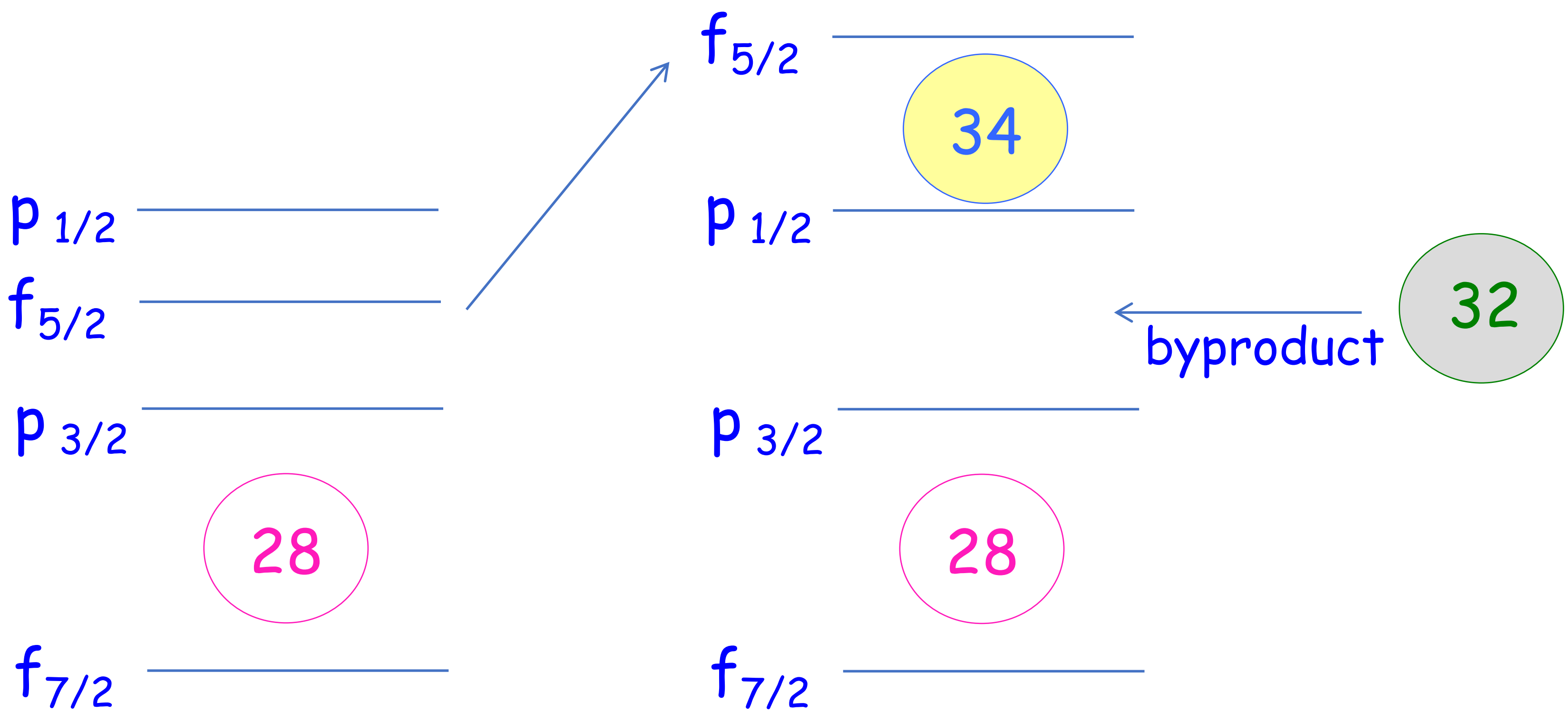


図2-23 1粒子軌道の順序．図は M. G. Mayer and J. H. D. Jensen, *Elementary Theory of Nuclear Shell Structure*, p. 58, Wiley, New York, 1955 からとった．

Basic picture

shell structure
for neutrons
in Ni isotopes
($f_{7/2}$ fully occupied)

N=34 magic number may appear
if proton $f_{7/2}$ becomes vacant (Ca)
($f_{5/2}$ becomes less bound)



Appearance of new magic number N=34

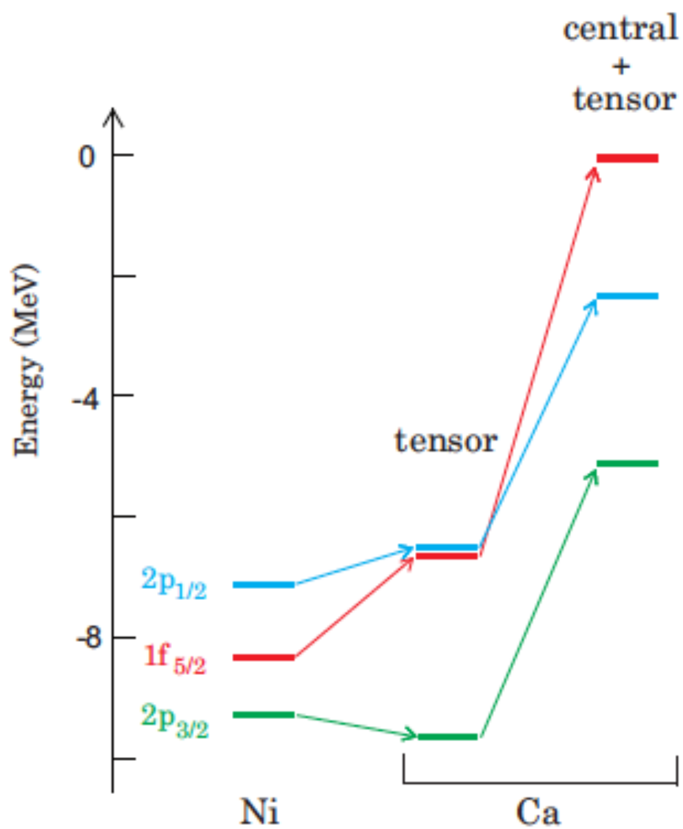


Figure 41 Change of single-particle energies from ^{56}Ni to ^{48}Ca.

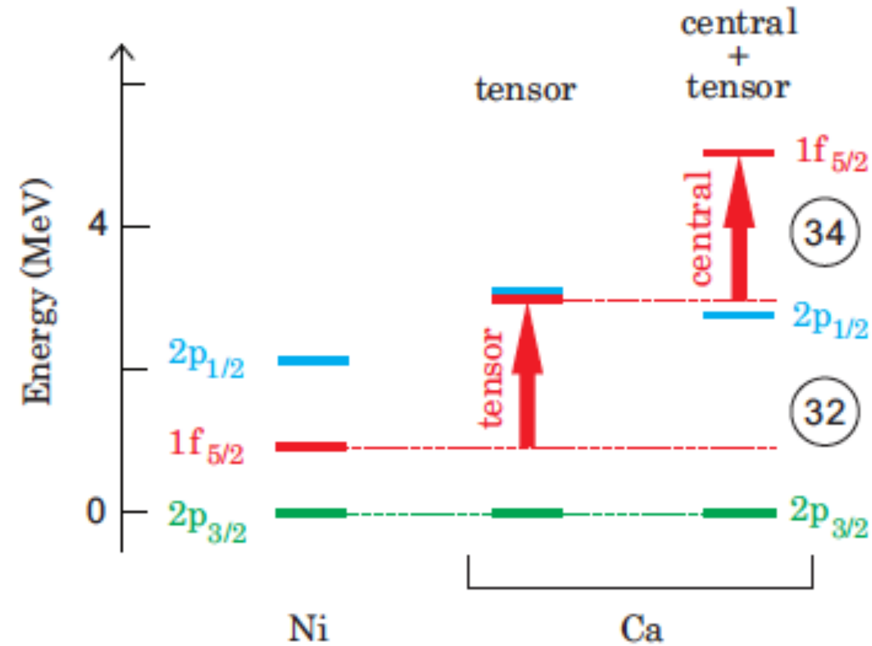
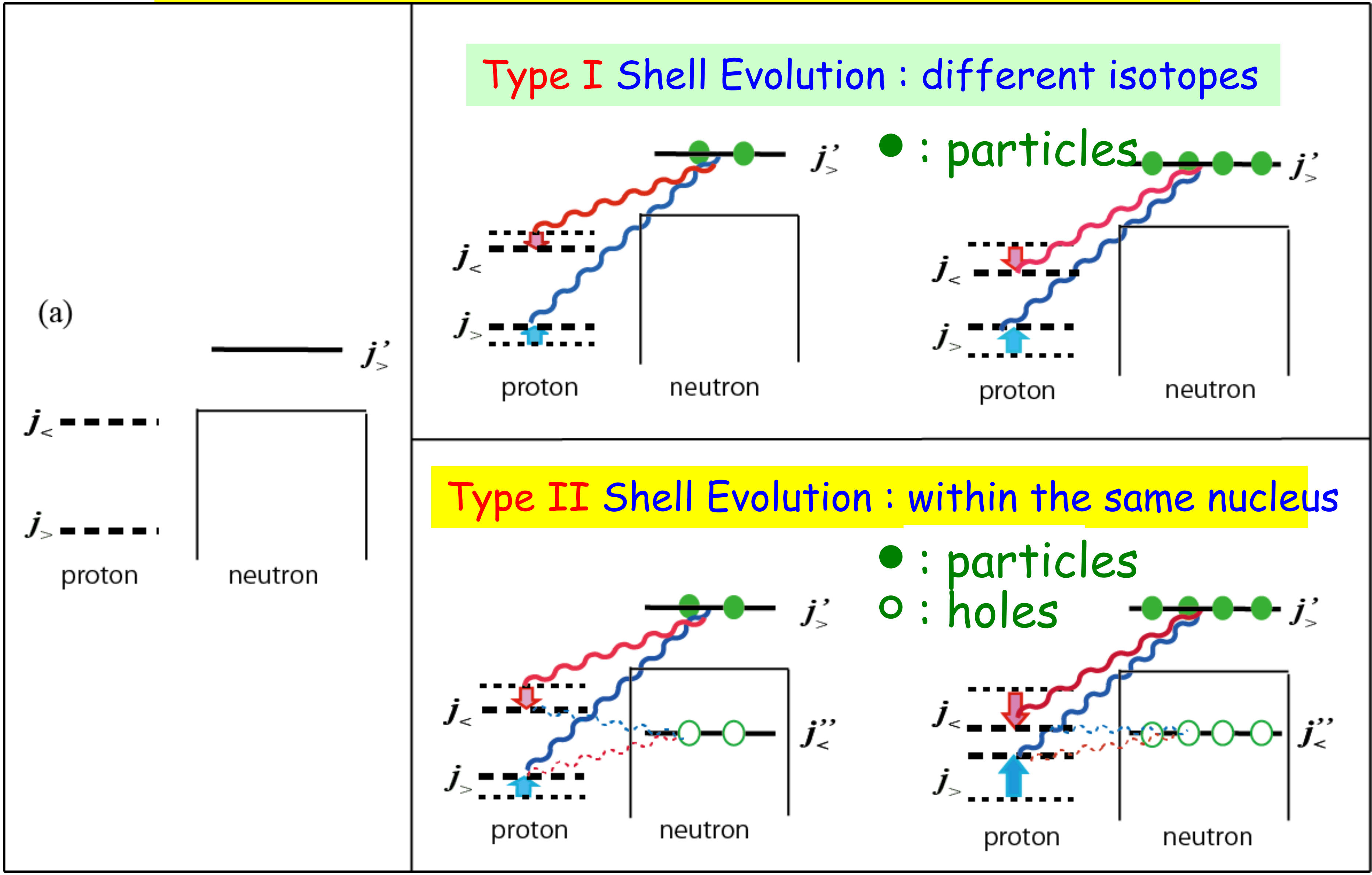


Figure 42 Change of single-particle energies from ^{56}Ni to ^{48}Ca relative to the $2p_{3/2}$ orbit. The red arrows indicate the change of the $1f_{5/2}$ ESPE. The arising magic numbers, N=32 and 34, are shown in black circles.

Shell Evolution - from Type I to Type II -



TO and Y. Tsunoda, J. Phys. G: Nucl. Part. Phys. 4

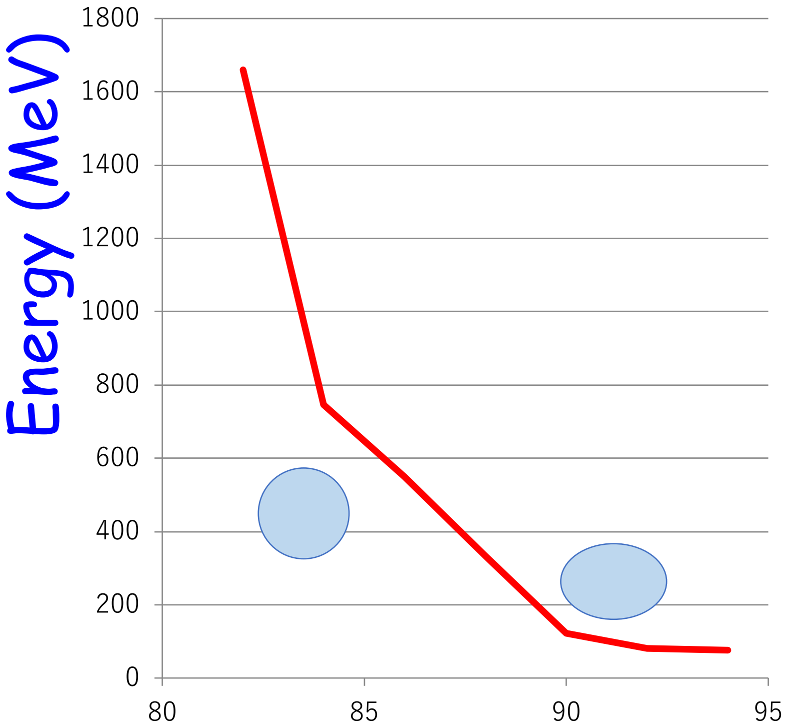
Quantum Phase Transition

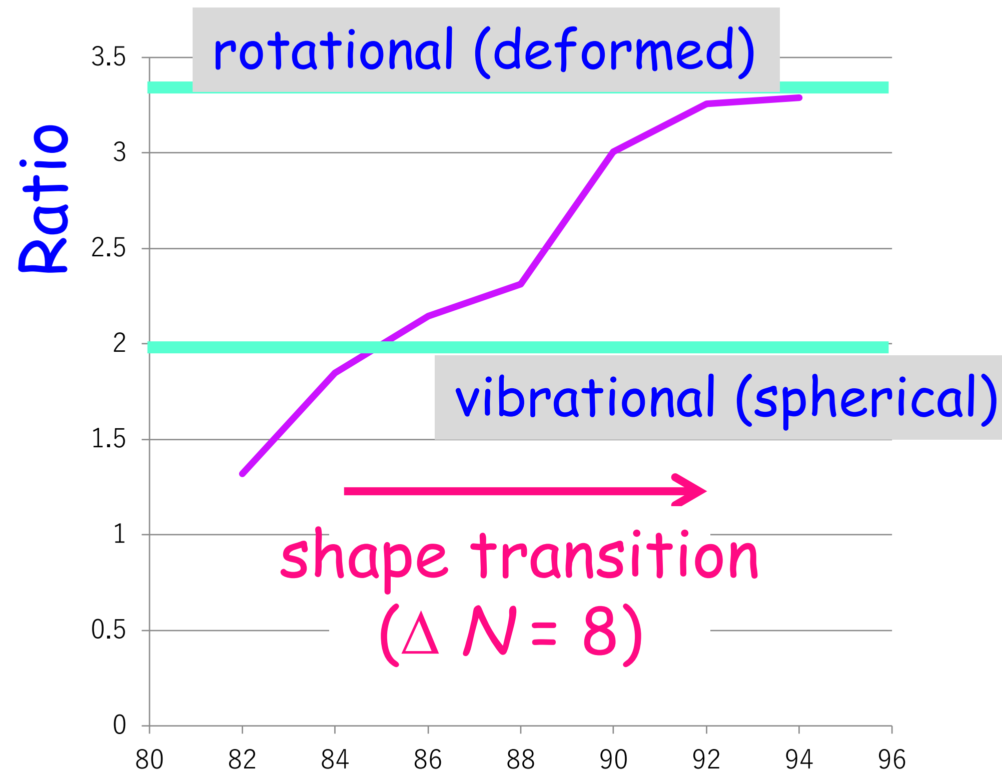
Shape change as a function of *N* (or *Z*)

2^+ and 4^+ level properties of Sm isotopes

Ex (2^+) :
excitation energy of first 2^+ state

$R_{4/2}$ = Ex (4^+) / Ex(2^+)





Neutron number, *N*

Neutron number, *N*

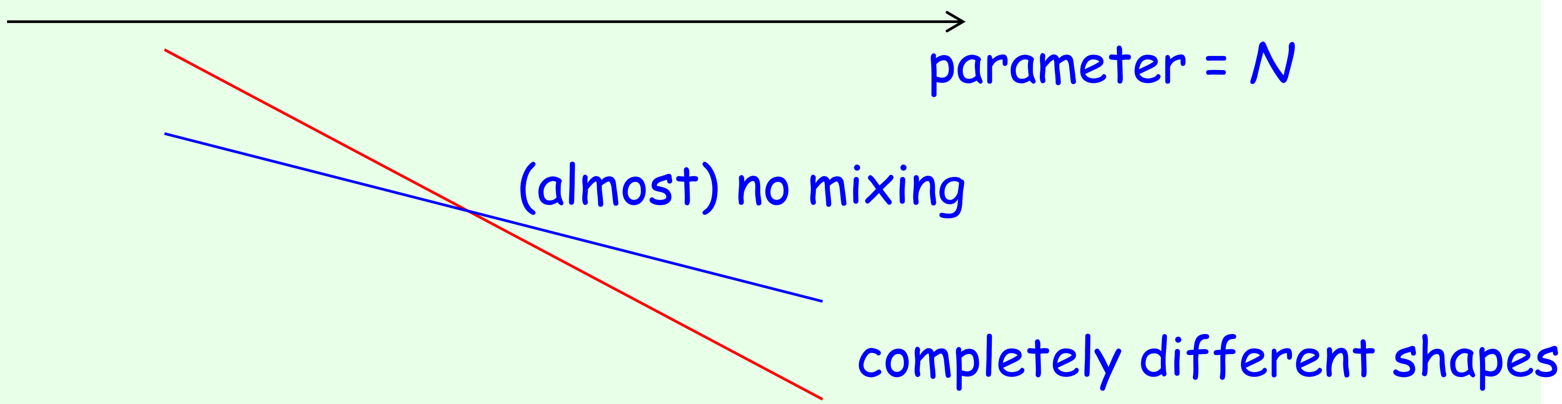
Can this be a kind of *Phase Transition* ?

Can the shape transition be a "Quantum Phase Transition" ?

The shape transition occurs rather gradually.

The definition of Quantum Phase Transition :
an abrupt change in the ground state of a many-body system by varying a physical parameter at zero temperature. (*cf., Wikipedi*

possible scenario



Sizable mixing occurs usually in finite quantum systems.

An example : shapes of Zr isotopes by Monte Carlo Shell Model

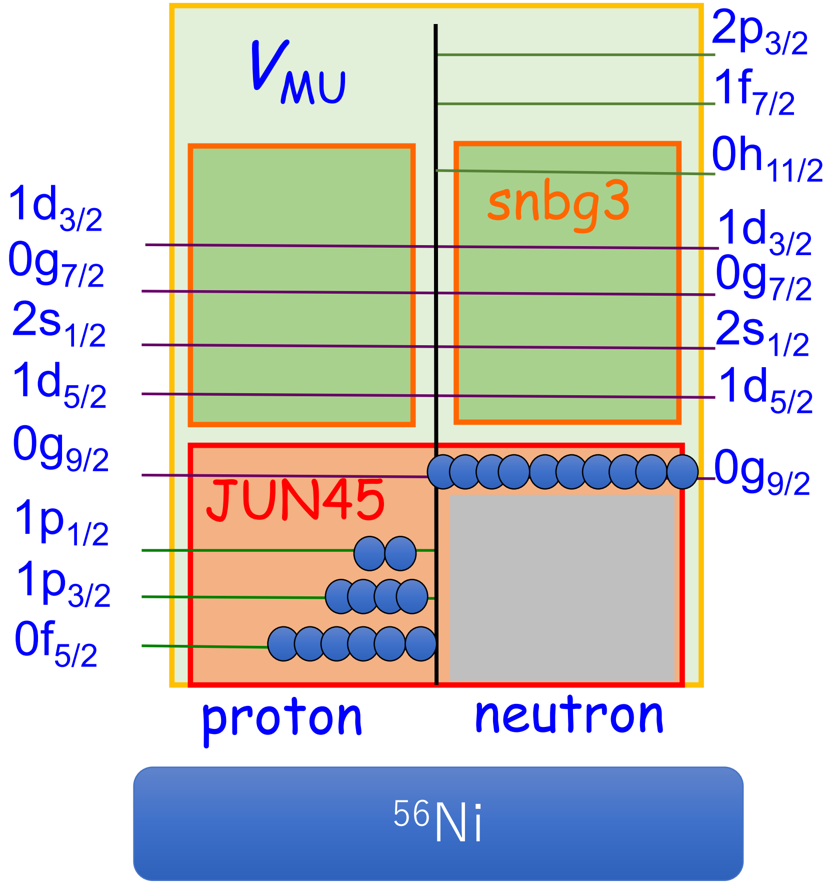
- Effective interaction:
  JUN45 + snbg3 + V_{MU}

  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, Tsunoda, TO *et al.* PRL 117, 172502 (2016)

From earlier shell-model works …

PHYSICAL REVIEW C VOLUME 20, NUMBER 2 AUGUST 1979

Unified shell-model description of nuclear deformation

P. Federman
Instituto de Fisica, Universidad Nacional Autonoma de Mexico, Apartado Postal 20-364, Mexico 20, D. F.

S. Pittel

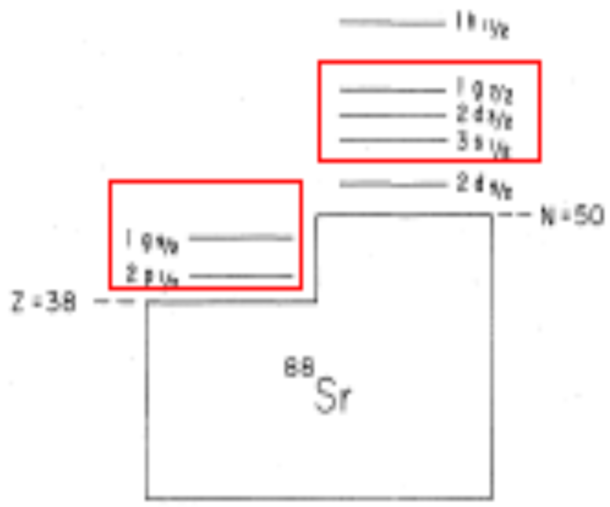


FIG. 3. Single-particle levels appropriate to a description of nuclei in the Zr-Mo region. An ^{88}Sr core is assumed.

PHYSICAL REVIEW C 79, 064310 (2009)

Shell model description of zirconium isotopes

K. Sieja,[1,2] F. Nowacki,[3] K. Langanke,[2,4] and G. Martínez-Pinedo[1]

In this paper, we perform for the first time a SM study of Zr isotopes in an extended model space ($1f_{5/2}$, $2p_{1/2}$, $2p_{3/2}$, $1g_{9/2}$) for protons and ($2d_{5/2}$, $3s_{1/2}$, $2d_{3/2}$, $1g_{7/2}$, $1h_{11/2}$) for neutrons, dubbed hereafter $\pi(r3-g)$, $\nu(r4-h)$.

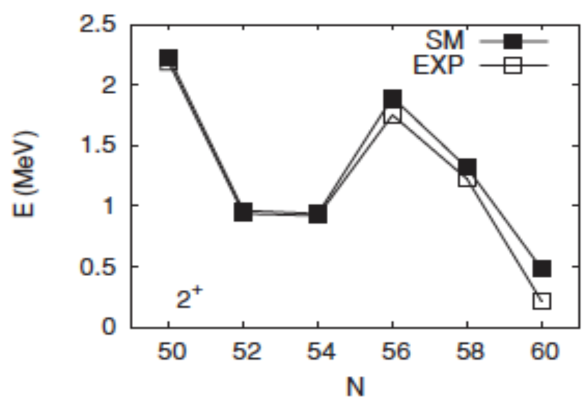
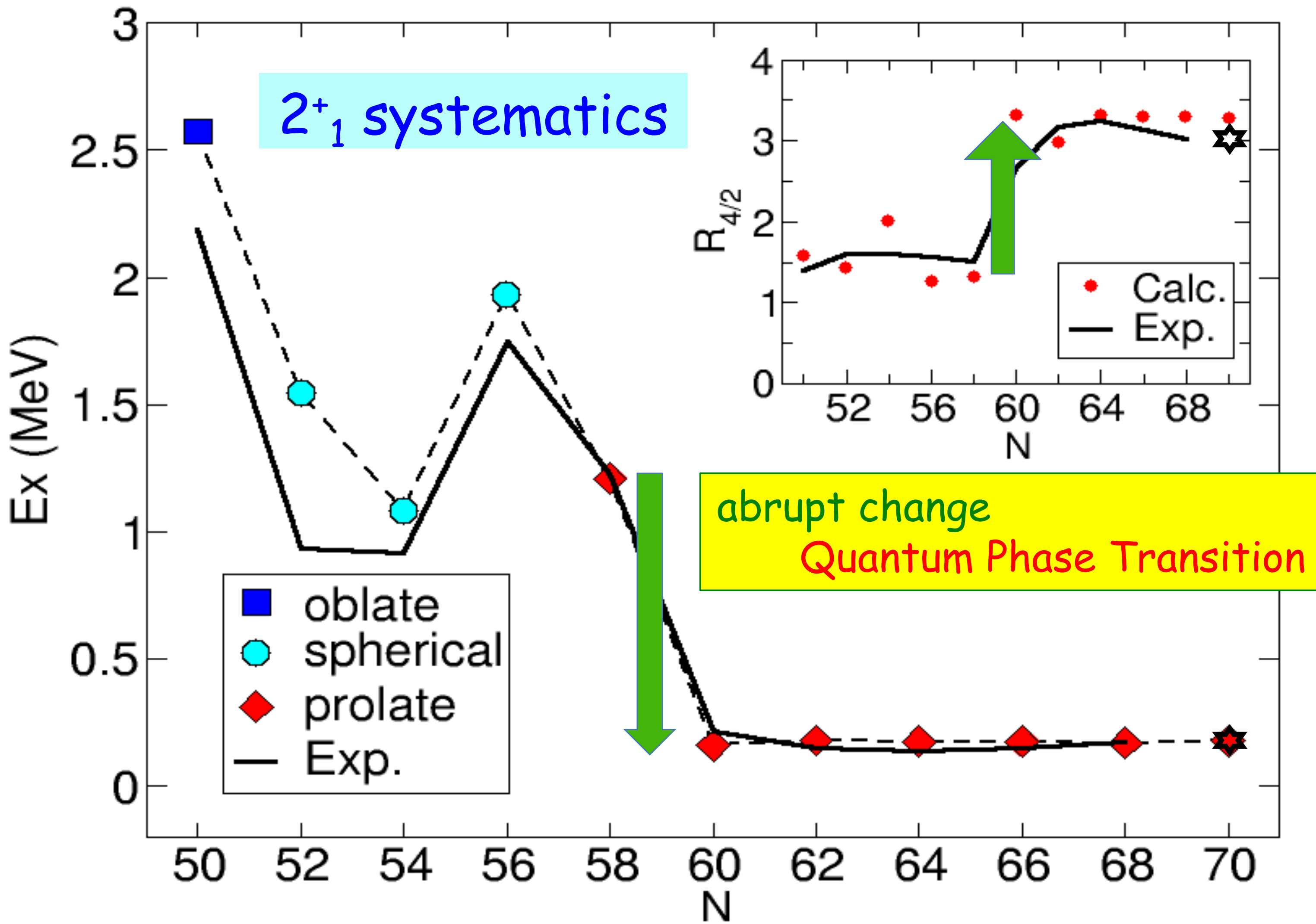


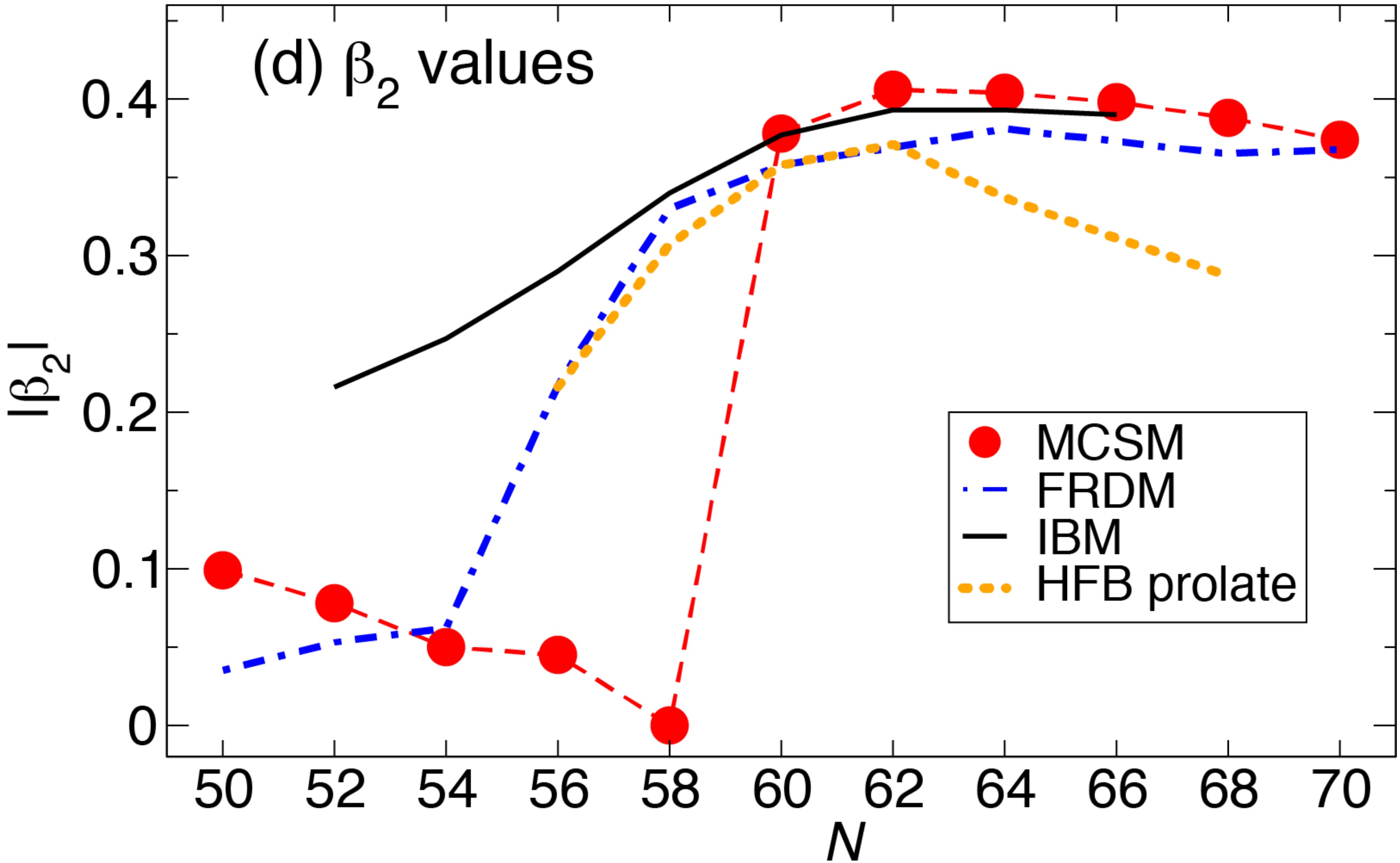
FIG. 12. Systematics of the experimental and theoretical first excited 2^+ states along the zirconium chain.

PRL 117, 172502 (2016) PHYSICAL REVIEW LETTERS week ending 21 OCTOBER 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]

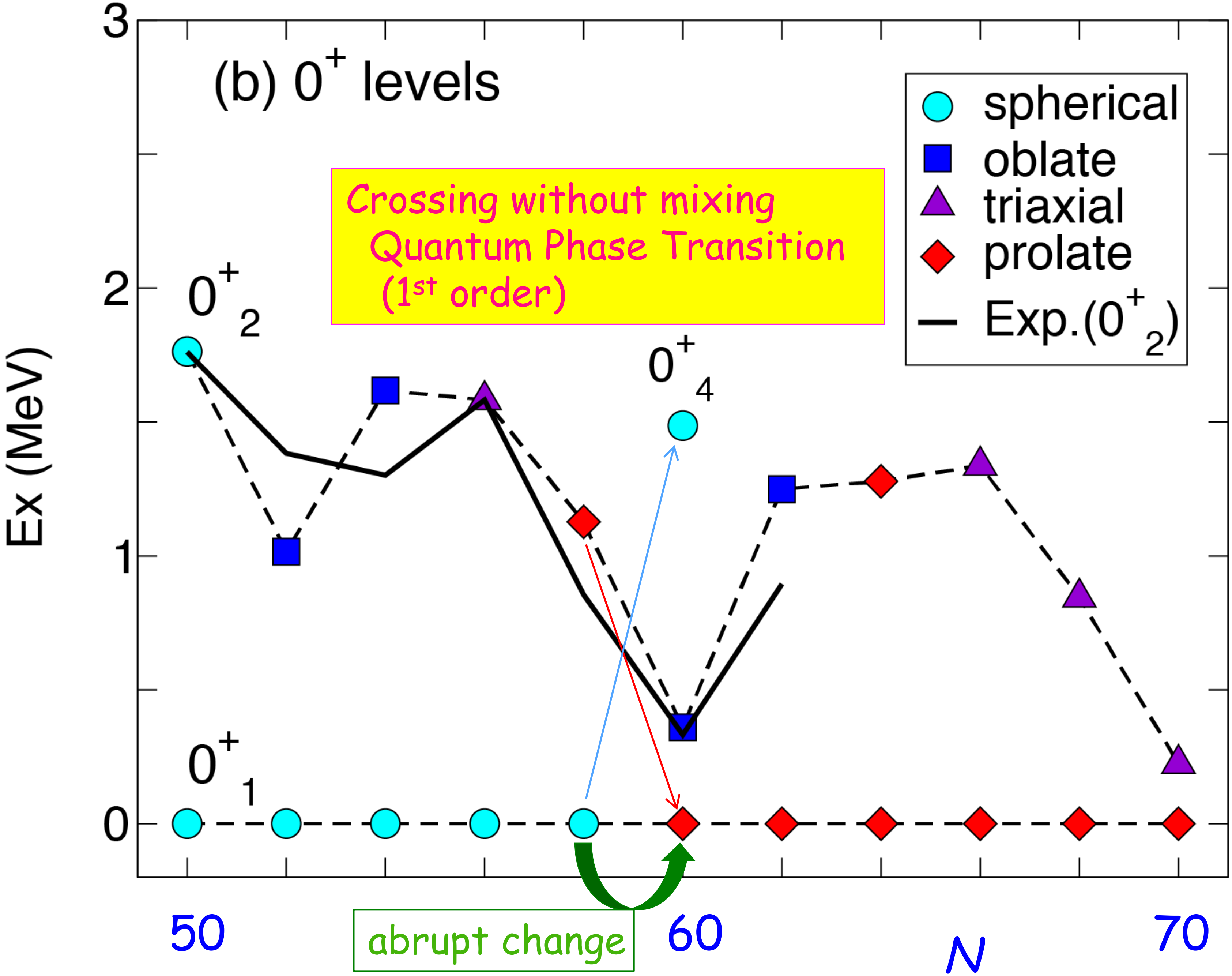




FRDM: S. Moeller et al. At. Data Nucl. Data Tables 59, 185 (1995).

IBM: M. Boyukata et al. J. Phys. G 37, 105102 (2010).

HFB: R. Rodriuez-Guzman et al. Phys. Lett. B 691, 202 (2010).

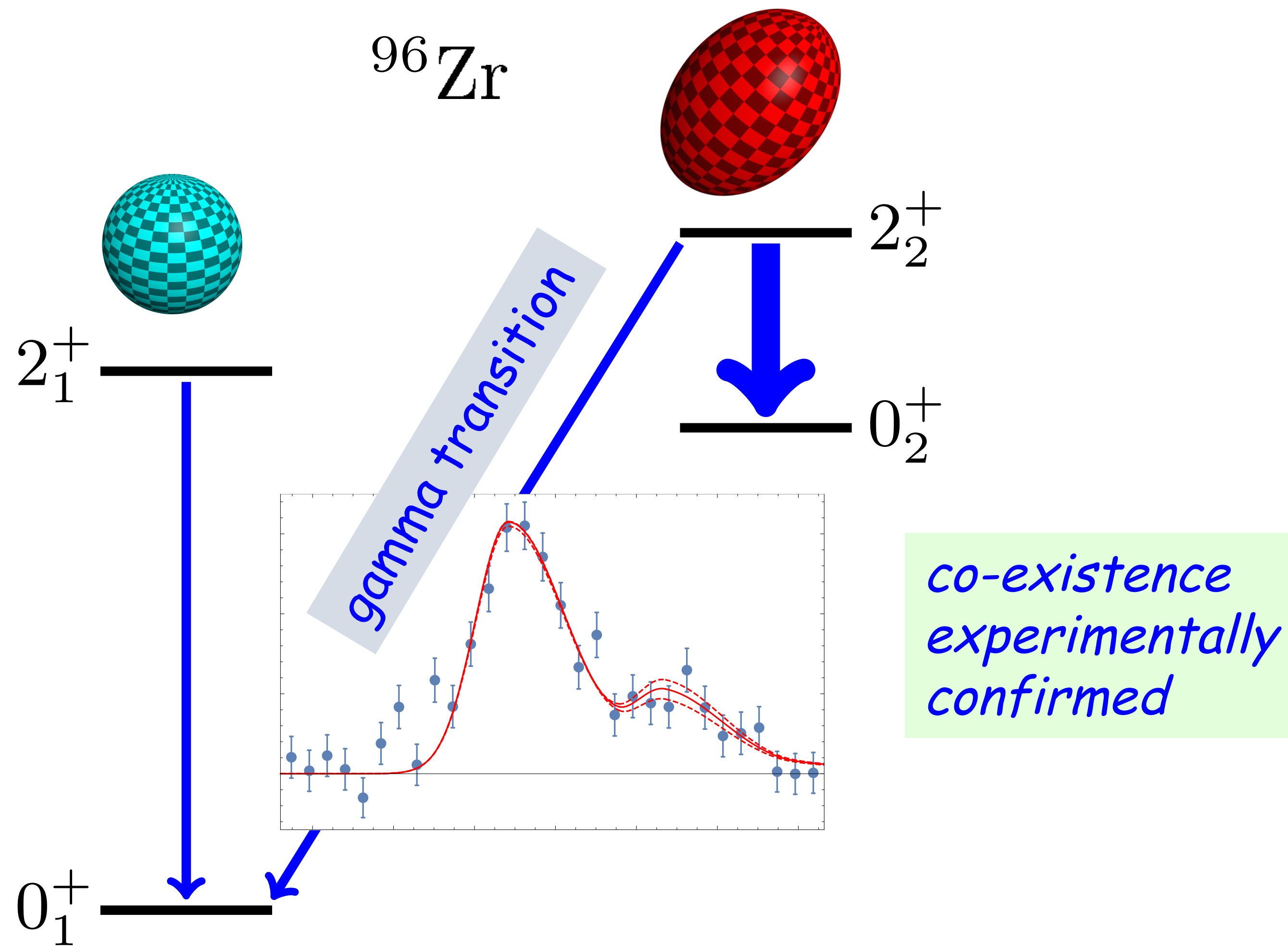


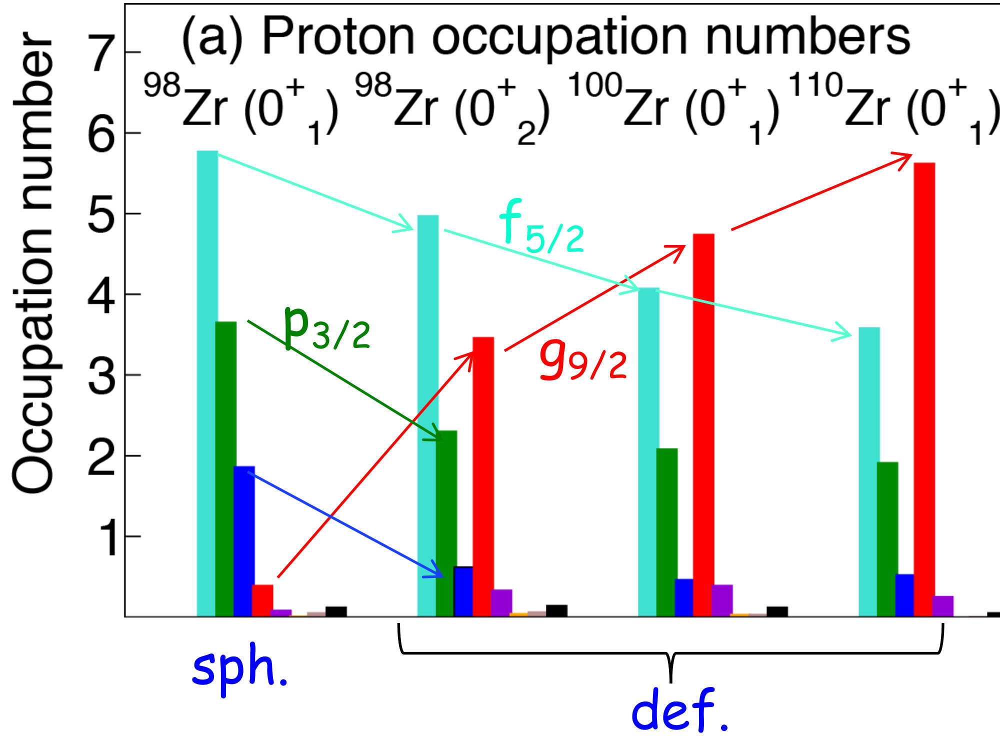
(b) 0+ levels
spherical
oblate
triaxial
prolate
Exp.(0+2)
Crossing without mixing
Quantum Phase Transition
(1st order)
0+2
0+4
0+1
Ex (MeV)
3
2
1
0
50
60
70
N
abrupt change

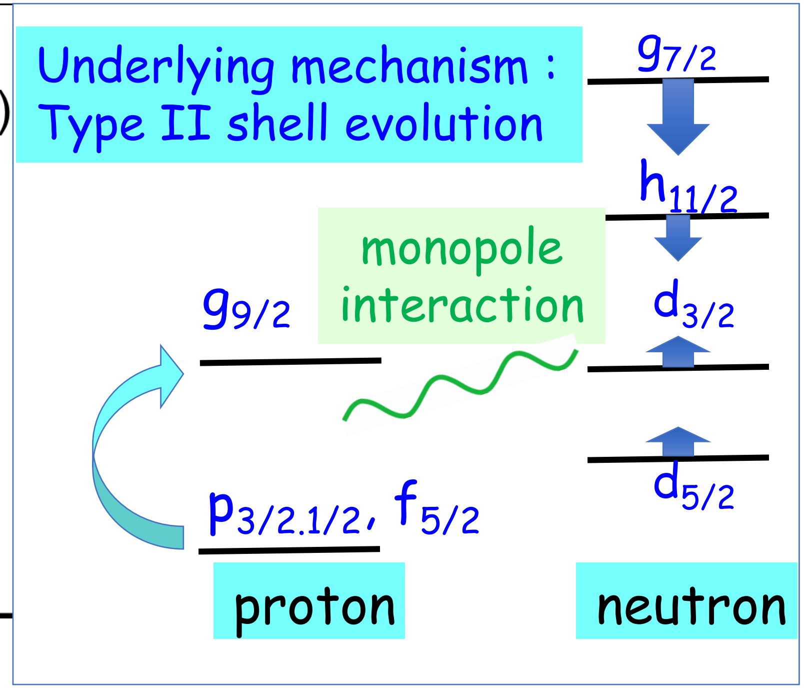
PRL 117, 172503 (2016) PHYSICAL REVIEW LETTERS week ending 21 OCTOBER 2016

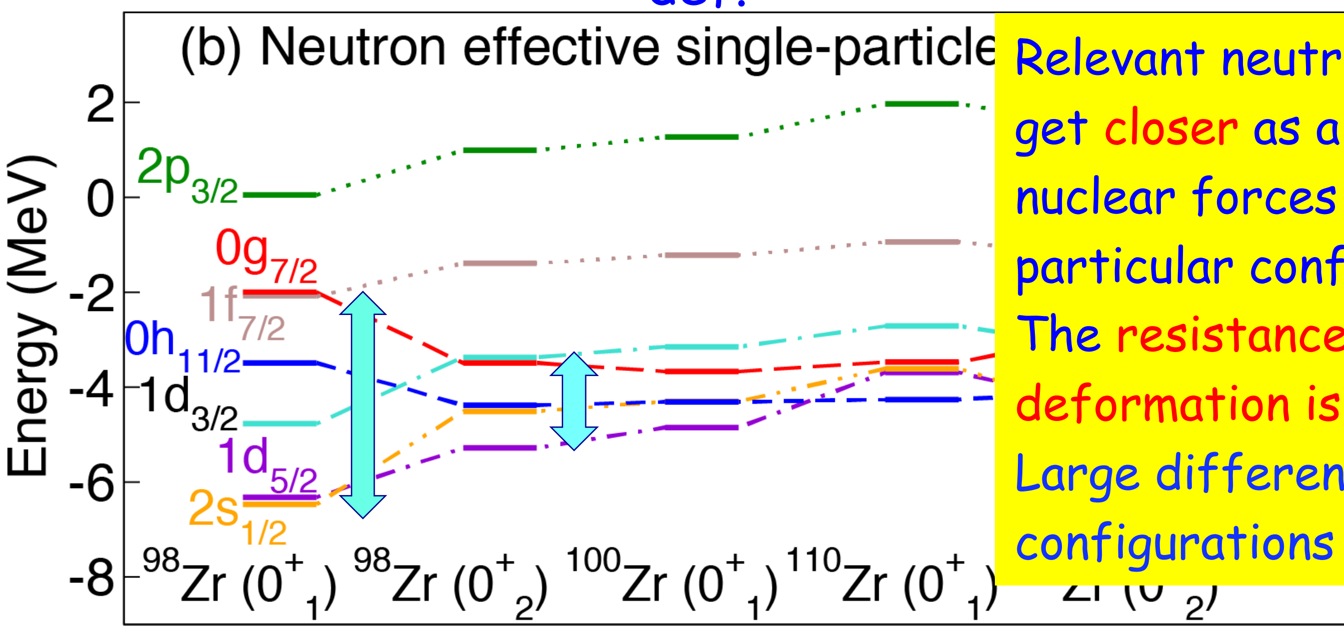
First Measurement of Collectivity of Coexisting Shapes Based on Type II Shell Evolution: The Case of ^{96}Zr

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

Type II shell evolution is a simplest and visible case of

Quantum Self Organization

$$\text{deformation} = \frac{\text{quadrupole force}}{\text{resistance power}}$$

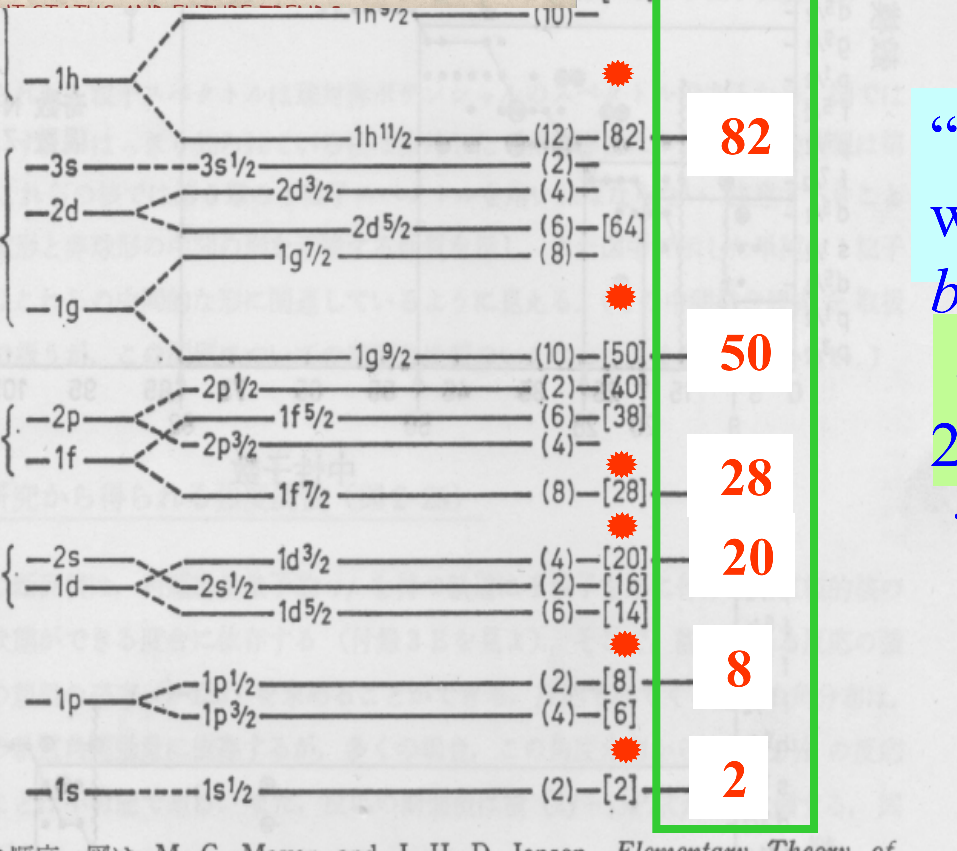
resistance power ← pairing force

single-particle energies

Atomic nuclei can "organize" their single-particle energies by taking particular configurations of protons and neutrons optimized for each eigenstate, thanks to orbit-dependences of monopole components of nuclear forces (*e.g.*, tensor force).

→ an enhancement of Jahn-Teller effect.

Magic numbers by Mayer and Jensen (1949)



126

82

50

28

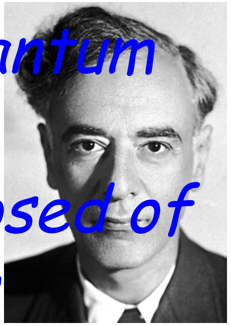
20

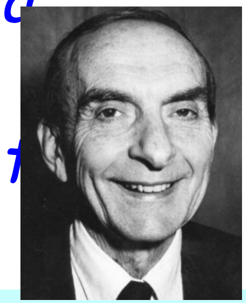
8

2

Atomic nucleus is a quantum Fermi liquid :

The nucleus is composed of almost free nucleons interacting weakly via residual forces in a (solid) (mean) pot

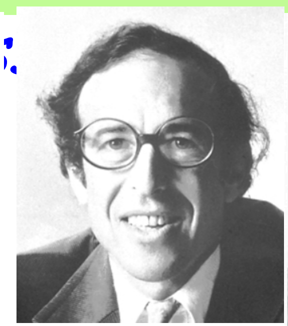




"how single-particle states can coexist with collective modes" *conceived also by Gerry Brown*

(T. Schaefer, Fermi Liquid theory ... 2014)

Surface deformation produced by additional deformed mean field



SVEN GÖSTA NILSSON

Nilsson model Hamiltonian

"*Nuclear structure II*" by Bohr and Mottelson

deformed nuclei, is obtained by a simple modification of the harmonic oscillator (Nilsson, 1955; Gustafson *et al*., 1967),

$$H = \frac{\mathbf{p}^2}{2M} + \underbrace{\boxed{\tfrac{1}{2}M\left(\omega_3^2 x_3^2 + \omega_\perp^2\left(x_1^2 + x_2^2\right)\right)}}_{\text{quadrupole deformed field}} + \underbrace{\boxed{v_{ll}\hbar\omega_0\left(\mathbf{l}^2 - \langle \mathbf{l}^2\rangle_N\right) + v_{ls}\hbar\omega_0(\mathbf{l}\cdot\mathbf{s})}}_{\text{spherical field}} \tag{5-10}$$

$$\langle \mathbf{l}^2\rangle_N = \tfrac{1}{2}N(N+3)$$

Figure	Region	$-v_{ls}$	$-v_{ll}$
5-1	N and Z < 20	0.16	0
5-2	$50 < Z < 82$	0.127	0.0382
5-3	$82 < N < 126$	0.127	0.0268
5-4	$82 < Z < 126$	0.115	0.0375
5-5	$126 < N$	0.127	0.0206

Table 5-1 Parameters used in the single-particle potentials of Figs. 5-1 to 5-5.

Spin-orbit force

$$\left.\begin{array}{ll} A=\ 68 & 1.28 \\ A=100 & 1.12 \\ A=186 & 0.91 \end{array}\right\} (\mathbf{l}\cdot\mathbf{s})$$

Intuitively speaking,

$$\text{deformation} = \frac{\text{quadrupole force}}{\text{resistance power}}$$

resitance power ← pairing force

single-particle energies

Atomic nuclei can "organize" their single-particle energies by taking particular configurations of protons and neutrons, thanks to orbit-dependences of nuclear forces (*e.g.*, tensor force).

Quantum Self Organization

Note : spherical single-particle energies are often treated being constant

After mastering the shell model,
three (possible) pillars combined for future

computation

Monte Carlo
Shell Model
(MCSM)

(almost)
unlimited
dimensionality

massive
parallel
computers

Hamiltonian

pf
pfg9d5 (A3DA) (Ni)
8+8 on ^{56}Ni core (Zr)
8+8 on ^{80}Zr core (Sn)
8+10 on ^{132}Sn core
(Sm)
...
island of stability
+
χEFT based
(multi-)shell int.

many-body dynamics

Shell evolution
(Type I & II)

Quantum Phase
Transition

Shape coexistence

Quantum
Self-organization