Int. School of Physics "Enrico Fermi" - Course 201 Nuclear Physics with Stable and Radioactive Ion Beams Varenna July 14-19, 2017

Recent developments shell model studies of atomic nuclei

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

From the shell model perspectives, 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 ⁵⁶Ni core (Zr) 8+8 on ⁸⁰Zr core (Sn) 8+10 on ¹³²Sn core (Sm)

island of stability +

 χ EFT based (multi-)shell int.

many-body dynamics

Shell evolution (Type I & II)

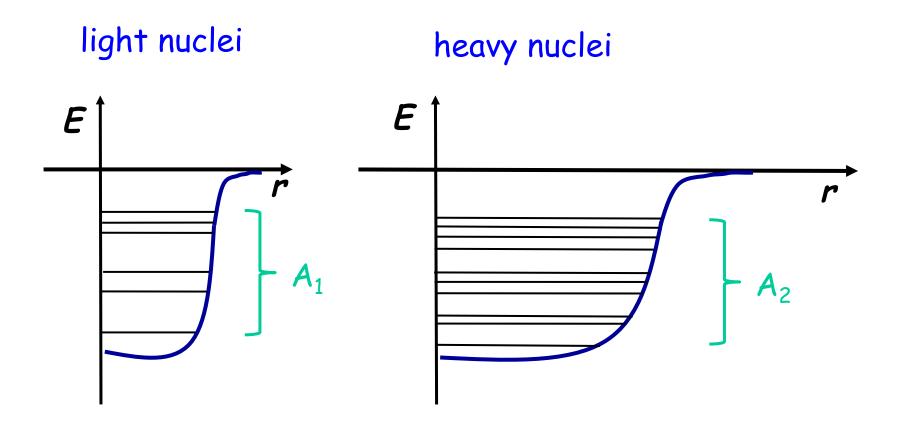
Quantum Phase Transition

Shape coexistence

Quantum Self-organization

Single-particle states - starting point -

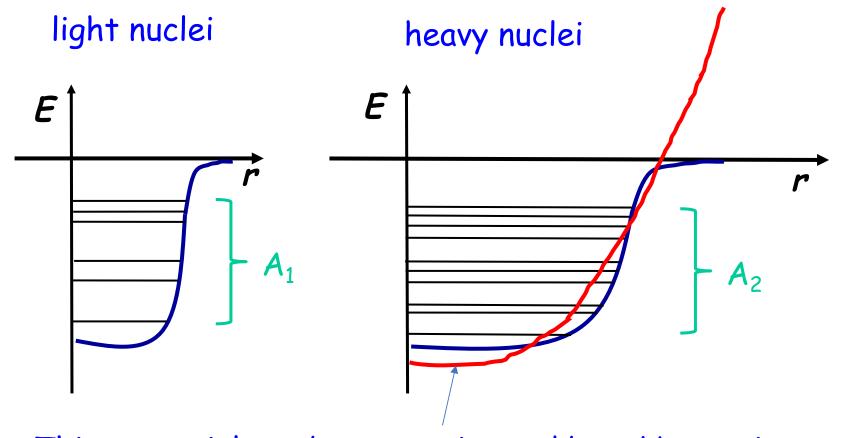
Mean potential becomes wider so as to cast A nucleons with the same separation energy, keeping its depth.



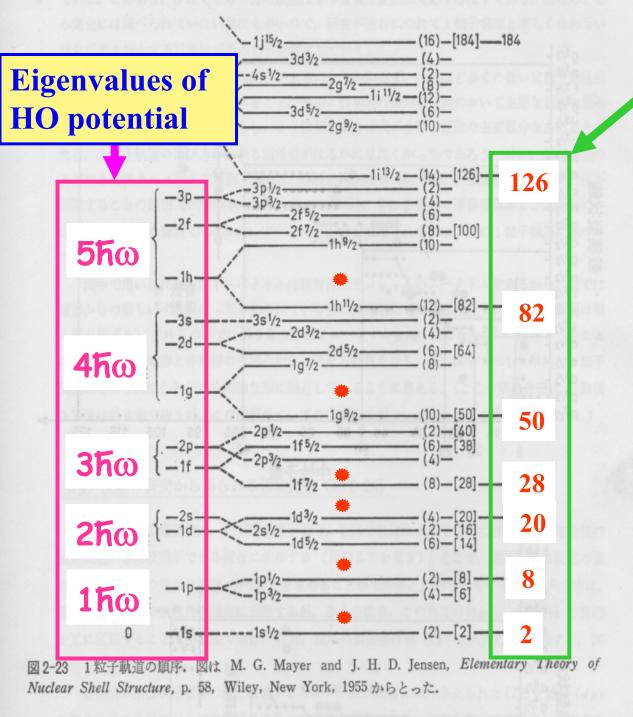
This potential can be approximated by a Harmonic Oscillator potential.

Single-particle states - starting point -

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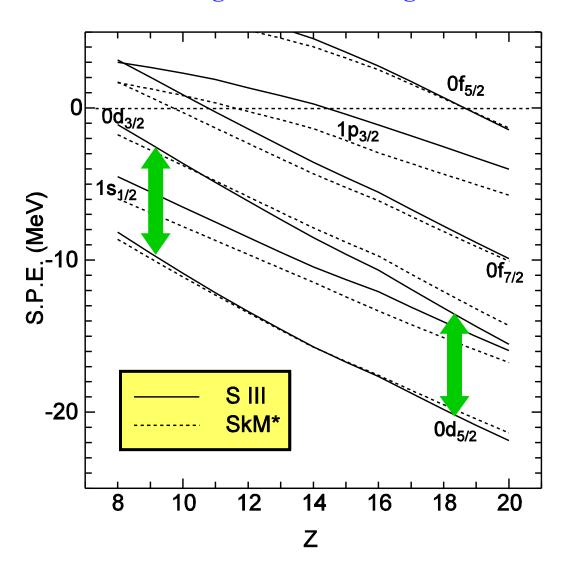
Magic numbers by Mayer and Jensen (1949)



R SHELL MODEL

Realization in Hartree-Fock energies by Skyrme model

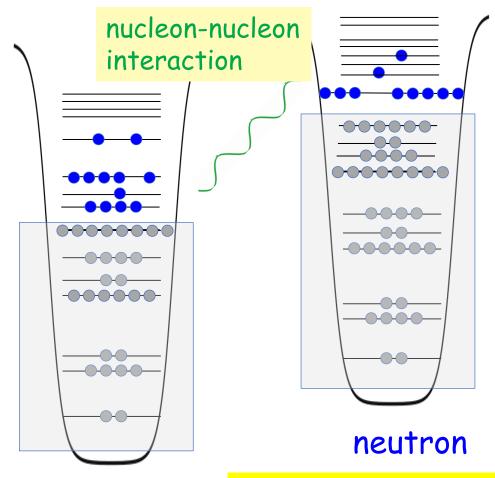
Neutron Single-Particle Energies at *N***=20**



The shell structure remain rather unchanged

- orbitals shifting together
- -- change of potential depth
- ~ Woods-Saxon.

shell structure and nucleon-nucleon interaction



Protons and neutrons are orbiting in the mean potential like a "vase"

→ single-particle energies

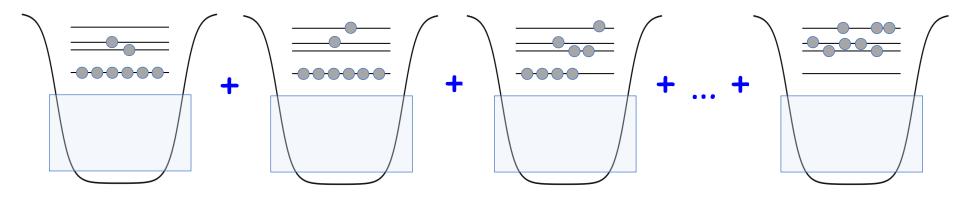
Lower orbits form the inert core (or closed shell) (shaded parts in the figure)

Upper orbits are only partially occupied (valence orbits and nucleons).

proton

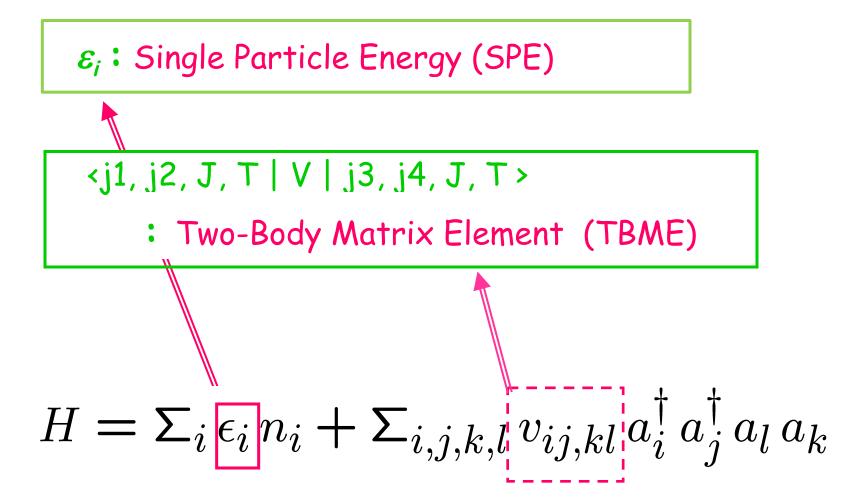
Valence nucleons are the major source of nuclear dynamics at low excitation energy, because the inert core is frozen (implicitly taken into account in terms of effective interaction and operators).

Possible configurations: dimension of the shell-model calculation



How can we find the solution of this problem?

Hamiltonian in shell model calculations



Step 1: Calculate matrix elements

$$<\phi_1 \mid H \mid \phi_1>$$
, $<\phi_1 \mid H \mid \phi_2>$, $<\phi_1 \mid H \mid \phi_3>$,

where ϕ_1 , ϕ_2 , ϕ_3 are Slater determinants

In the second quantization, closed shell
$$\phi_1 = a_\alpha^+ a_\beta^+ a_\gamma^+ \dots | 0 >$$

$$\phi_2 = a_\alpha^{++} a_\beta^{++} a_\gamma^{++} \dots | 0 >$$

$$\phi_3 = \dots$$

$$H = \sum_{i} \epsilon_{i} n_{i} + \sum_{i,j,k,l} v_{ij,kl} a_{i}^{\dagger} a_{j}^{\dagger} a_{l} a_{k}$$

Step 2: Obtain the matrix of Hamiltonian, H

Step 3: Solve the eigenvalue problem: $H \Psi = E \Psi$

 $\Psi = \mathbf{c_1} \; \phi_1 + \mathbf{c_2} \; \phi_2 + \mathbf{c_3} \; \phi_3 + \dots$ $\mathbf{c_i} \quad \text{probability amplitudes}$

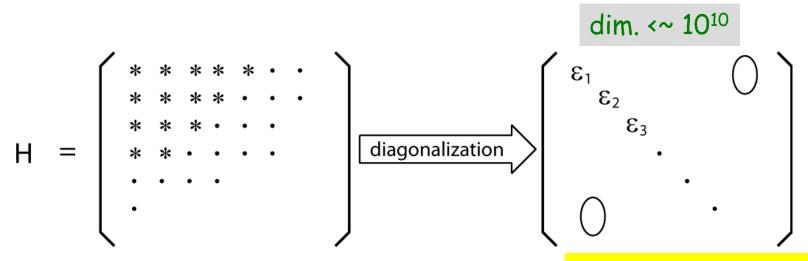
With Slater determinants $\phi_1, \phi_2, \phi_3, ...,$ the eigen wave function is expanded as

$$\Psi = \mathbf{c_1} \, \phi_1 + \mathbf{c_2} \, \phi_2 + \mathbf{c_3} \, \phi_3 + \dots$$

c_i probability amplitudes

With this, we can calculate various physical quantities by $\langle \Psi' | T | \Psi \rangle$.

Two types of shell-model calculations



Conventional Shell Model

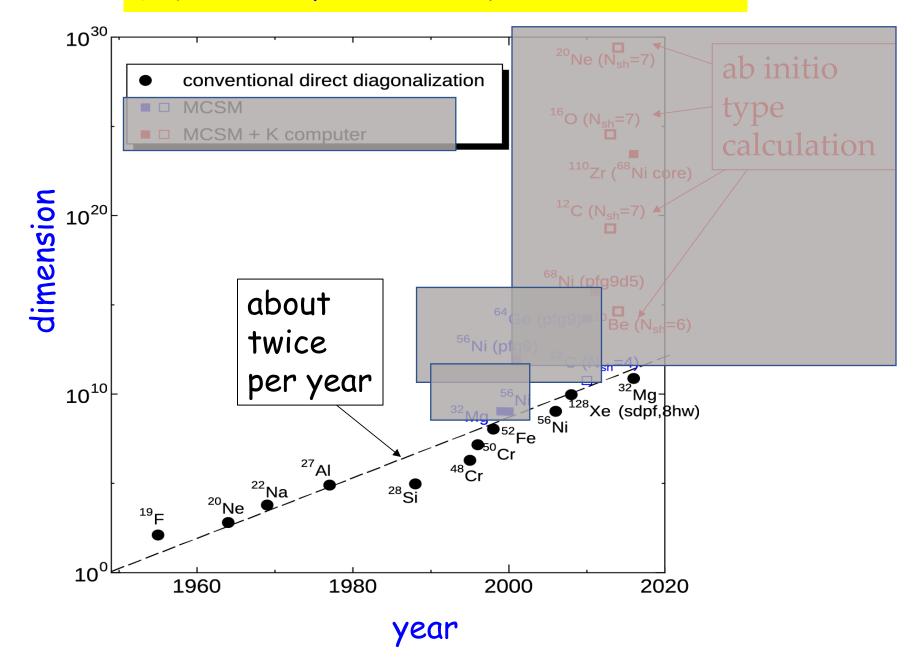
all Slater determinants

Direct diagonalization

For even bigger problem,

Monte Carlo Shell Model bases important for a specific eigenstate important basis vectors

Dimension of the shell-model calculation



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) Σ_{α} v_{α} O_{α}^{2}

 α : index

 O_{α} : one-body operators (rearranged by diagonalization)

Hubberd-Stratonovichi transformation

True eigenstate: $\psi = \Sigma_{\sigma} e^{-\beta h(\sigma)} e^{-\beta h(\sigma')} ... \psi_{o}$ imaginary time (β) evolution by one-body field h(σ)

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

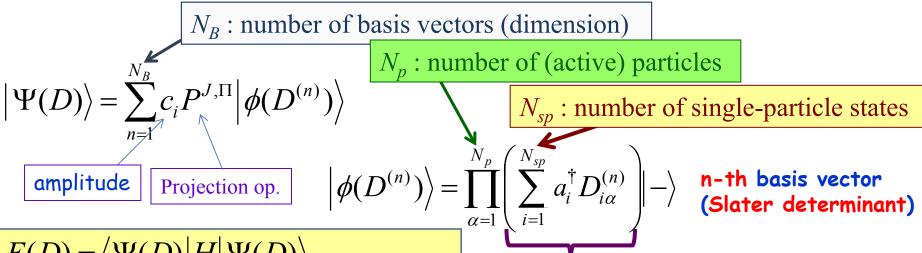
 ϕ (σ , σ' ,...) are selected and refined :

- (i) Random sampling -> only those lowering energy are kept
- (ii) Polished by varying $\sigma_i \sigma'_{i}$ 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)



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

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

Stochastically "deformed" single-particle state

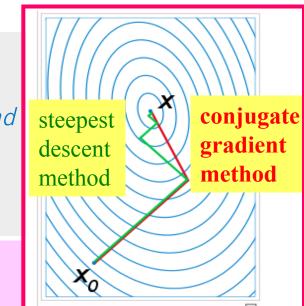
Step 1: stochastic generation of candidates of the n-th MCSM basis vector

$$|\phi(\sigma)\rangle = e^{\Delta \phi h(\sigma)} \cdot |\phi^{(0)}\rangle$$
 only theoretical background

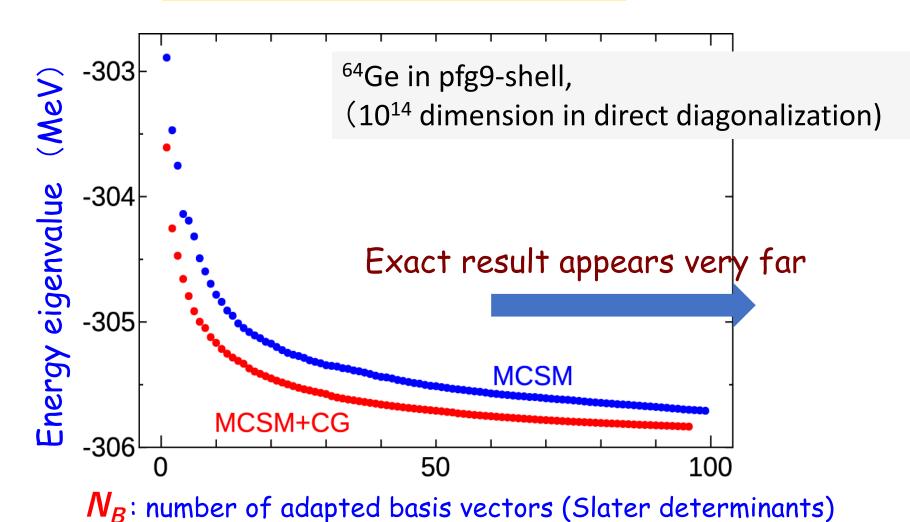
Shift randomly matrix elements of the matrix D.

(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".

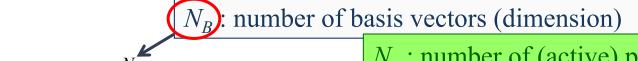


Example of MCSM calculation



Numerous MC trials and CG optimization for each basis vector

Advanced Monte Carlo Shell Model (currently used)



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

amplitude

Projection op.

$$N_p$$
: number of (active) particles

 N_{sp} : number of single-particle states

$$\left|\phi(D^{(n)})\right\rangle = \prod_{\alpha=1}^{N_p} \left(\sum_{i=1}^{N_{sp}} a_i^{\dagger} D_{i\alpha}^{(n)}\right) - \left\langle \text{ (Slater determinant)} \right\rangle$$

Deformed single-particle state

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

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

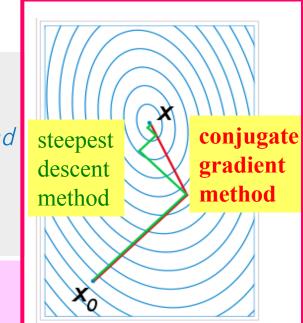
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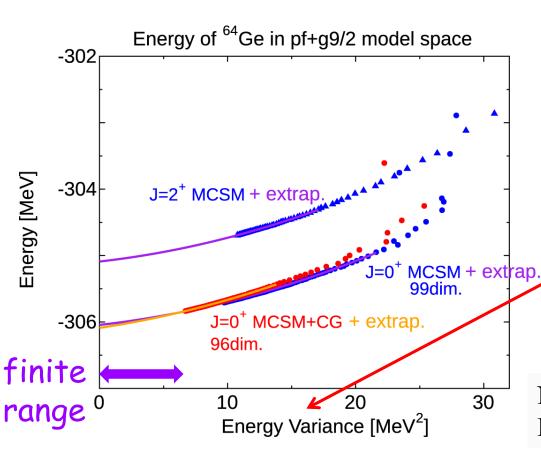
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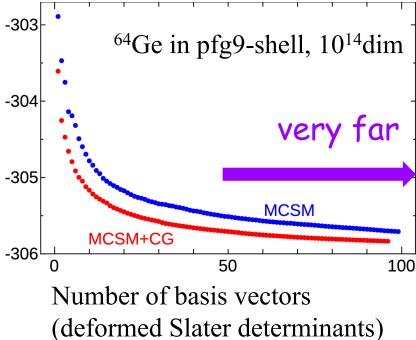
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Extrapolation by Energy Variance





Energy (MeV)

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)

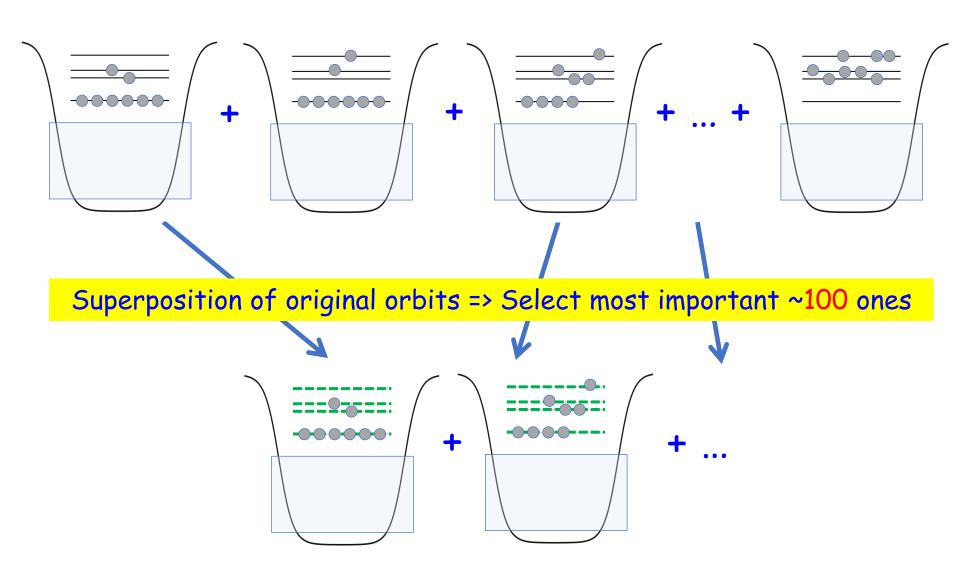


K computer (in Kobe) 10 peta flops machine
 ⇒ Projection of basis vectors
 Rotation with three Euler angles

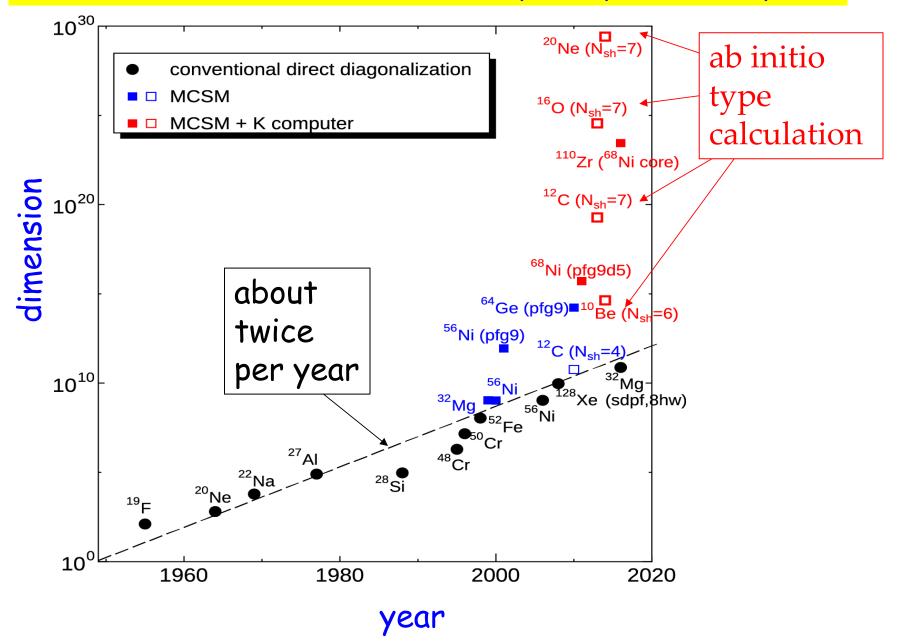
with about 50,000 mesh points

Example: 8+ 68Ni 7680 core x 14 h

Possible configurations: 10²³ ways at maximum for Zr isotopes to be discussed



Dimension of the shell-model many-body Hilbert space

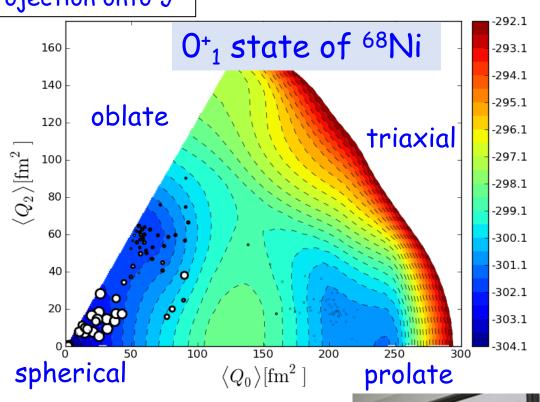


MCSM basis vectors on Potential Energy Surface

eigenstate $\Psi = \sum_{i} c_{i} P[J^{\pi}] \Phi_{i}$ Slater determinant of deformed s. p. states \rightarrow intrinsic shape projection onto J^{π}

- 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



Y. Tsunoda

Called T-plot in reference to

Y. Tsunoda, et al.

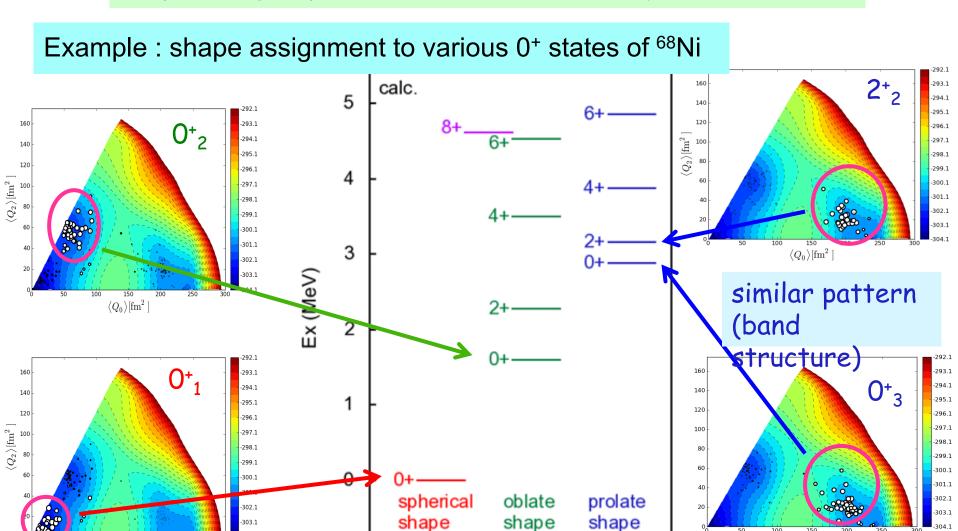
PRC 89, 031301 (R) (2014)

General properties of T-plot:

 $\langle Q_0 \rangle [\mathrm{fm}^2$

Certain number of large circles in a small region of PES pairing correlations

Spreading beyond this can be due to shape fluctuation



 $\left\langle Q_{0}\right\rangle [\mathrm{fm}^{2}\mid$

Three pillars combined for future

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Hamiltonian

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island of stability
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many-body dynamics

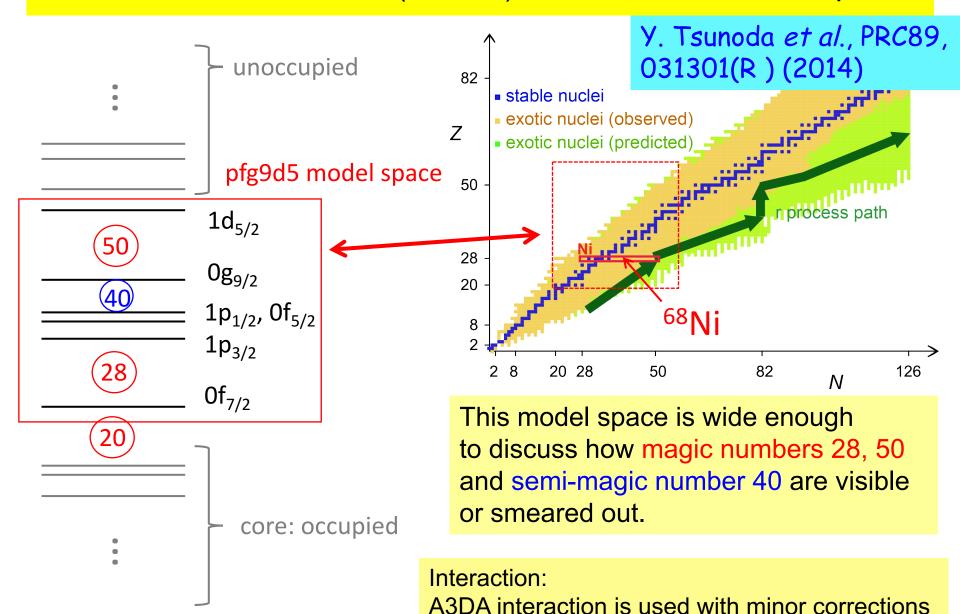
Shell evolution (Type I & II)

Quantum Phase Transition

Shape coexistence

Quantum Self-organization

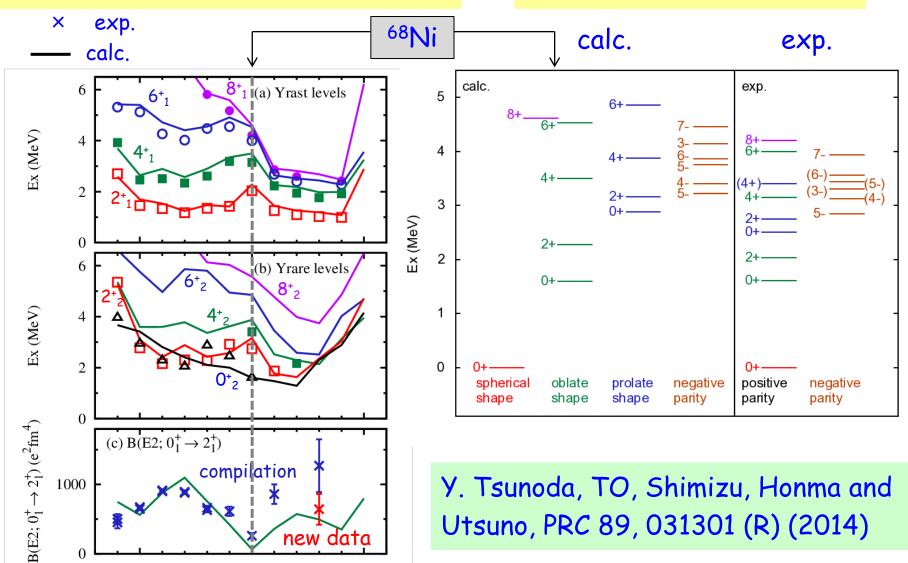
Monte Carlo Shell Model (MCSM) calculation on Ni isotopes



Energy levels and B(E2) values of Ni isotopes



Shape coexistence in ⁶⁸Ni



new data

50

40

N

30

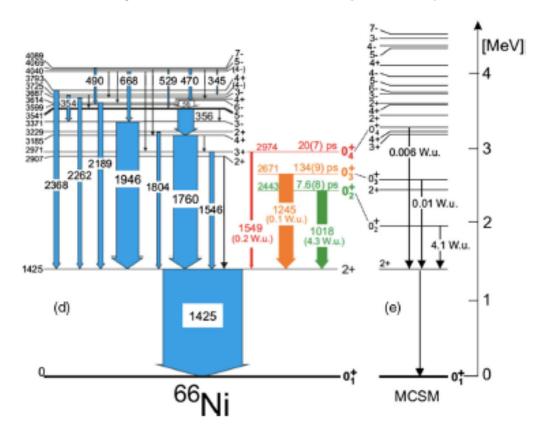
Y. Tsunoda, TO, Shimizu, Honma and Utsuno, PRC 89, 031301 (R) (2014)

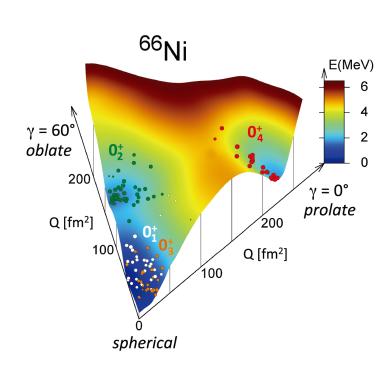


Multifaceted Quadruplet of Low-Lying Spin-Zero States in ⁶⁶Ni: Emergence of Shape Isomerism in Light Nuclei

S. Leoni, 12,* B. Fornal, N. Mărginean, M. Sferrazza, Y. Tsunoda, T. Otsuka, 67,89 G. Bocchi, 12 F. C. L. Crespi, 12
A. Bracco, 12 S. Aydin, M. Boromiza, 11 D. Bucurescu, N. Cieplicka-Orynczak, 23 C. Costache, S. Călinescu, N. Florea, D. G. Ghiţă, T. Glodariu, A. Ionescu, 11 Ł. W. Iskra, M. Krzysiek, R. Mărginean, C. Mihai, R. E. Mihai, A. Mitu, A. Negreţ, C. R. Niţă, A. Olăcel, A. Oprea, S. Pascu, P. Petkov, C. Petrone, G. Porzio, A. Şerban, 11 C. Sotty, L. Stan, I. Ştiru, L. Stroe, R. Şuvăilă, S. Toma, A. Turturică, S. Ujeniuc, and C. A. Ur Dipartimento di Fisica, Università degli Studi di Milano, I-20133 Milano, Italy

1 Institute of Nuclear Physics, PAN, 31-342 Kraków, Poland



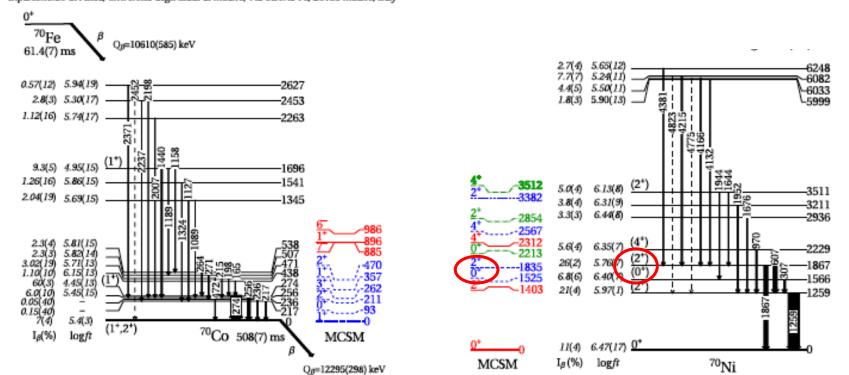


Physics Letters B 765 (2017) 328-333 What is this?

Type II shell evolution in A = 70 isobars from the $N \ge 40$ island of inversion

```
A.I. Morales a,b,*, G. Benzoni a, H. Watanabe c,d, Y. Tsunoda e, T. Otsuka f,g,h, S. Nishimura d, F. Browne i,d, R. Daido j, P. Doornenbal d, Y. Fang j, G. Lorusso d, Z. Patel k,d, S. Rice k,d, L. Sinclair l,d, P.-A. Söderström d, T. Sumikama m, J. Wu d, Z.Y. Xu f,d, A. Yagi j, R. Yokoyama f, H. Baba d, R. Avigo a,b, F.L. Bello Garrote n, N. Blasi a, A. Bracco a,b, F. Camera a,b, S. Ceruti a,b, F.C.L. Crespi a,b, G. de Angelis o, M.-C. Delattre p, Zs. Dombradi q, A. Gottardo o, T. Isobe d, I. Kojouharov f, N. Kurz f, I. Kuti q, K. Matsui f, B. Melon s, D. Mengoni f,u, T. Miyazaki f, V. Modamio-Hoybjor o, S. Momiyama f, D.R. Napoli o, M. Niikura f, R. Orlandi h,v, H. Sakurai d,f, E. Sahin n, D. Sohler q, H. Schaffner f, R. Taniuchi f, J. Taprogge w,x, Zs. Vajta q, J.J. Valiente-Dobón o, O. Wieland a, M. Yalcinkaya y
```

b Dipartimento di Fisica, Università degli Studi di Milano, Via Celoria 16, 20133 Milano, Italy



^a Istituto Nazionale di Fisica Nucleare, Sezione di Milano, Via Celoria 16, 20133 Milano, Italy

End of the 1st lecture

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2nd lecture











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Three pillars combined for future

In order to understand the physics behind these calculations, let us jump to

computation

Monte Carlo Shell Model (MCSM)

(almost) unlimited dimensionality

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Hamiltonian

pfq9d5 (A3DA) (Ni) 8+8 on ⁵⁶Ni core (Zr) 8+8 on 80Zr core (Sn) 8+10 on ¹³²Sn core (Sm)

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χEFT based multi-shell int. many-body dynamics

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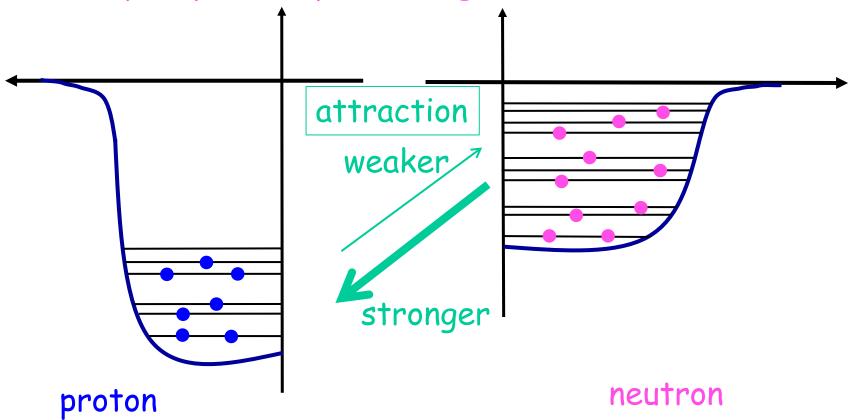
Quantum Phase Transition

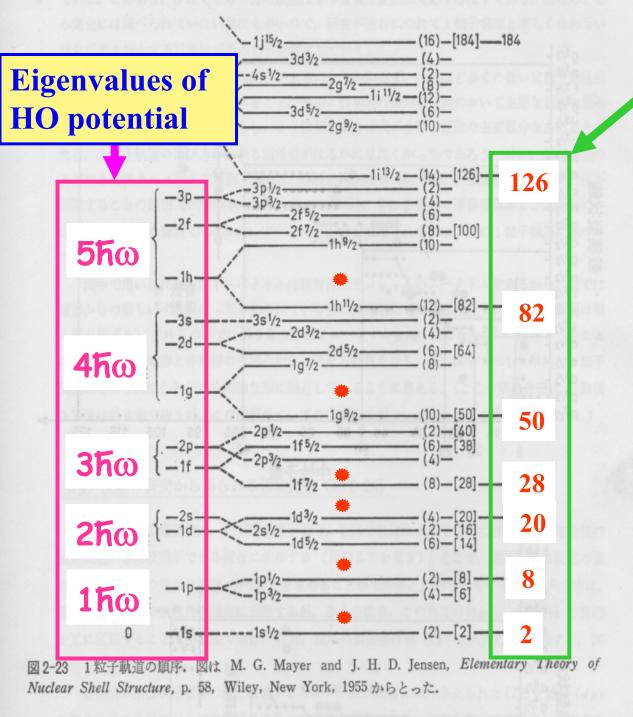
Shape coexistence

Quantum Self-organization

If $Z \ll N$, protons are more bound.

Relative relations among orbits are preserved, because basically only the depths change. Can we assume this?





Magic numbers by Mayer and Jensen (1949)



R SHELL MODEL

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 question leads us to one of the major developments of recent nuclear structure studies.

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

In other words, let's discuss whether the shell evolution, the change of the shell structure, occurs or not.

If it occurs, how?

The key tool is the monopole interaction.

Monopole matrix element between orbits j and j'

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

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

Monopole matrix element between orbits j and j'

$$\langle \downarrow \downarrow \downarrow | v | \downarrow \downarrow \downarrow \rangle + \langle \downarrow \downarrow \downarrow v | \downarrow \downarrow \downarrow \rangle + \langle \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \rangle + \dots$$

$$+ \langle \vee \Diamond | v | \vee \Diamond \rangle + \dots + \langle \Diamond \Diamond | v | \Diamond \Diamond \rangle$$

number of matrix elements in the summation

Monopole matrix elements can be written equivalently by usual TBMEs as

$$\begin{split} V_T^m(j,\,j') &= \frac{\sum_J (2J+1)\langle j,j';J,T|\hat{v}|j,j';J,T\rangle}{\sum_J (2J+1)}. \\ \text{for } T=0 \text{ and } 1, \end{split}$$

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

$$\hat{v}_{nn}^{m}(j,j') = \begin{cases} V_{nn}^{m}(j,j) \frac{1}{2} \hat{n}_{j} (\hat{n}_{j} - 1) & \text{for } j = j' \\ V_{nn}^{m}(j,j') \hat{n}_{j} \hat{n}_{j'} & \text{for } j \neq j' \end{cases}$$

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

$$\begin{split} \hat{v}_{pn,mono,T=1} &= \sum_{j,\,j'} V_{T=1}^m(j,\,j') \, \frac{1}{2} \, \hat{n}_j^p \, \hat{n}_{j'}^n \\ &+ \sum_{j < j'} V_{T=1}^m(j,\,j') \, \frac{1}{2} \, \Big\{ \, \hat{\tau}_j^+ \hat{\tau}_{j'}^- \, + \hat{\tau}_j^- \hat{\tau}_{j'}^+ \, \Big\} \\ &+ \sum_{j} V_{T=1}^m(j,\,j) \, \frac{1}{2} : \hat{\tau}_j^+ \hat{\tau}_j^- : \, . \end{split}$$

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

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

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

$$\hat{v}_{pn,mono} = \sum_{j,j'} \frac{1}{2} \left\{ V_{T=0}^{m}(j,j') + V_{T=1}^{m}(j,j') \right\} \hat{n}_{j}^{p} \hat{n}_{j'}^{n}$$

$$- \sum_{j < j'} \frac{1}{2} \left\{ V_{T=0}^{m}(j,j') - V_{T=1}^{m}(j,j') \right\}$$

$$\left\{ \hat{\tau}_{j}^{+} \hat{\tau}_{j'}^{-} + \hat{\tau}_{j}^{-} \hat{\tau}_{j'}^{+} \right\}$$

$$- \sum_{j} \frac{1}{2} \left\{ V_{T=0}^{m}(j,j) - V_{T=1}^{m}(j,j) \right\} : \hat{\tau}_{j}^{+} \hat{\tau}_{j}^{-} :$$

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!

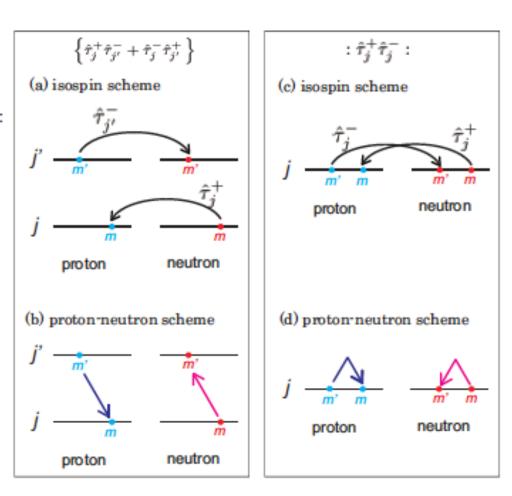
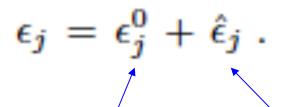


Figure 16 Implication of $\hat{\tau}_{j}^{+}\hat{\tau}_{j'}^{-}$ terms. Panels (a) and (c) are for the $\{\hat{\tau}_{j}^{+}\hat{\tau}_{j'}^{-}+\hat{\tau}_{j}^{-}\hat{\tau}_{j'}^{+}\}$ and : $\hat{\tau}_{j}^{+}\hat{\tau}_{j}^{-}$: cases in the isospin scheme, respectively. Panels (b) and (d) are similar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

Effective single-particle energy (ESPE)



Contribution from valence nucleons through the monopole interaction

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

Changes of ESPEs between nuclei

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, $\Delta \hat{n}_{j'}^n$ denotes the change of the neutron number in the orbit j'.

If monopole matrix elements, $V_{T=1}^m(j,j')$ and $V_{pn}^m(j,j')$, are uniform, nothing happens.

However, the shell evolution occurs, if $V_{T=1}^m(j,j')$ or $V_{pn}^m(j,j')$ change significantly depending on j and j'.

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

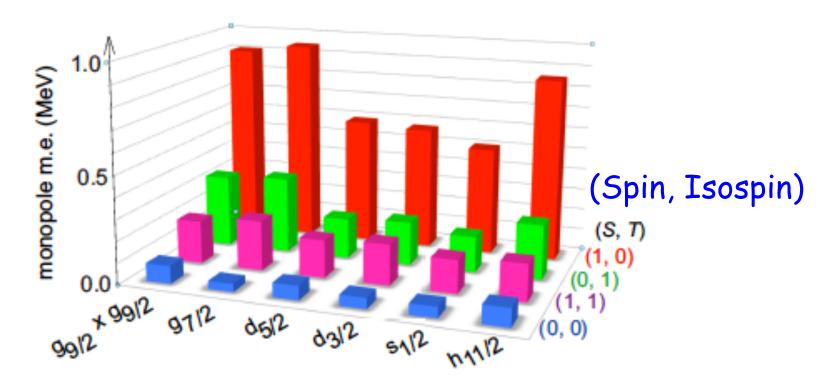


Figure 24 Monopole matrix elements of central gaussian interactions for (S,T) channels with an equal strength parameter (see the text). One of the orbit is $1g_{9/2}$, and the other is shown.

Monopole matrix element from a central force: A=70

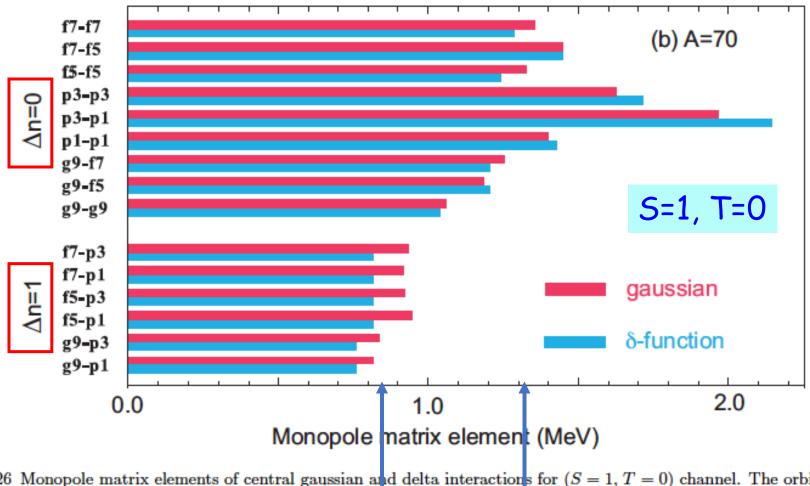


Figure 26 Monopole matrix elements of central gaussian and delta interactions for (S = 1, T = 0) channel. The orbit labeling is abbreviated like g9 for $1g_{9/2}$, etc. The orbits are from valence shell for (a) A = 100 and (b) A = 70

mean values ~0.8 MeV ~1.3 MeV
variations ~0.1 MeV ~0.3 MeV

difference

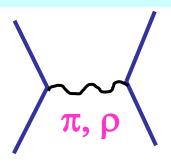
~ < 0.5 MeV

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

Tensor Force

 π meson : primary source

ρ meson ($\sim \pi + \pi$): minor ($\sim 1/4$) cancellation



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

Multiple pion exchanges

- \rightarrow 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)

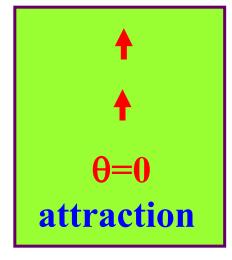
One pion exchange \rightarrow Tensor force

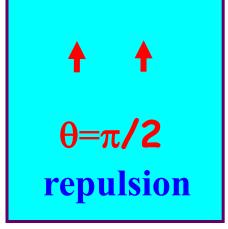
How does the tensor force work?

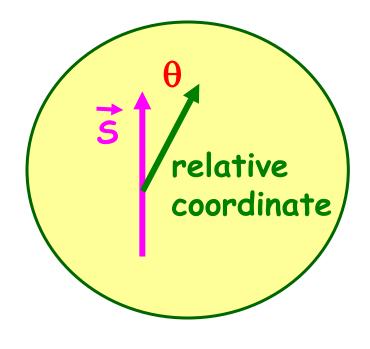
Spin of each nucleon \uparrow is parallel, because the total spin must be S=1

The potential has the following dependence on the angle θ with respect to the total spin 5.

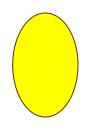
$$V \sim Y_{2,0} \sim 1 - 3 \cos^2 \theta$$







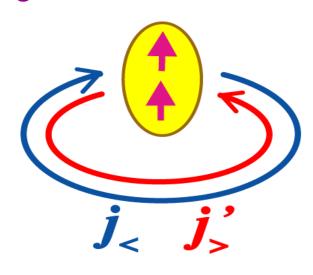
Monopole effects due to the tensor force



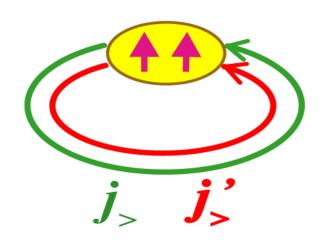
wave function of relative motion

spin of nucleon

large relative momentum small relative momentum



attractive

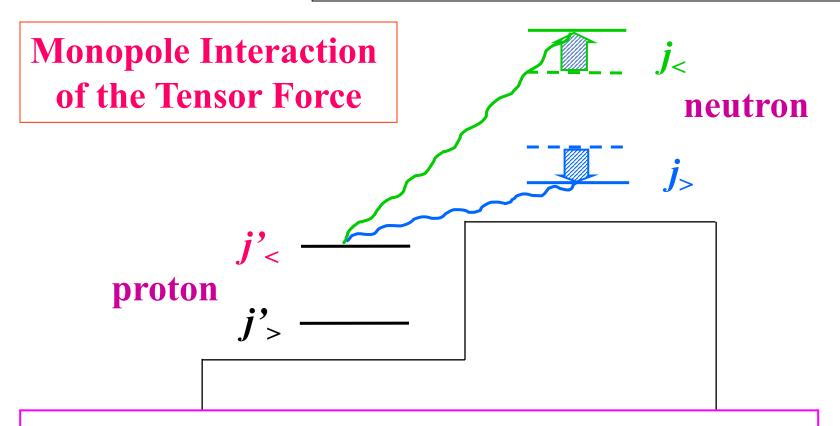


repulsive

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

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

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



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

Variation of monopole matrix element from tensor force: A=70

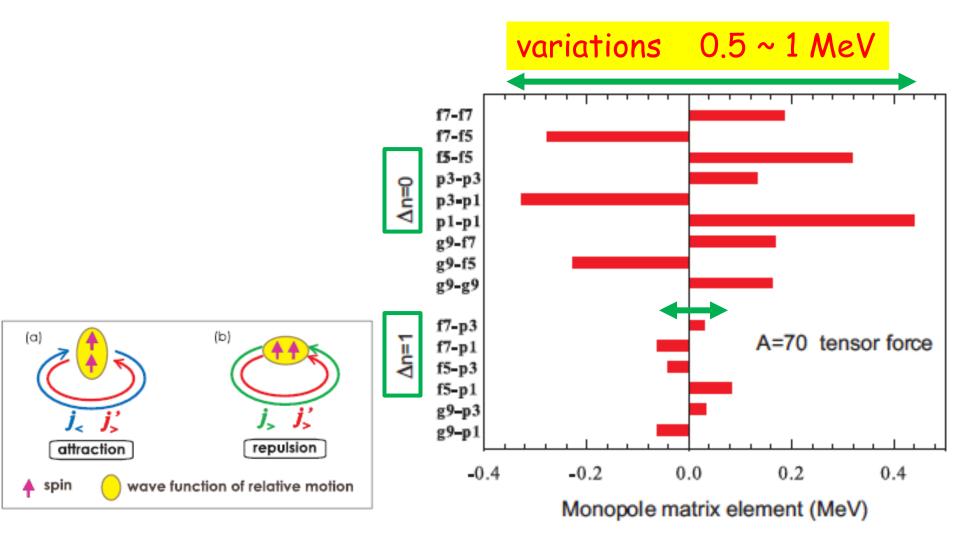


Figure 34 Monopole matrix elements of the tensor force in the T=0 channel. The orbit labeling is abbreviated like f7 for $1f_{7/2}$, etc. The orbits are from valence shell for A=70.

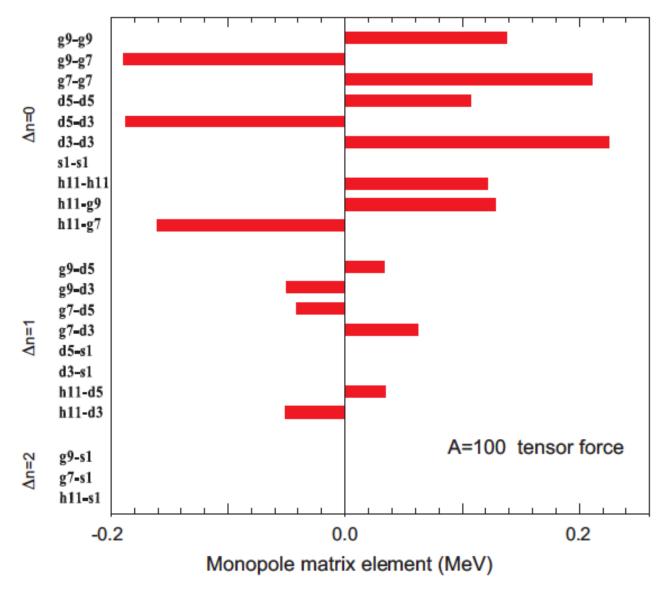
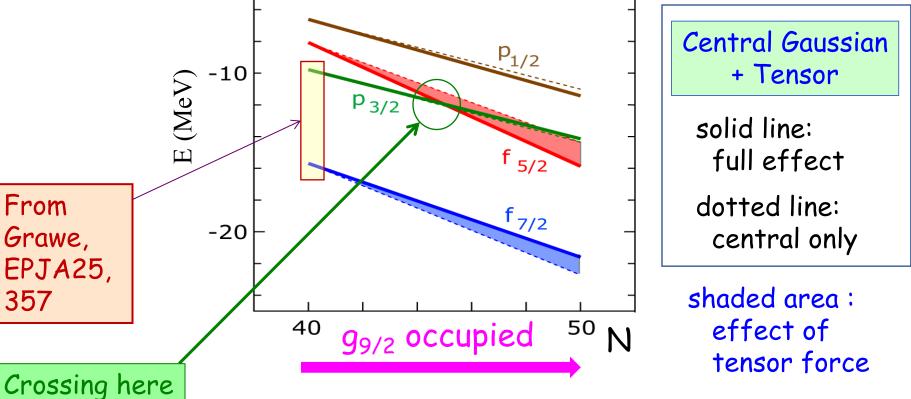


Figure 33 Monopole matrix elements of the tensor force in the T=0 channel. The orbit labeling is abbreviated like g9 for $1g_{9/2}$, etc. The orbits are from valence shell for A=100.

Proton single-particles levels of Ni isotopes



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. Matema, 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. Volkov¹³

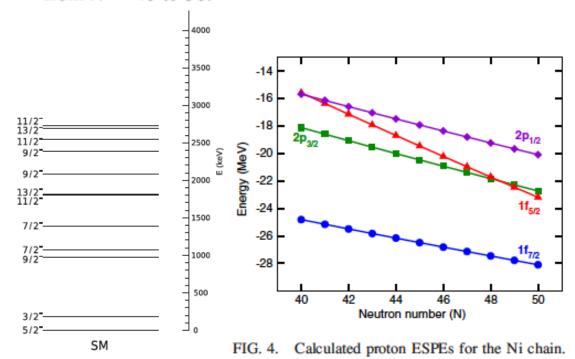
¹Instituut voor Kern- en Stralingsfysica, Katholieke Universiteit Leuven, B-3001 Leuven, Belgium

Shell Evolution towards ⁷⁸Ni: Low-Lying States in ⁷⁷Cu

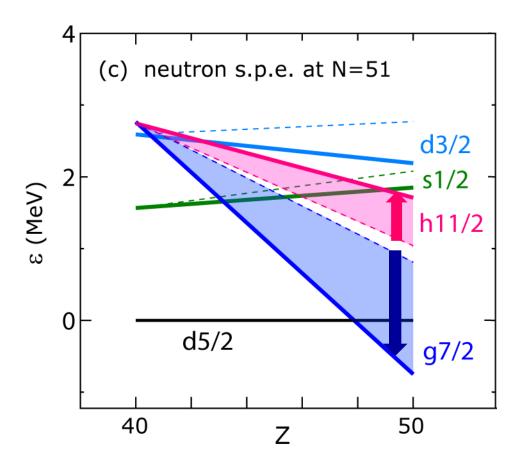
E. Sahin,^{1,*} F. L. Bello Garrote,¹ Y. Tsunoda,² T. Otsuka,^{2,3,4,5} G. de Angelis,⁶ A. Görgen,¹ M. Niikura,³ S. Nishimura,⁷

2.5% >5.7 (7/2, 9/2, 11/2-) 3954 3.9% >5.6 (9/2, 11/2") 3410 (9/2, 11/2°) 2909 (11/2, 13/2°) 2869 $(11/2, 13/2^{-})$ 2604 2068 (7/2")-1954 (11/2") 8.3% >5.6 1775 $(13/2^{-})$ 3.1% >6.1 1154 $(7/2^{-})$ 6.4% >5.9 (9/2")-22.0% >5.4 ళి 293 1.2% >6.8 (3/2") 5/2 ⁷⁷Cu log(ft)

above \sim 1 MeV. A rather large Z=28 gap is consistent with this, while the gap decreases modestly by \sim 2 MeV from N=40 to 50.



Shell structure of a key nucleus 100 Sn



```
solid line: full (central + tensor)
```

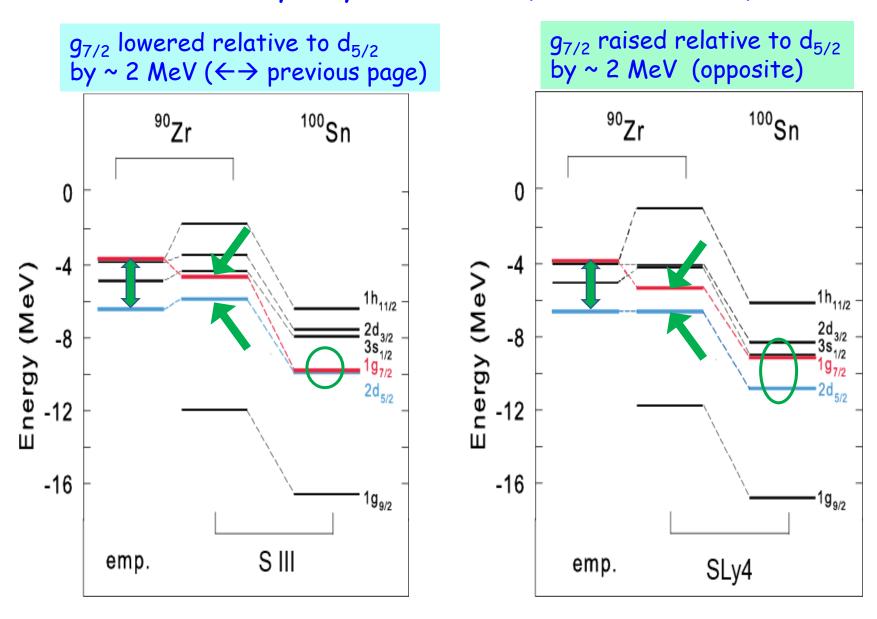
dashed line: central only Fedderman-Pittel (1977)

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.

Predictions by Skyrme model (HF calculation)



An example with 51Sb isotopes

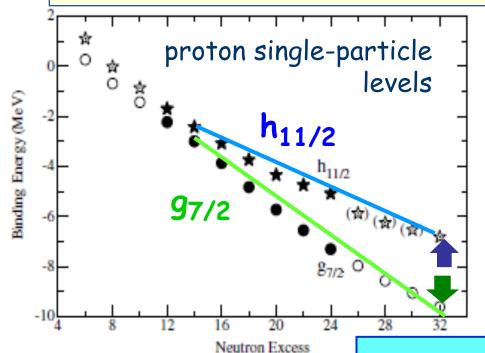
Volume 92, Number 16

PHYSICAL REVIEW LETTERS

week ending 23 APRIL 2004

Is the Nuclear Spin-Orbit Interaction Changing with Neutron Excess?

J. P. Schiffer, S. J. Freeman, J. A. Caggiano, C. Deibel, A. Heinz, C.-L. Jiang, R. Lewis, A. Parikh, P. D. Parker, K. E. Rehm, S. Sinha, and J. S. Thomas



Z=51 isotopes

change driven by neutrons in 1h_{11/2}

 $h_{11/2} - h_{11/2}$ repulsive \blacksquare

 $h_{11/2} - g_{7/2}$ attractive \blacksquare

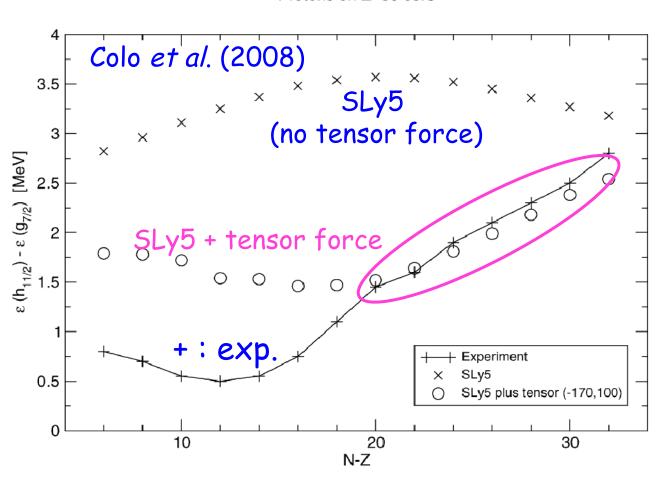
 $\pi + \rho$ meson exchange tensor force (splitting increased by ~ 2 MeV)

TO et al., PRL 95, 232502 (2005)

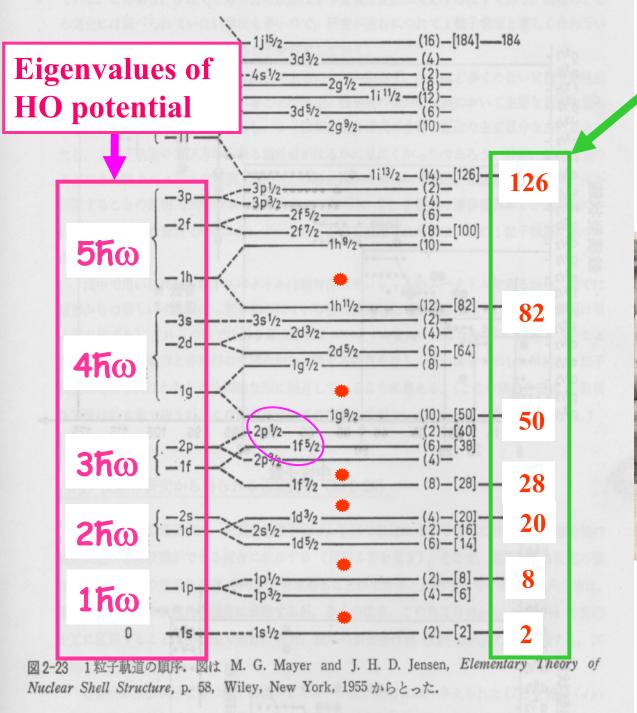
No mean field theory, (Skyrme, Gogny, RMF) explained this before.

Tensor force effect added to the Skyrme (maen-field) model: Proton $g_{7/2}$ and $h_{11/2}$ single-particle orbits on the Z=50 core with N=64-82

Protons on Z=50 core



New magic number ?



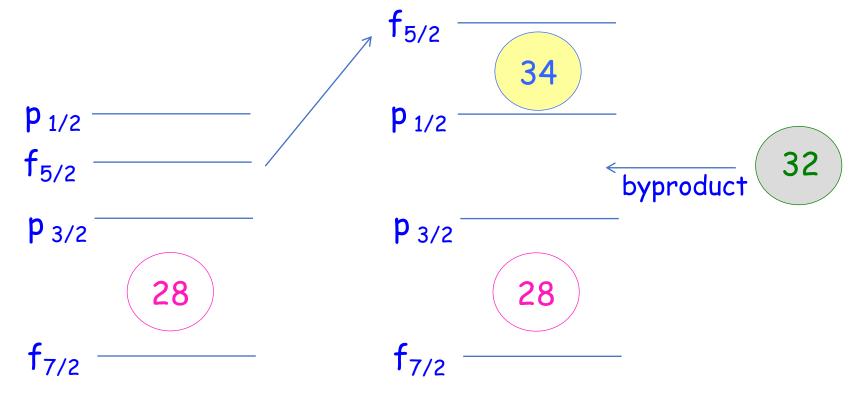
Magic numbers Mayer and Jensen (1949)



R SHELL MODEL

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

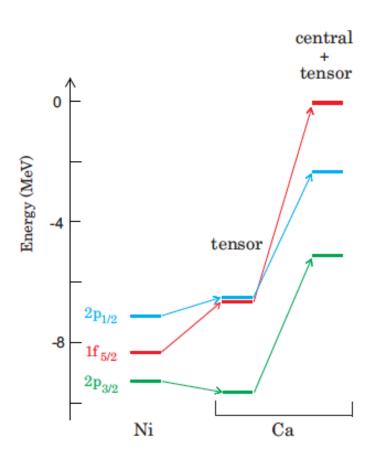


Figure 41 Change of single-particle energies from ⁵⁶Ni to ⁴⁸Ca.

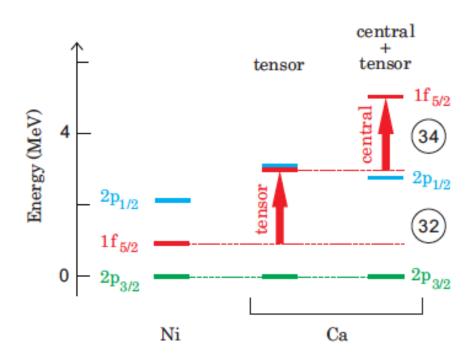


Figure 42 Change of single-particle energies from 56 Ni to 48 Ca relative to the $2p_{3/2}$ orbit. The red arrows indicate the change of the $1f_{5/2}$ ESPE. The arising magic numbers, N=32 and 34, are shown in black circles.

Is there N=34 magic number?

In comparison to N=32 magic number known experimentally for nearly 30 years.

Moving back to heavier nuclei, from the strong interaction in Fig. 1(c), we can predict other magic numbers, for instance, N = 34 associated with the $0f_{7/2}$ - $0f_{5/2}$ interaction. In heavier nuclei, $0g_{7/2}$, $0h_{9/2}$, etc. are shifted upward in neutron-rich exotic nuclei, disturbing the magic numbers N = 82, 126, etc. It is of interest how the r process of nucleosynthesis is affected by it.

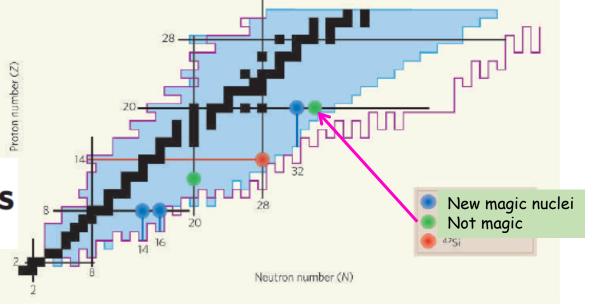
TO et al. PRL 87 (2001)

NATURE | Vol 435 | 16 June 2005

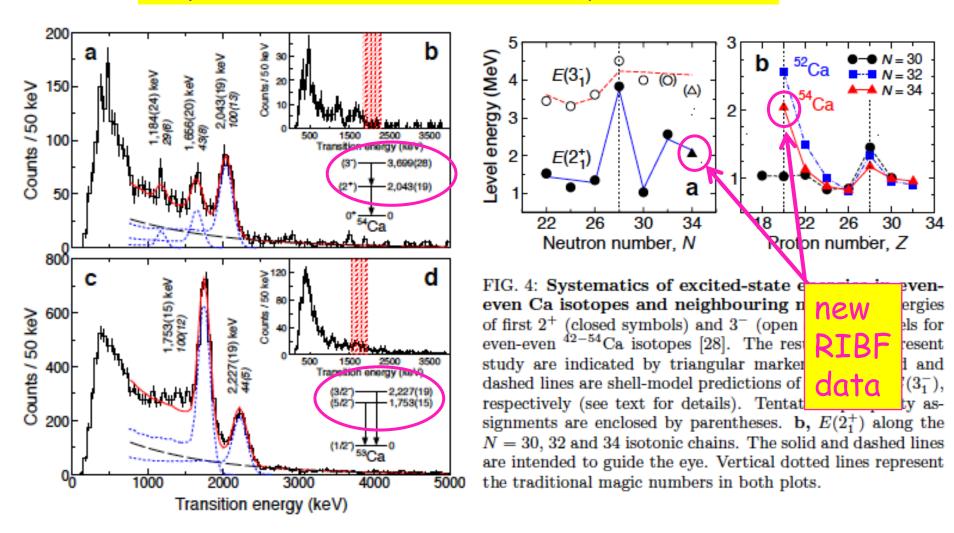
NUCLEAR PHYSICS

Elusive magic numbers

Robert V. F. Janssens



Experiment @ RIBF -> Finally confirmed



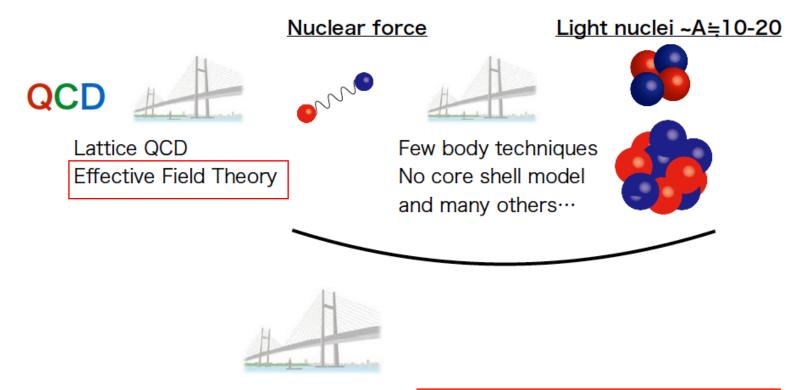
er-corrected γ -ray energy spectra. De-excitation γ rays measured in coinci-

4Ca and c, 53Ca reaction products. Peaks a Steppenbeck et al. Nature, 502, 207 (2013)

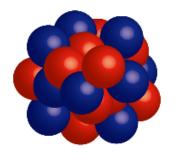
ve intensities are indicated by italic fonts. The short-blue and long-black dashed

Shell evolution with the modern nuclear forces

shell model powered by modern nuclear forces



Medium mass nuclei~A≒20-100



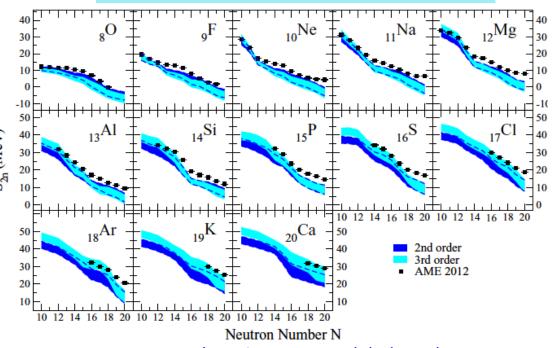
shell model with core via the effective interaction derived from nuclear force

Examples of structure calculations starting from chiral EFT forces

NN force: N3LO + 3N force: N2LO

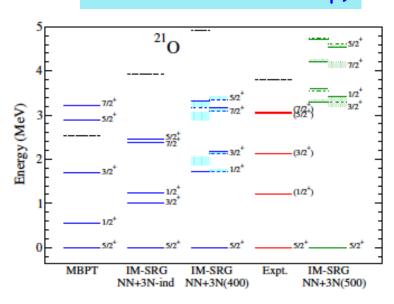
-> valence shell interaction

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)



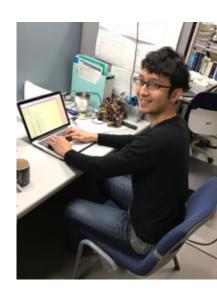
Bogner et al. PRL 113, 142501 (2014)

+ 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

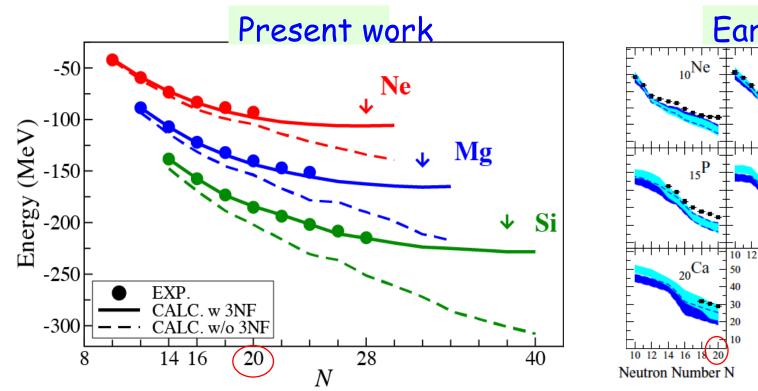
Naofumi Tsunoda,¹ Takaharu Otsuka,^{1,2,3,4} Noritaka Shimizu,¹ Morten Hjorth-Jensen,^{5,6} Kazuo Takayanagi,⁷ and Toshio Suzuki⁸

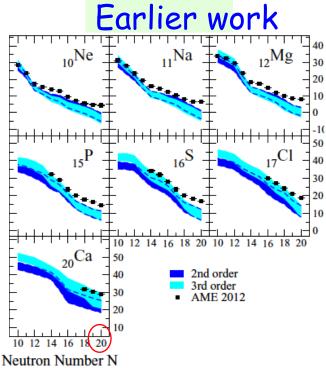
^{*}E. M. Krenciglowa and T. T. S. Kuo, Nucl. Phys. A 235, 171 (1974).

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

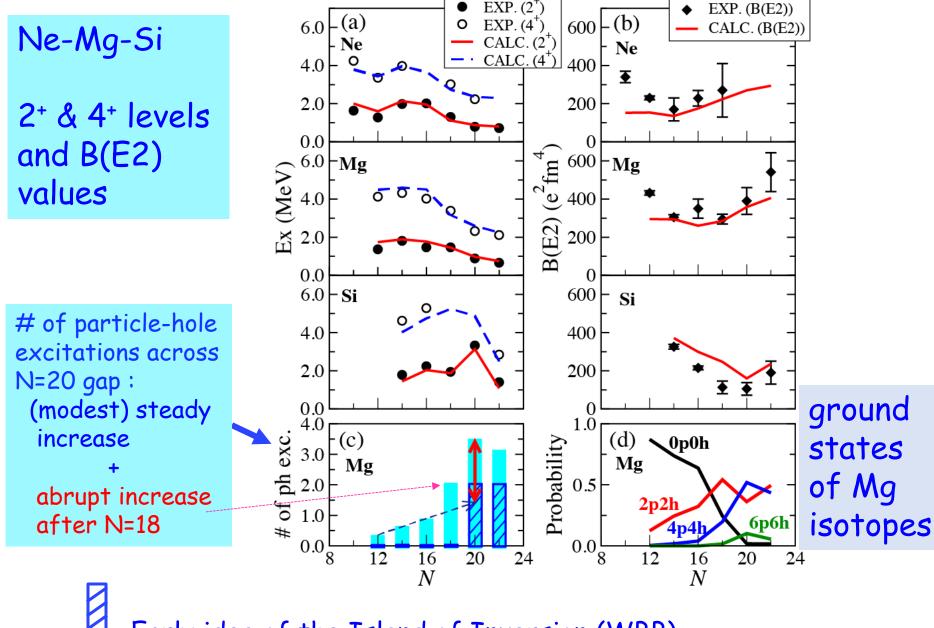
Calculations with full sd + pf shell

ground-state energies



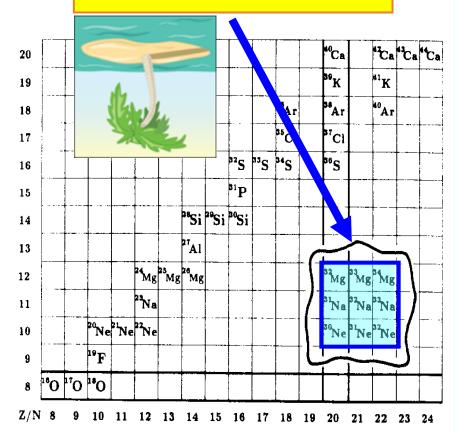


Simonis et al. PRC 93, 011302(R) (2016)



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

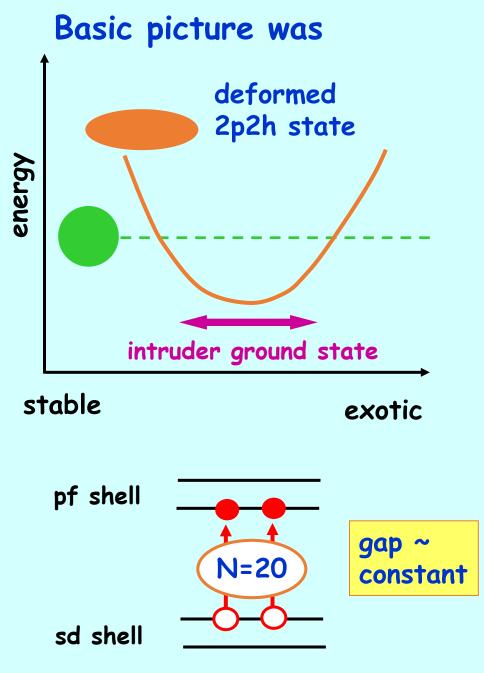
Island of Inversion



9 nuclei:

Ne, Na, Mg with N=20-22

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



³¹₁₂Mg₁₉: very difficult to fit by the shell model

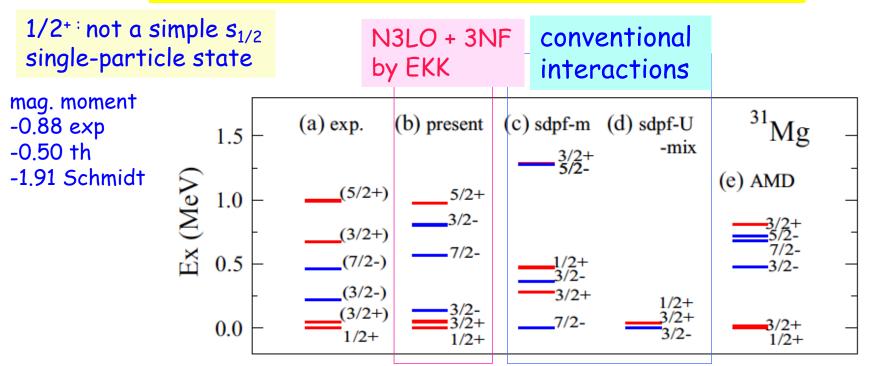


FIG. 4. Energy levels of ³¹Mg. (a) experimental values, (b) present work, (c) sdpf-m [16], (d) sdpf-U-mix [17], and (e) AMD+calculation [52].

exp. by laser spectroscopy: PRL 94, 022501 (2005), G. Neyens, et al.

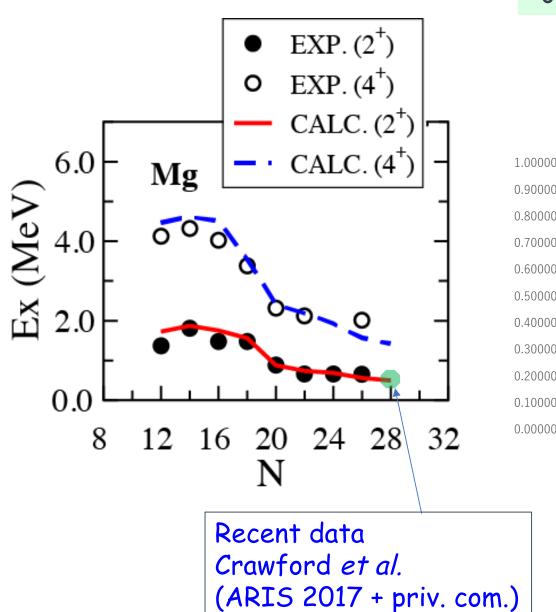
Mixing between sd and pf shells is crucial

Fit of relevant TRME's is infeasible: too many TRME

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).

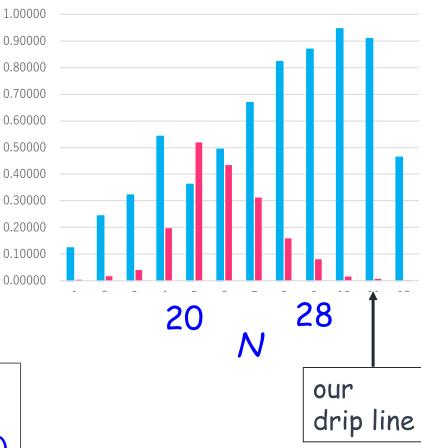
Mg up to N=28 2^+ & 4^+ levels



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

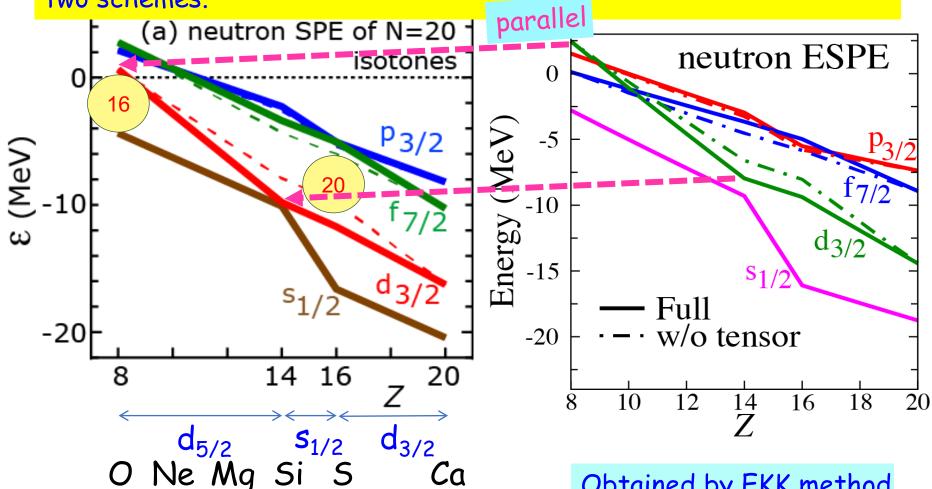
2 ph excitations over N=20

4 ph excitations over N=20



Neutron single-particle energy (SPE) at N=20

Tensor and central force effects are almost identical between the two schemes.



Obtained from VMU interaction : phenomenological central (Gaussian) and π + ρ meson-exchange tensor interaction

Obtained by EKK method from chiral EFT NN interaction

The traditional picture such as the Island of Inversion is being re-visited and re-examined, leading to a renewed picture!

The shell structure can be indeed changed in many cases!

The same physics drives the shape coexistence and in the quantum phase transition. Tomorrow ...

Int. School of Physics "Enrico Fermi" - Course 201 Nuclear Physics with Stable and Radioactive Ion Beams Varenna July 14-19, 2017

Recent developments shell model studies of atomic nuclei

Takaharu Otsuka

3rd lecture











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

Summary of shell evolution

p-n monopole interaction between orbits j and j'

```
particularly strong, if \Delta n=0 (n: # of nodes of radial wave func.)
```

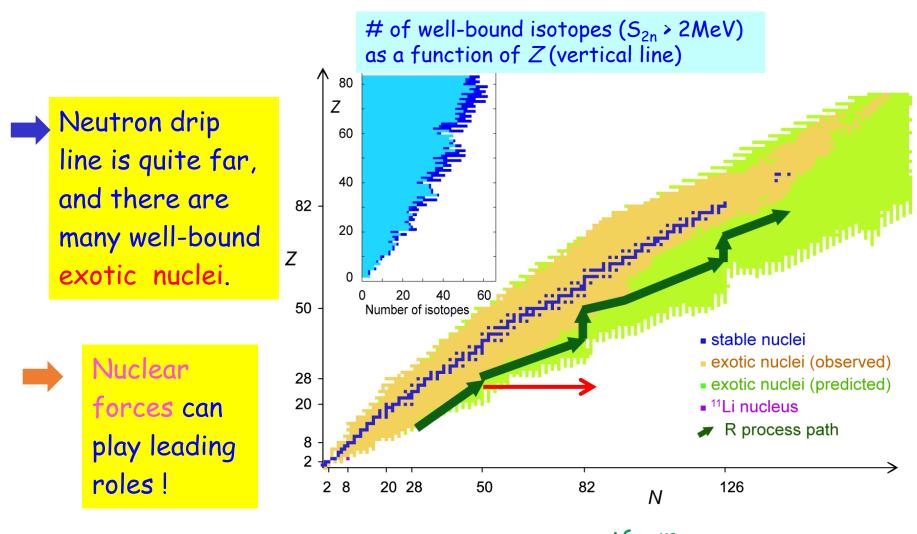
central: attractive

tensor: attractive (j, -j',) or repulsive (j, -j',)

example: $g_{9/2}$ - $f_{5/2}$: coherent $g_{9/2}$ - $f_{7/2}$: cancellation

monopole interaction changes ESPE (effective single-particle energy) with linear dependence on the occupation number $n_{j'}$ \rightarrow effect can be magnified \rightarrow shell evolution

change of spin-orbit splitting
change of shell gap
change of the ordering of orbits
new magic numbers, disappearance of usual magic numbers



Effective single-particle energy

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

This is not uniform as a function of j and j'.

$$\sum_{j'} V_{pn}^m(j,j') \Delta \hat{n}_{j'}^n,$$

This can be large.

Three pillars combined for future

computation

Monte Carlo Shell Model (MCSM)

(almost)
unlimited
dimensionality

massive parallel computers

Hamiltonian

pfg9d5 (A3DA) (Ni) 8+8 on ⁵⁶Ni core (Zr) 8+8 on ⁸⁰Zr core (Sn) 8+10 on ¹³²Sn core (Sm)

island of stability
+

χEFT based multi-shell int.

many-body dynamics

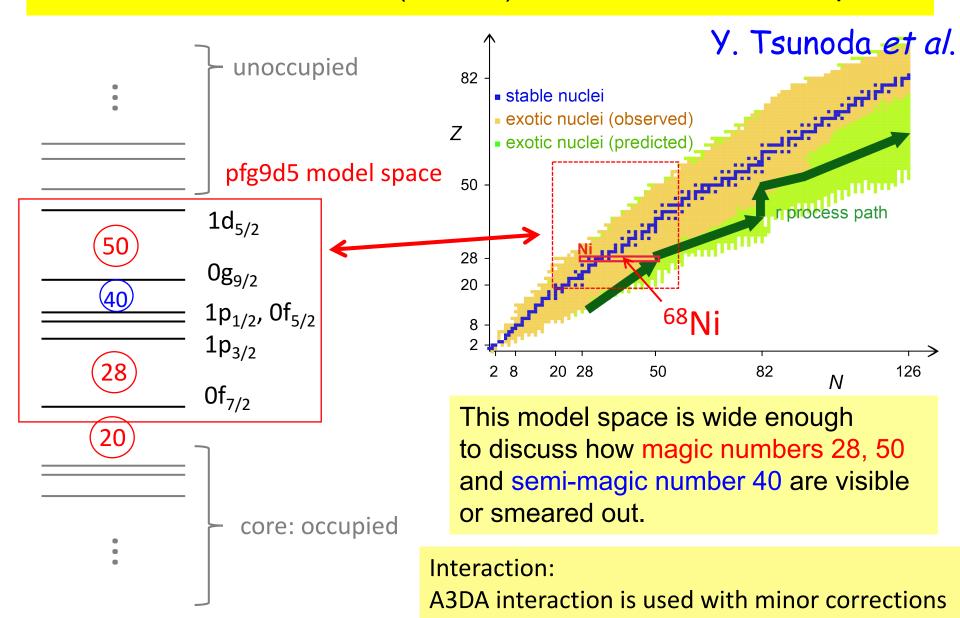
Shell evolution (Type I & II)

Quantum Phase Transition

Shape coexistence

Quantum Self-organization

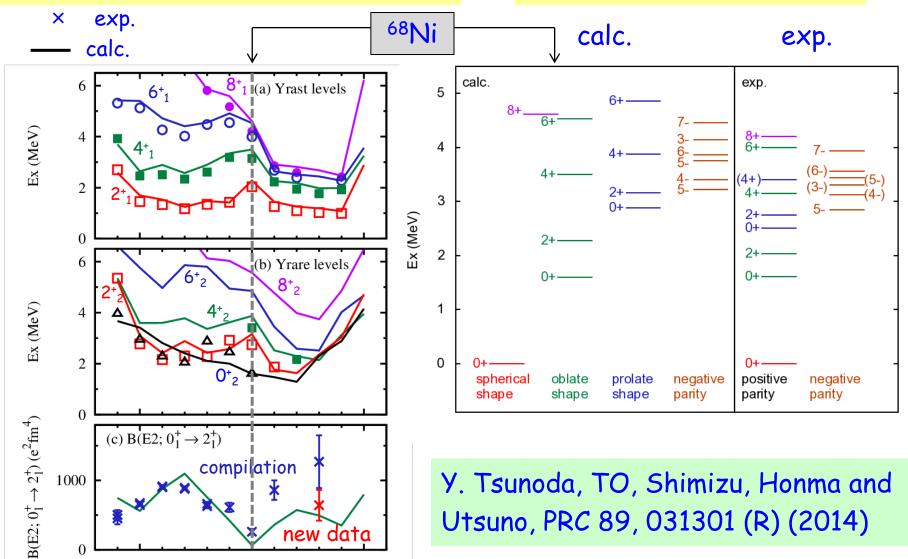
Monte Carlo Shell Model (MCSM) calculation on Ni isotopes



Energy levels and B(E2) values of Ni isotopes



Shape coexistence in ⁶⁸Ni



new data

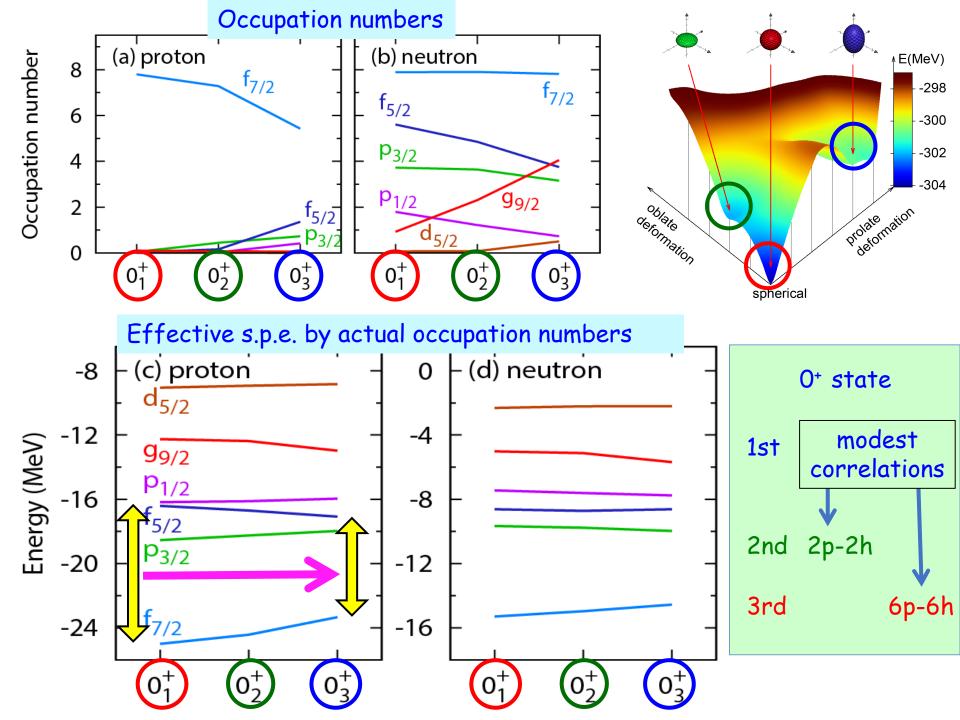
50

40

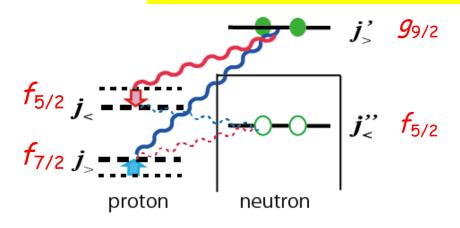
N

30

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



Type II Shell Evolution in ⁶⁸Ni (Z=28, N=40)



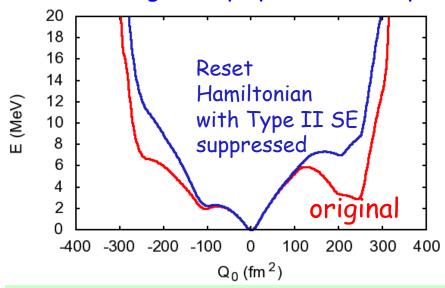
Spin-orbit splitting works against quadrupole deformation (cf. Elliott's SU(3)).

weakening of spin-orbit splitting

Type II shell evolution

⇒ more neutron p-h excitation

PES along axially symmetric shape



Type II shell evolution is suppressed by resetting monopole interactions as

$$\pi f_{7/2} - v g_{9/2} = \pi f_{5/2} - v g_{9/2}$$

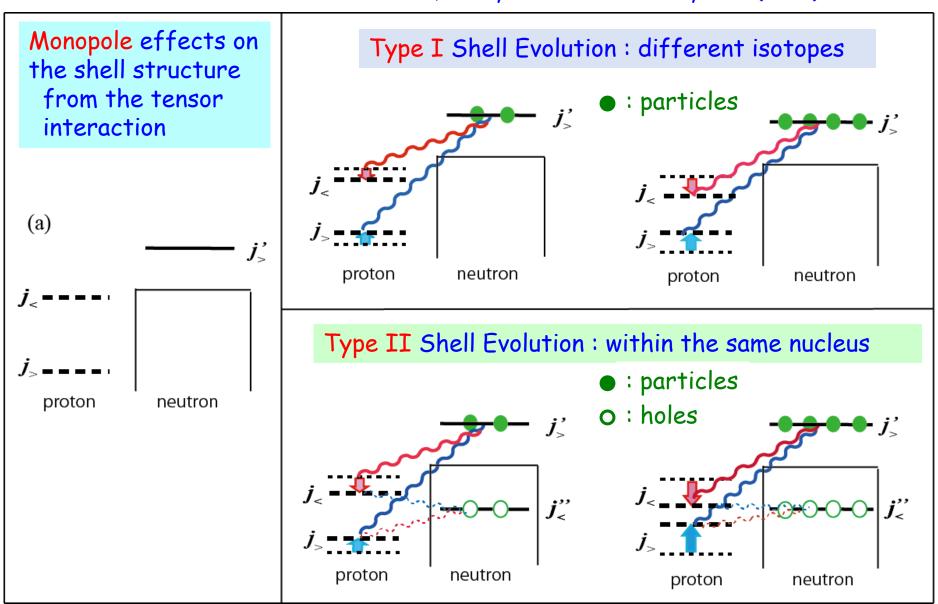
 $\pi f_{7/2} - v f_{5/2} = \pi f_{5/2} - v f_{5/2}$

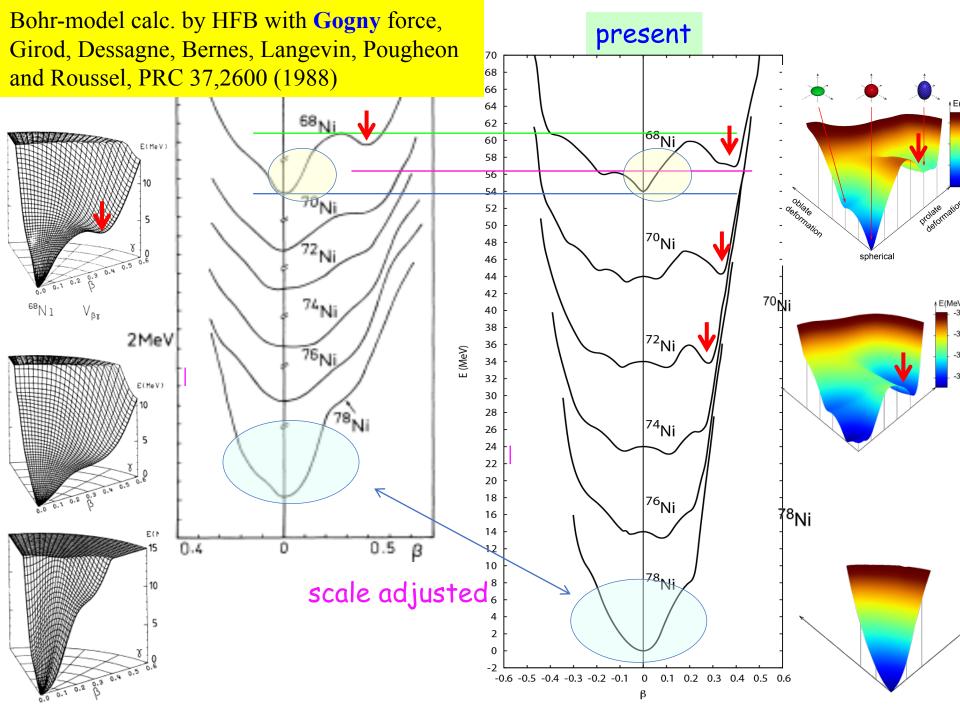
The local minima become much less pronounced.

Shape coexistence is enhanced by type II shell evolution because the same quadrupole interaction can work more efficiently.

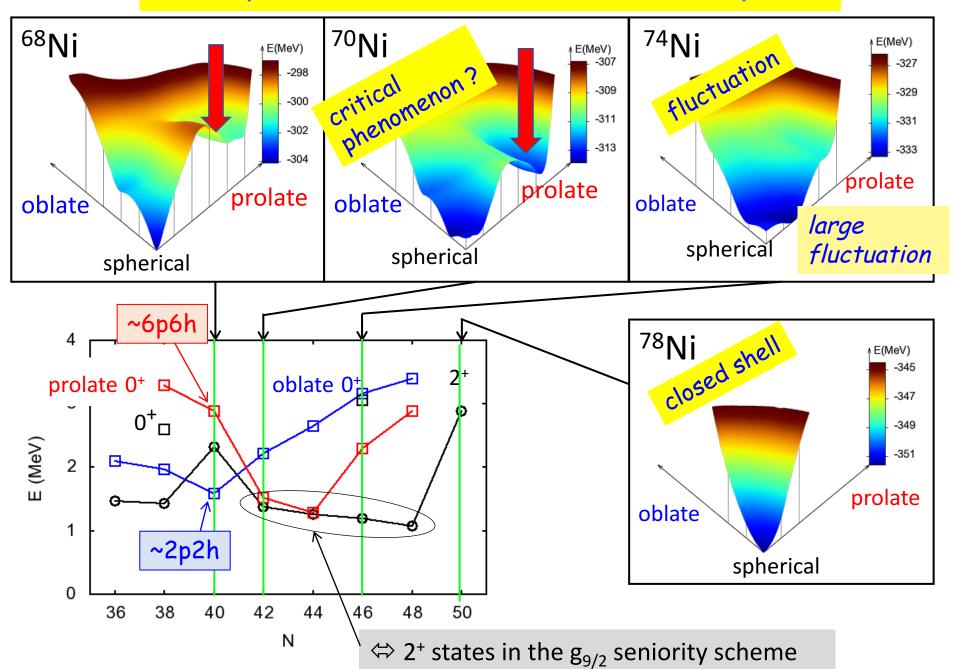
Underlying mechanism of the appearance of low-lying deformed states : Type II Shell Evolution

TO and Y. Tsunoda, J. Phys. G: Nucl. Part. Phys. 43 (2016) 024009





Shape or structure evolution of Ni isotopes

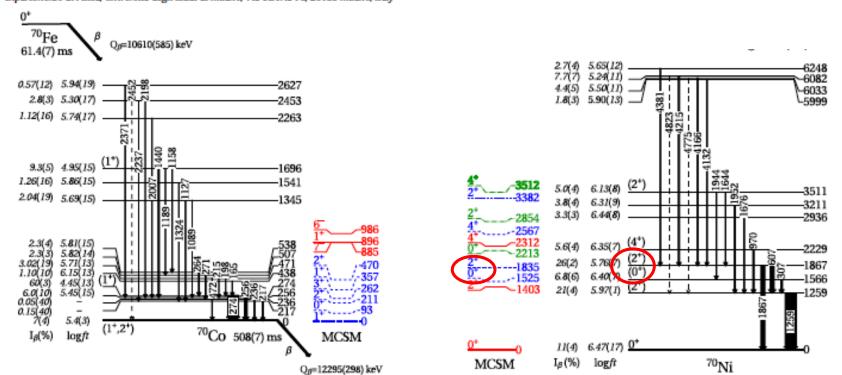


Physics Letters B 765 (2017) 328-333 What is this?

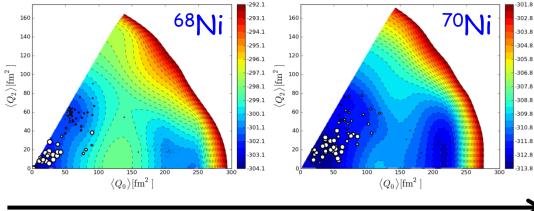
Type II shell evolution in A = 70 isobars from the $N \ge 40$ island of inversion

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b Dipartimento di Fisica, Università degli Studi di Milano, Via Celoria 16, 20133 Milano, Italy



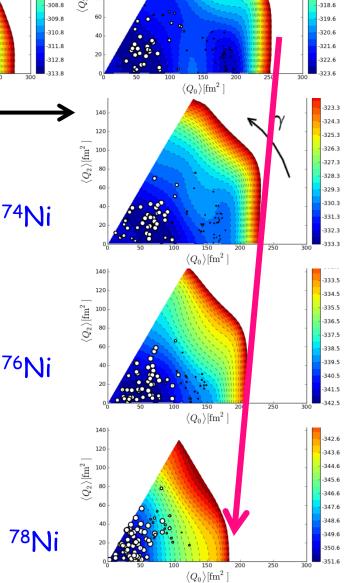
^a Istituto Nazionale di Fisica Nucleare, Sezione di Milano, Via Celoria 16, 20133 Milano, Italy



Energy of prolate state comes down. Barrier becomes low.

T-plot for 0⁺1 states of ⁶⁸⁻⁷⁸Ni

The ground state is always like seniority-zero (BCS-type) spherical state.



72Ni

-316.6

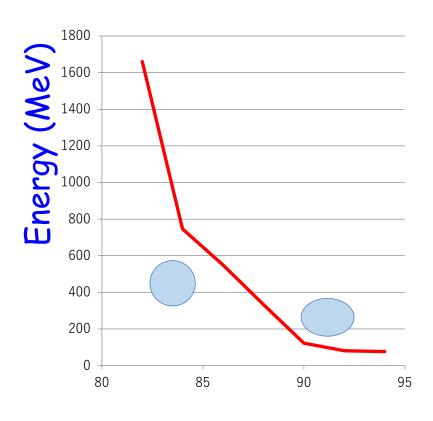
Shape transition and quantum phase transition

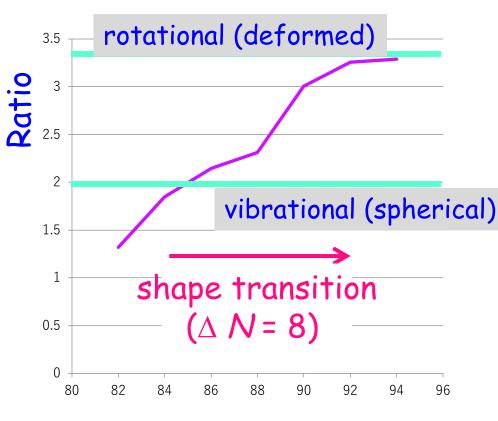
Shape change as a function of N(or Z)

2+ and 4+ level properties of Sm isotopes

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

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



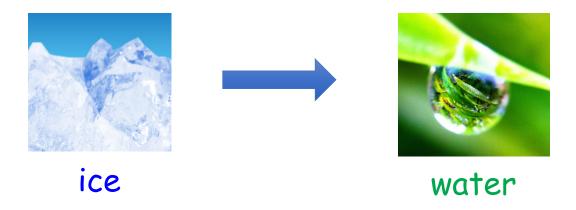


Neutron number, N

Neutron number, N

Can this be a kind of *Phase Transition*?

Can the shape transition in nuclei 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).

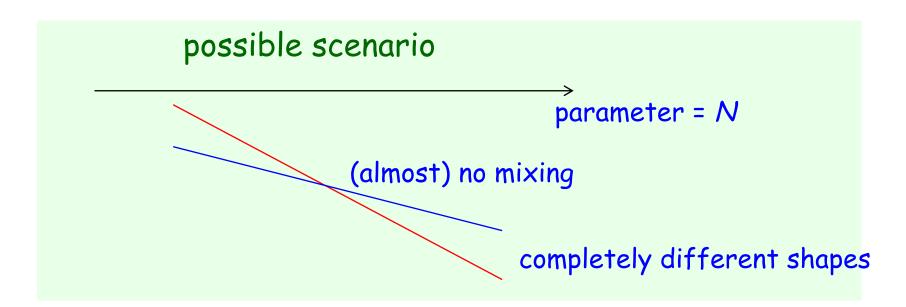
The phase transition implies this kind of phenomena of macroscopic systems consisting of almost infinite number of molecules.

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

The shape transition occurs rather gradually.

Quantum Phase Transition:

an abrupt change in the ground state of a many-body system by varying a physical parameter at zero temperature. (cf., Wikipedia)



Sizable mixing occurs usually in finite quantum systems.

Quest for Quantum Phase Transition: Shapes of Zr isotopes by Monte Carlo Shell Model

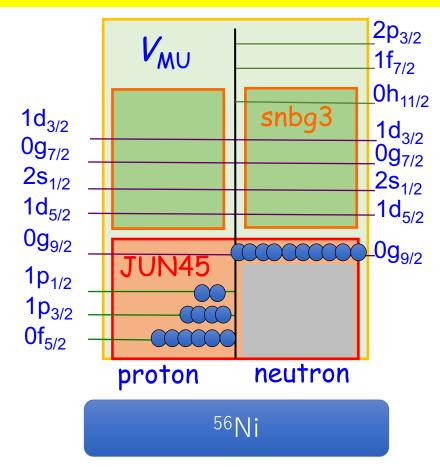
- Effective interaction: $JUN45 + snbg3 + V_{MU}$

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 x 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 Física, Universidad Nacional Autonoma de Mexico, Apartado Postal 20-364, Mexico 20, D. F.

S. Pittel

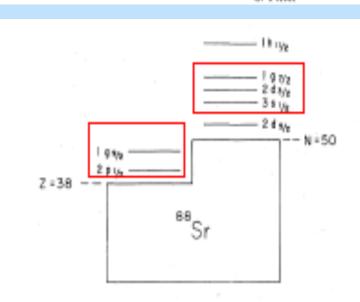


FIG. 3. Single-particle levels appropriate to a description of nuclei in the Zr-Mo region. An ⁵⁸Sr core is assumed.

PHYSICAL REVIEW C 79, 064310 (2009)

Shell model description of zirconium isotopes

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

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 $\pi(r3 - g)$, $\nu(r4 - h)$.

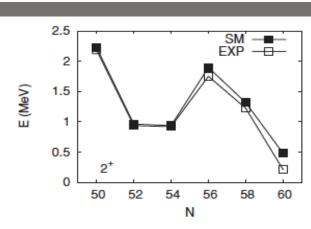


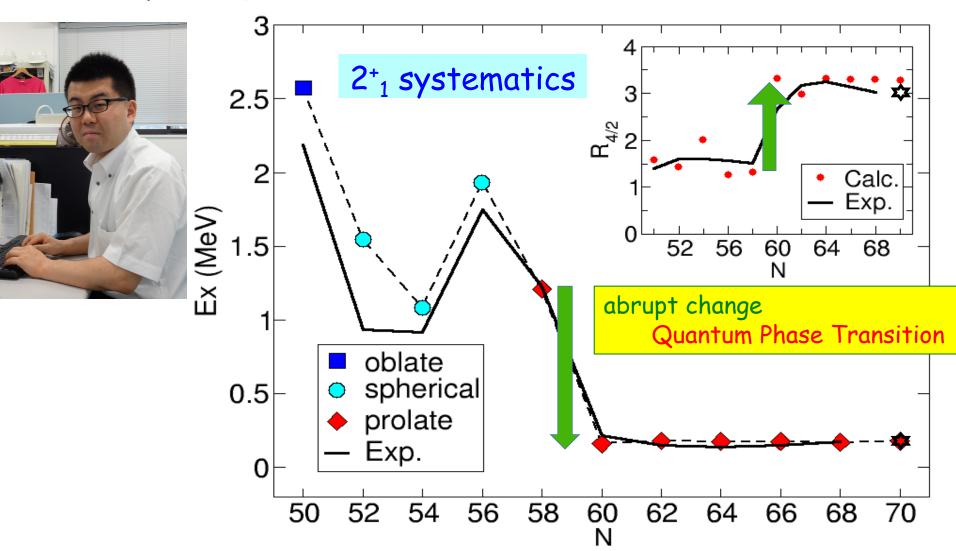
FIG. 12. Systematics of the experimental and theoretical first excited 2⁺ states along the zirconium chain.

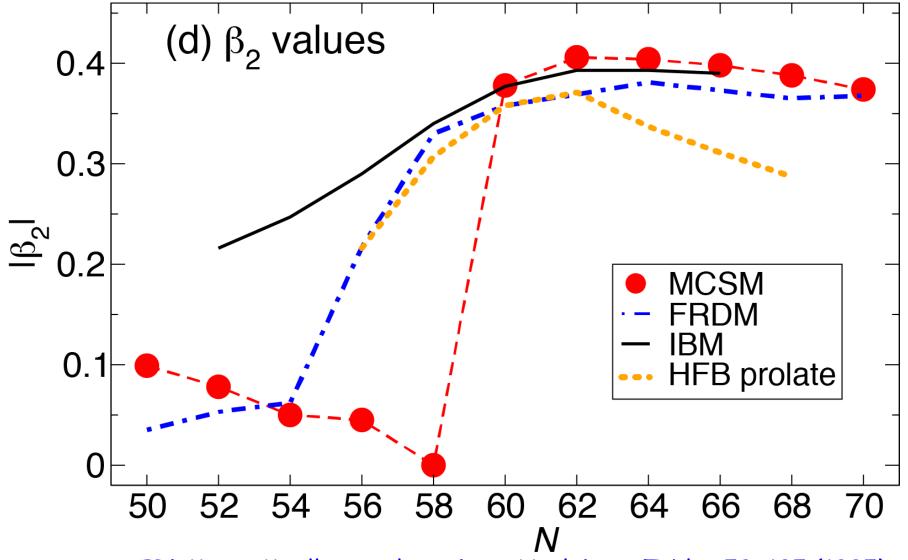


PRL 117, 172502 (2016)

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

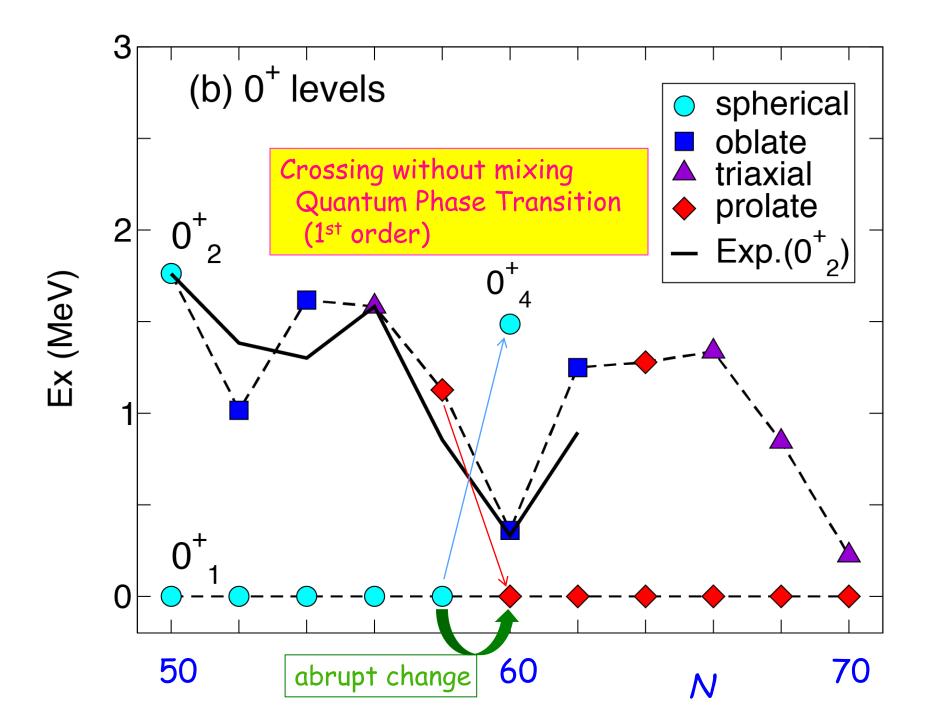




FRDM: S. Moeller et al. At. Data Nucl. Data Tables 59, 185 (1995).

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

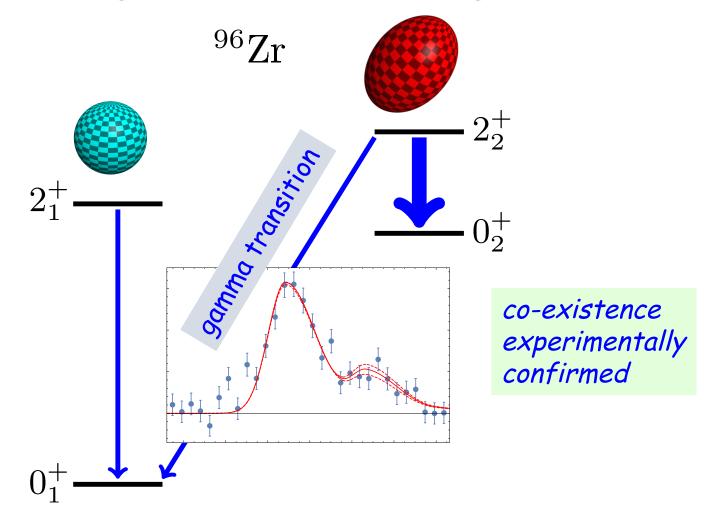
HFB: R. Rodriuez-Guzman et al. Phys. Lett. B 691, 202 (2010).98

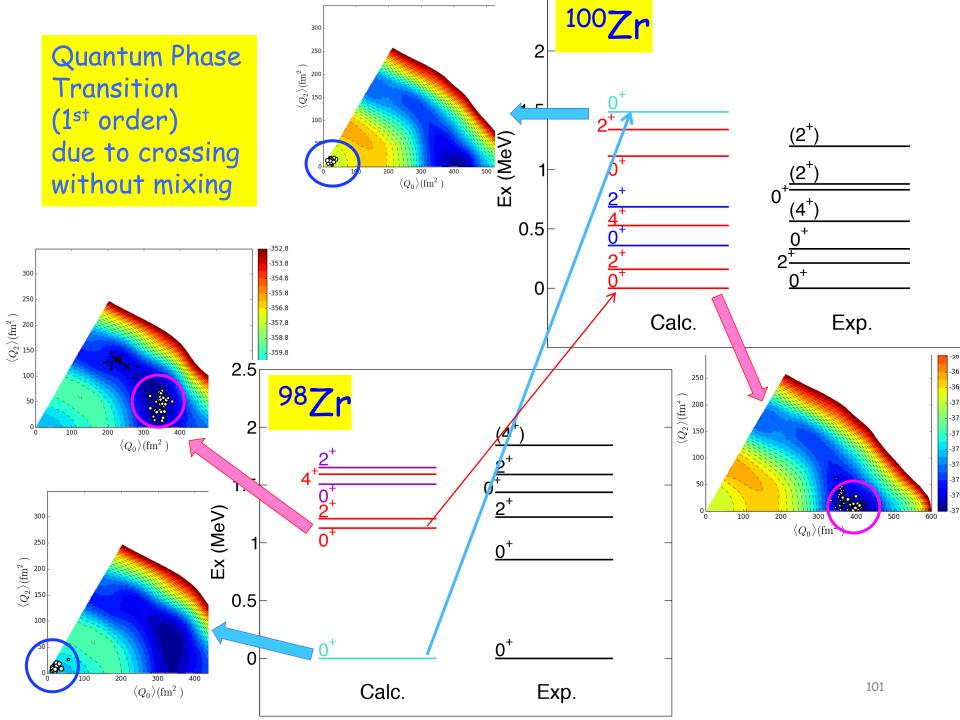


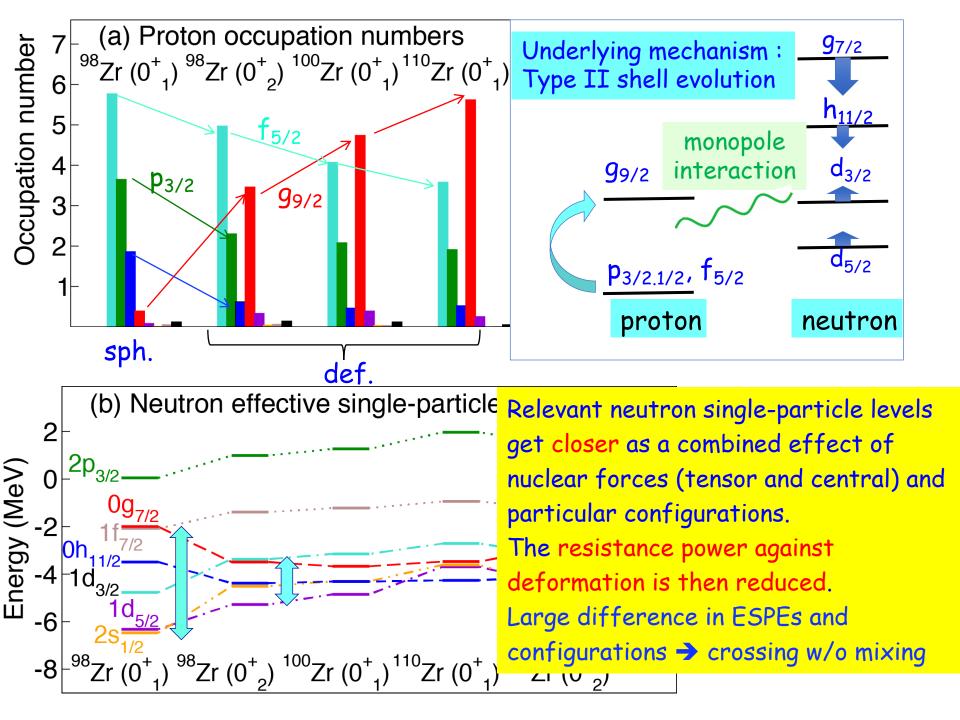


First Measurement of Collectivity of Coexisting Shapes Based on Type II Shell Evolution: The Case of ⁹⁶Zr

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

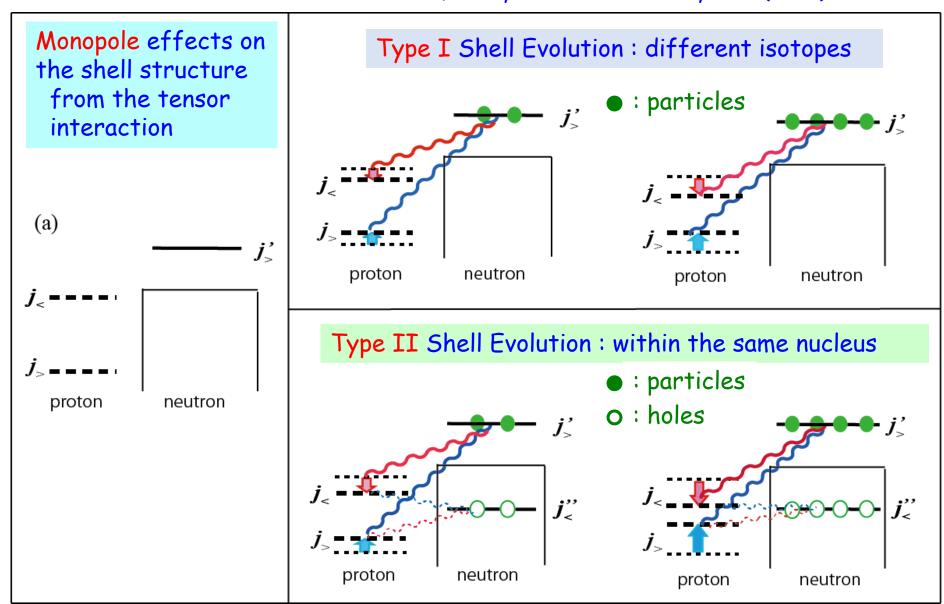






Underlying mechanism of the appearance of low-lying deformed states : Type II Shell Evolution

TO and Y. Tsunoda, J. Phys. G: Nucl. Part. Phys. 43 (2016) 024009



Type II shell evolution is a simplest and visible case of

Quantum Self Organization

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.

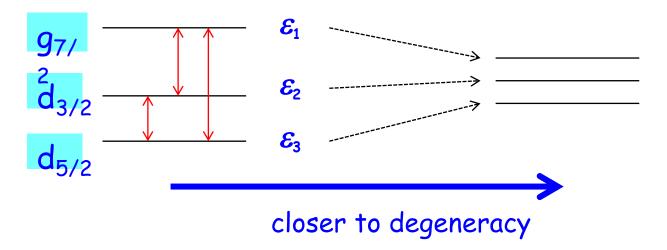
Reminder: Jahn-Teller effect for nuclear deformation

(Self-consistent) quadrupole deformed field $\propto Y_{2,0}$ (θ,ϕ) mixes the orbits below

$$\Psi(J_z=1/2) = c_1 |g_{7/2}; j_z=1/2\rangle + c_2 |d_{3/2}; j_z=1/2\rangle + c_3 |d_{5/2}; j_z=1/2\rangle$$

stronger mixing = larger quadrupole deformation

Mixing depends not only on the strength of the $Y_{2,0}$ (θ,ϕ) field, but also the spherical single-particle energies ε_1 , ε_2 , ε_3 , etc.



larger deformation for the same deformed field

Let's shed light on an old problem

Atomic nucleus is a quantum Fermi liquid :

The nucleus is composed of almost free nucleons interacting weakly via residual forces in a (solid) (mean) potential like a solid vase.

"how single-particle states can coexist with collective modes" *conceived* also *by Gerry Brown* as an open unresolved problem (T. Schaefer, Fermi Liquid theory: A brief survey in memory of Gerald E. Brown, NPA 2014)

Surface deformation produced by additional deformed mean field → Nilsson model (deformed "vase", monopole effect missing)



Sven Gösta Nilsson

Renewed picture:

Single-particle levels can be re-organized to enhance collective modes.

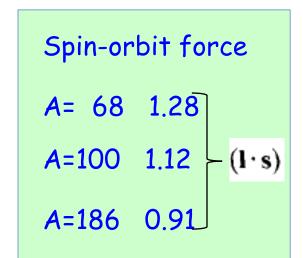
SP states and coll. mode are not enemies but friends!

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

$$H = \frac{\mathbf{p}^2}{2M} + \frac{1}{2}M\left(\omega_3^2x_3^2 + \omega_\perp^2(x_1^2 + x_2^2)\right) + v_{ll}\hbar\omega_0(\mathbf{l}^2 - \langle \mathbf{l}^2\rangle_N) + v_{ls}\hbar\omega_0(\mathbf{l} \cdot \mathbf{s})$$
quadrupole deformed field spherical field (5-10)
$$\langle \mathbf{l}^2\rangle_N = \frac{1}{2}N(N+3)$$

	$-v_{ls}$	$-v_{ll}$
N and $Z < 20$	0.16	0
50 < Z < 82	0.127	0.0382
82 < N < 126	0.127	0.0268
82 < Z < 126	0.115	0.0375
126 < N	0.127	0.0206
	50 < Z < 82 82 < N < 126 82 < Z < 126	50 < Z < 82 0.127 82 < N < 126 0.127 82 < Z < 126 0.115

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



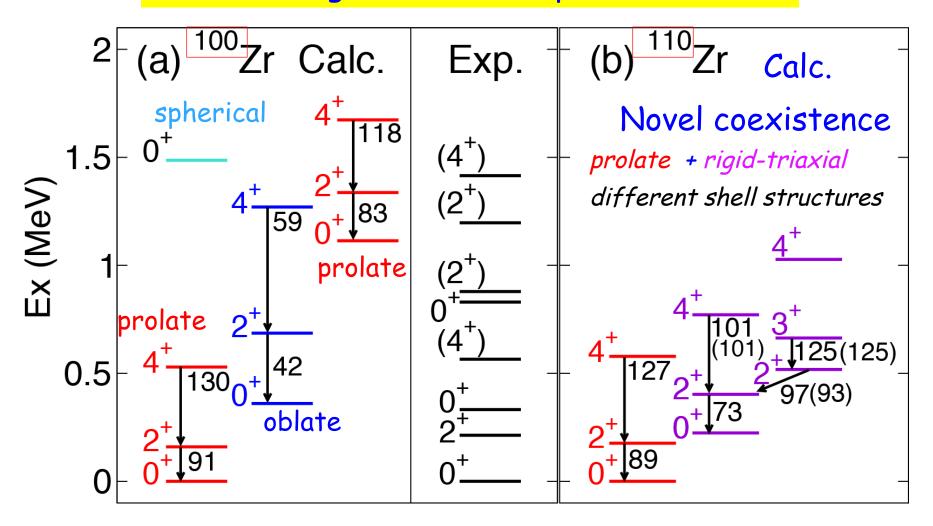
resistance power ← pairing force

single-particle energies

Analogy to electric current,

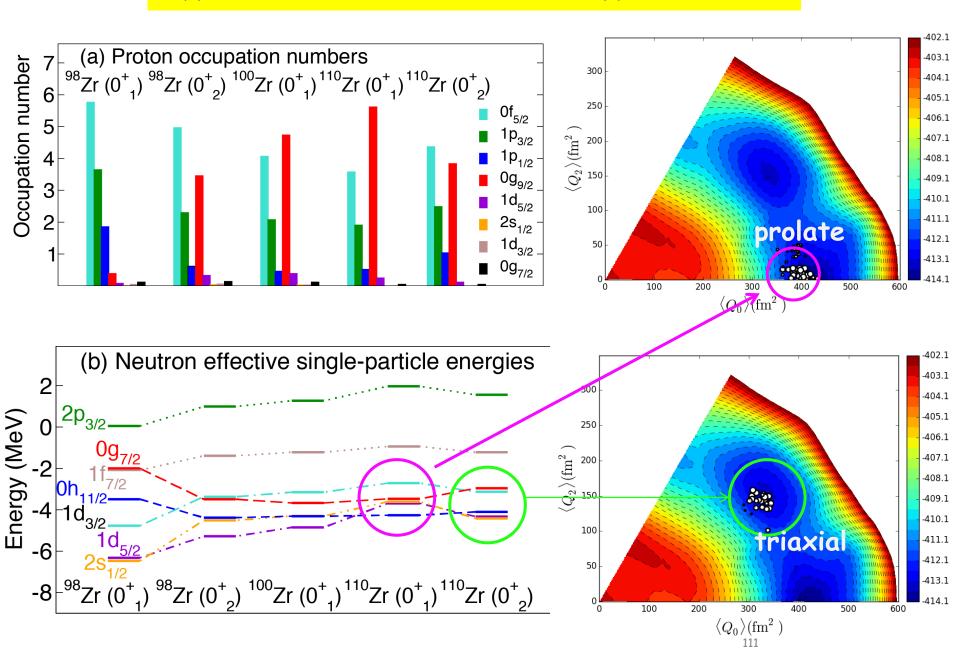
Anatomy of this effect: 98Zr spherical O₁ and deformed O₂ PES with T-plot monopole active Frozen monopole -353.8 98Zr 0+1 10.5 -354.8 (original result) spherical -355.8 -356.8 98Zr 0+ $\langle Q_2
angle
angle (ext{fm}^2)$ ground state -357.8 do not change -359.8 -360.8 100 (overlap~0.98) 3.0 -361.8 -362.8 1.5 (0) -363.8 500 $\langle Q_0 \rangle (\text{fm}^2)$ prolate Effective SPE -354.8 -355.8 - configuration dependent 250 -356.8 is gone -357.8200 98Zr 0⁺₂ -358.8 -359.8 2p_{3/2} Energy (MeV) -360.8 100 -361.8 $0g_{7/2}$ -362.8 -363.8 -364.8 0h_{11/2} 500 $\langle Q_0 \rangle (\text{fm}^2)$ Use them as constant SPEs $1d_{5/2}$ independent of configurations, putting 2s_{1/2} monopole int. aside > Frozen monopole treatment

Prolate - rigid-triaxial shape coexistence



(): Rigid-triaxial rotor with gamma=28 degrees normalized at $2^+_2 \rightarrow 0^+_2$

different shell structures ~ like "different nuclei"



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 ⁵⁶Ni core (Zr) 8+8 on ⁸⁰Zr core (Sn) 8+10 on ¹³²Sn core (Sm)

island of stability

 χ EFT based (multi-)shell int.

many-body dynamics

Shell evolution (Type I & II)

Quantum Phase Transition

Shape coexistence

Quantum Self-organization

Remark on Fermi liquid picture of nuclei

Naïve Fermi liquid picture (a la Landau) is revised, as atomic nuclei are not necessarily like simple solid vases containing almost free nucleons.

Nuclear forces are rich enough to optimize single-particle energies for each eigenstate (especially in the cases of collective-mode states), as referred to as quantum self-organization.

The quantum self-organization produces sizable effects with

- (i) two quantum fluids (protons and neutrons),
- (ii) two major forces : e.g., quadrupole interaction to drive collective mode monopole interaction to control resistance

Type II shell evolution is one of the most visible cases of the quantum self-organization, with massive p-h excitations across the shell gap. Quantum phase transition, shape coexistence, various deformation, fission, ... are releted to the quantum self-organization.

The beauty of the collective modes is enhanced. Time-dependent version for reactions is of great interest (beyond thermalisation *etc.*).

The microscopic foundation of the IBM (Interacting Boson Model) is also related, for instance, regarding the origin of the Majorana interaction.

