「京からポスト京に向けて」シンポジウム
筑波大学東京キャンパス
２月１６日（１６−１７日）, ２０１７

京で見えてきた原子核の新たな構造原理

大塚 孝治 *University of Tokyo / MSU / KU Leuven*

Yusuke Tsunoda (CNS, Tokyo)
Tomoaki Togashi (CNS, Tokyo)
Noritaka Shimizu (CNS, Tokyo)

Outline

- 序
  - 原子核の形と相転移

- 数値計算上の背景 : advanced Monte Carlo shell model (MCSM)

  - *T-plot*： 多体波動関数から古典論的な形の情報を引き出す

- 形の量子相転移から量子自己組織化

  - ジルコニウムのエキゾチック･アイソトープ

- 八重極振動、サマリウムの形の遷移

- さらなる展望

計算規模を拡大すれば、それまで手が届かなかったことができるようになる

原子核の場合には、例えば、より重い原子核の計算が可能になる

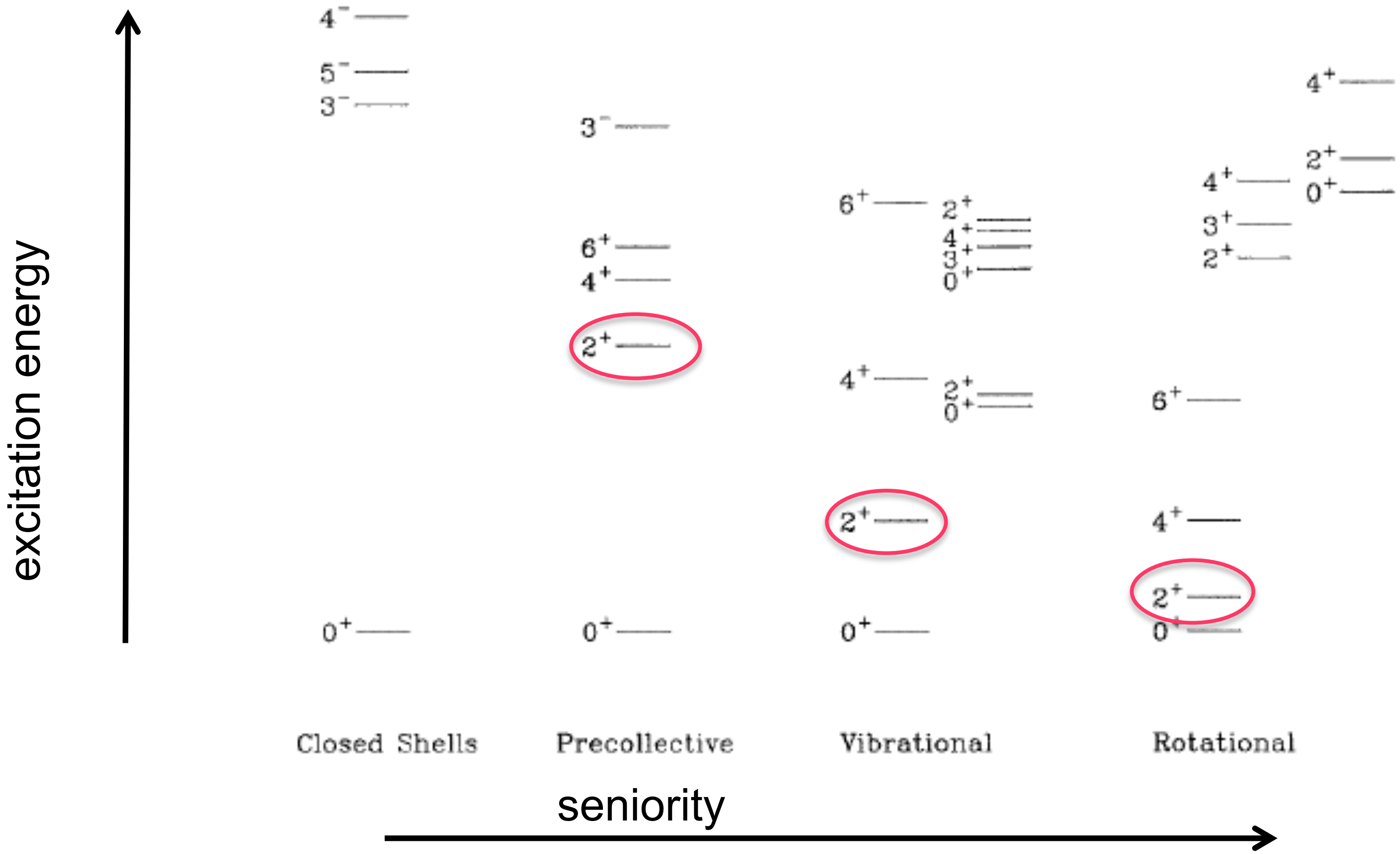
原子核のデータが増えるという意味は大きいがそれだけだろうか？

あらたな概念的な発見や展開があれば、さらに（ずっと）素晴らしい

「量子相転移」と「量子自己組織化」をキーワードに話したい

Schematic picture of shape evolution (sphere to ellipsoid & vice versa)

- gradual changes throughout the nuclear chart –



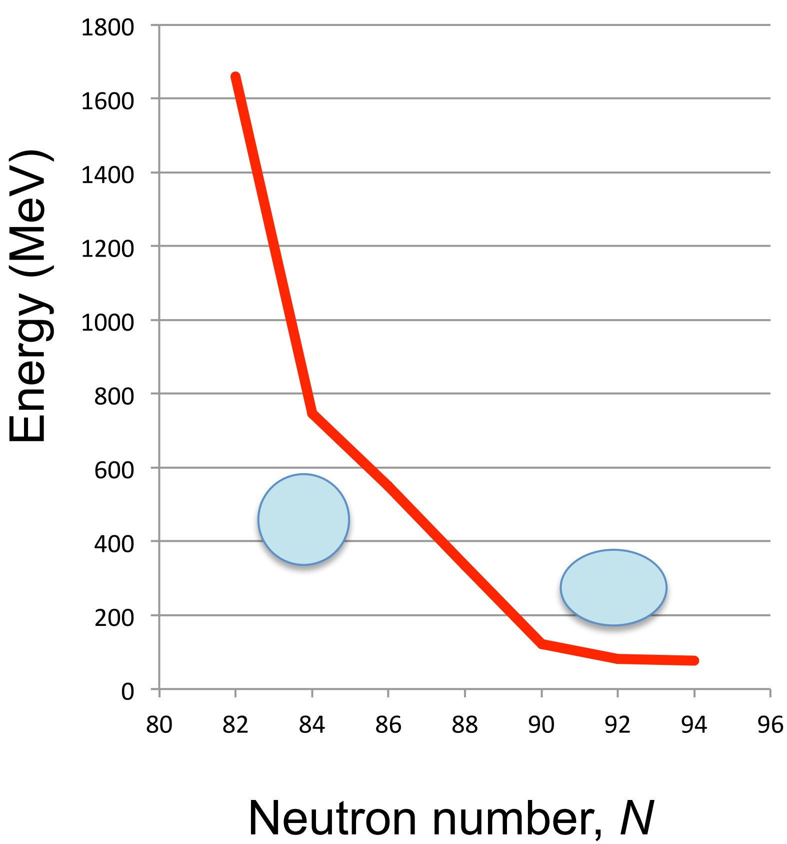
Distance from the nearest closed shell in *N* or *Z*

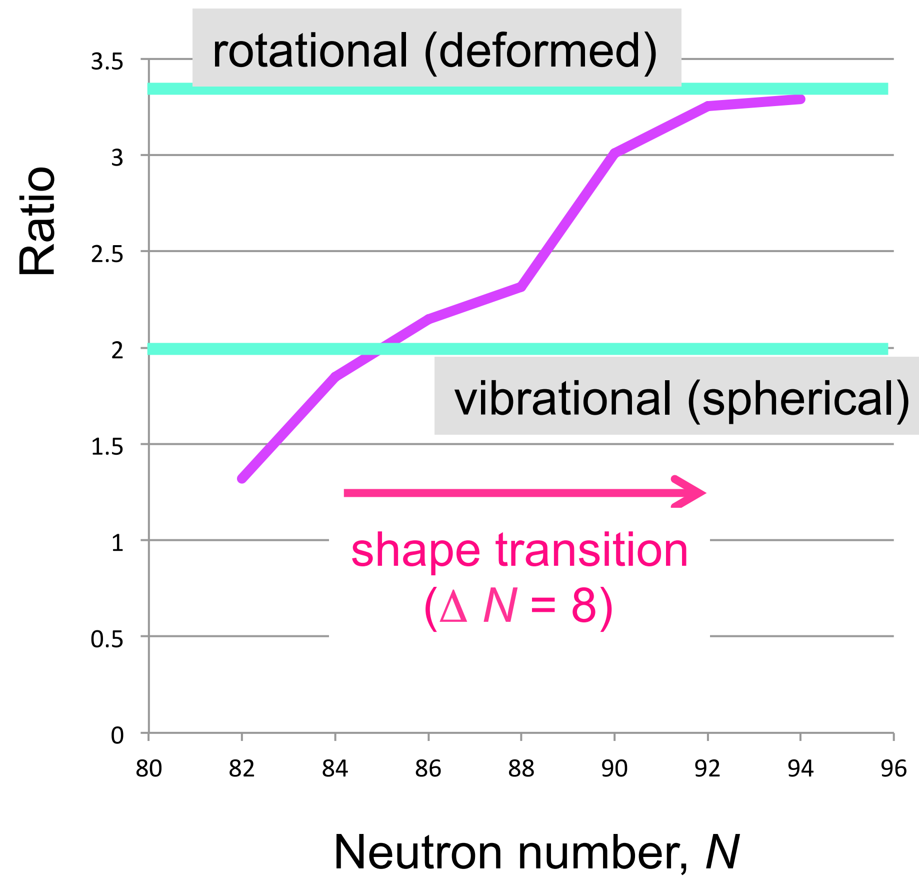
From "Nuclear Structure from a Simple Perspective", R.F. Casten (2001)

2^+ and 4^+ level properties of Sm isotopes サマリウム(Z＝62) アイソトープ

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

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



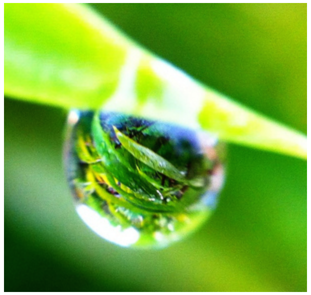


これは相転移とは言えないのではないか？

（言っている人は多いが　（岩波講座））

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,
where thermodynamics can be applied.



Quantum Phase Transition (QPT)

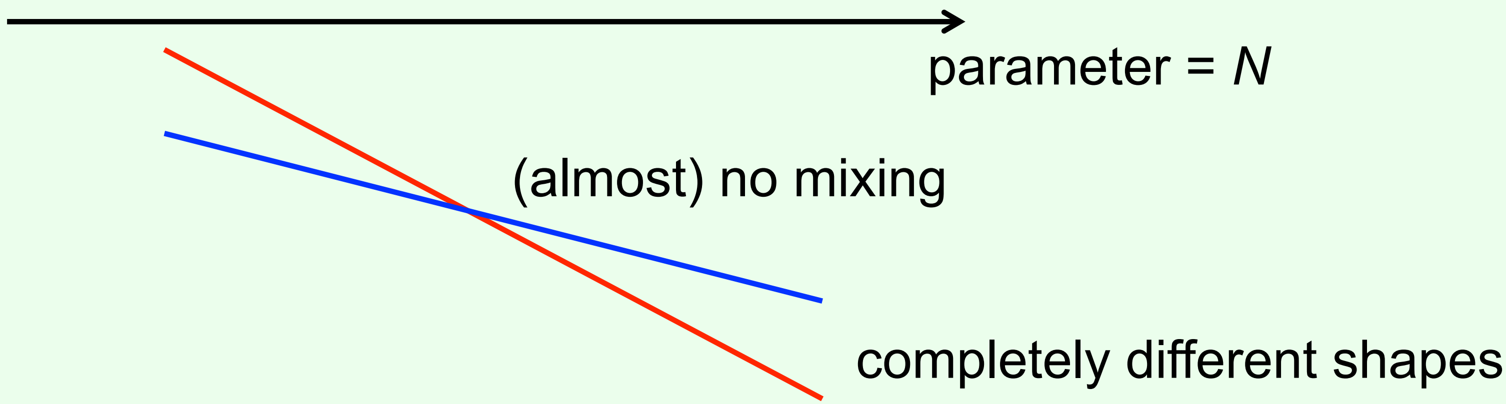
The concept of the phase transition cannot be applied to microscopic systems as it is. In the QPT, the ground state of a quantum (microscopic) system undergoes abrupt and qualitative change (of order parameter) as a (control) parameter changes (little).

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., Wikipedia*)

possible scenario



The usual shape transition may not fulfill the condition being *abrupt*.
Where can we see it ?
If it occurs in atomic nuclei, what is the underlying mechanism ?
Note that sizable mixing occurs usually in finite quantum systems.

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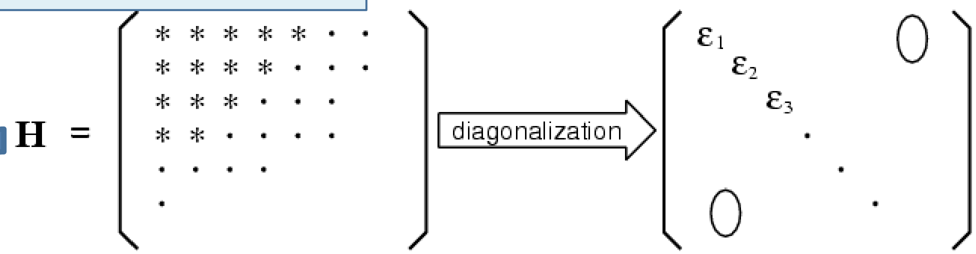
Advanced Monte Carlo shell model (MCSM)

Superposition of the projected Slater determinants
+ Extrapolation by energy variance

$$|\Psi\rangle = \sum_{k=1}^{N_{MCSM}} f_k P^{J,\pi} |\phi_k\rangle \qquad |\phi_k\rangle = \prod_{\alpha=1}^{N} \left(\sum_{i=1}^{N_{sp}} c_i^\dagger D_{i\alpha}^{(k)} \right) |-\rangle$$

MCSM basis, deformed Slater det.

$>10^{10}$ basis vectors



Conventional Shell Model
all Slater determinants

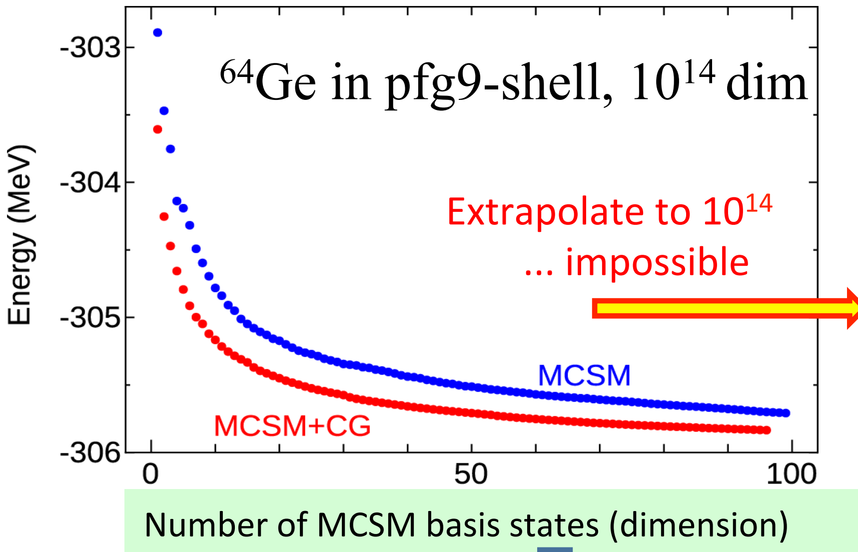
Monte Carlo Shell Model
bases important for a specific eigenstate

$\sim 10^2$ basis vectors

Step 1
- Select D stochastically from many candidates generated by the auxiliary-field Monte Carlo technique

Step 2
- optimize D variationally by the conjugate gradient method so as to minimize the energy eigenvalue of this small matrix

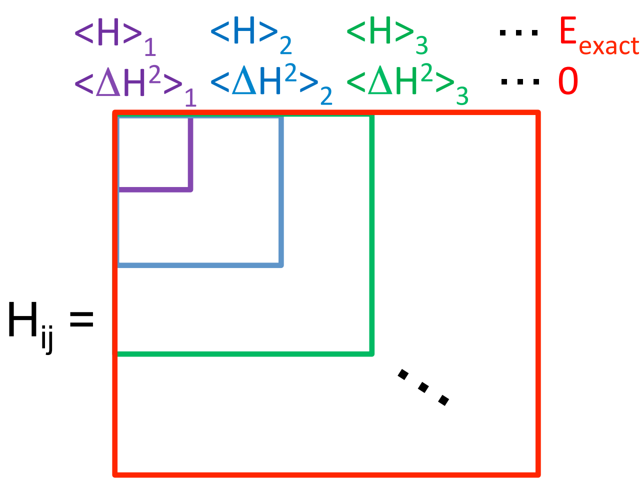
Step 3 : Energy variance extrapolation

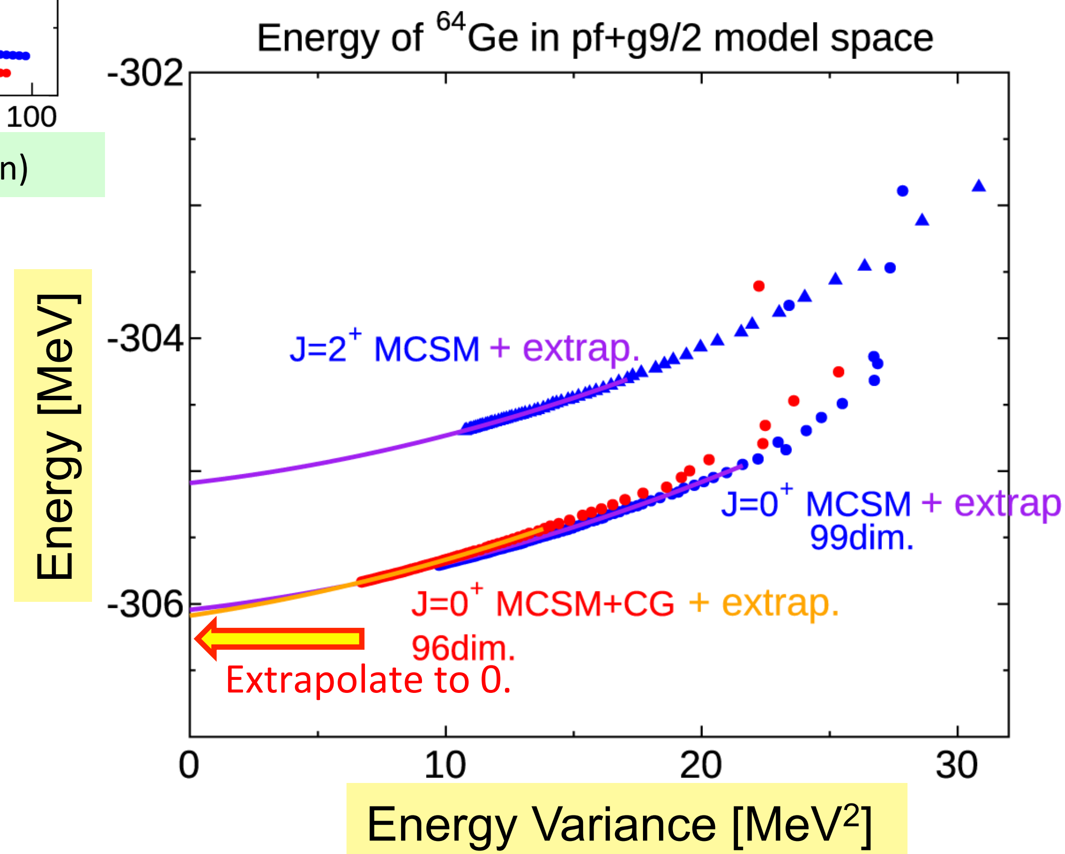


Energy variance : $\langle \Delta H^2 \rangle = \langle H^2 \rangle - \langle H \rangle^2$

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

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





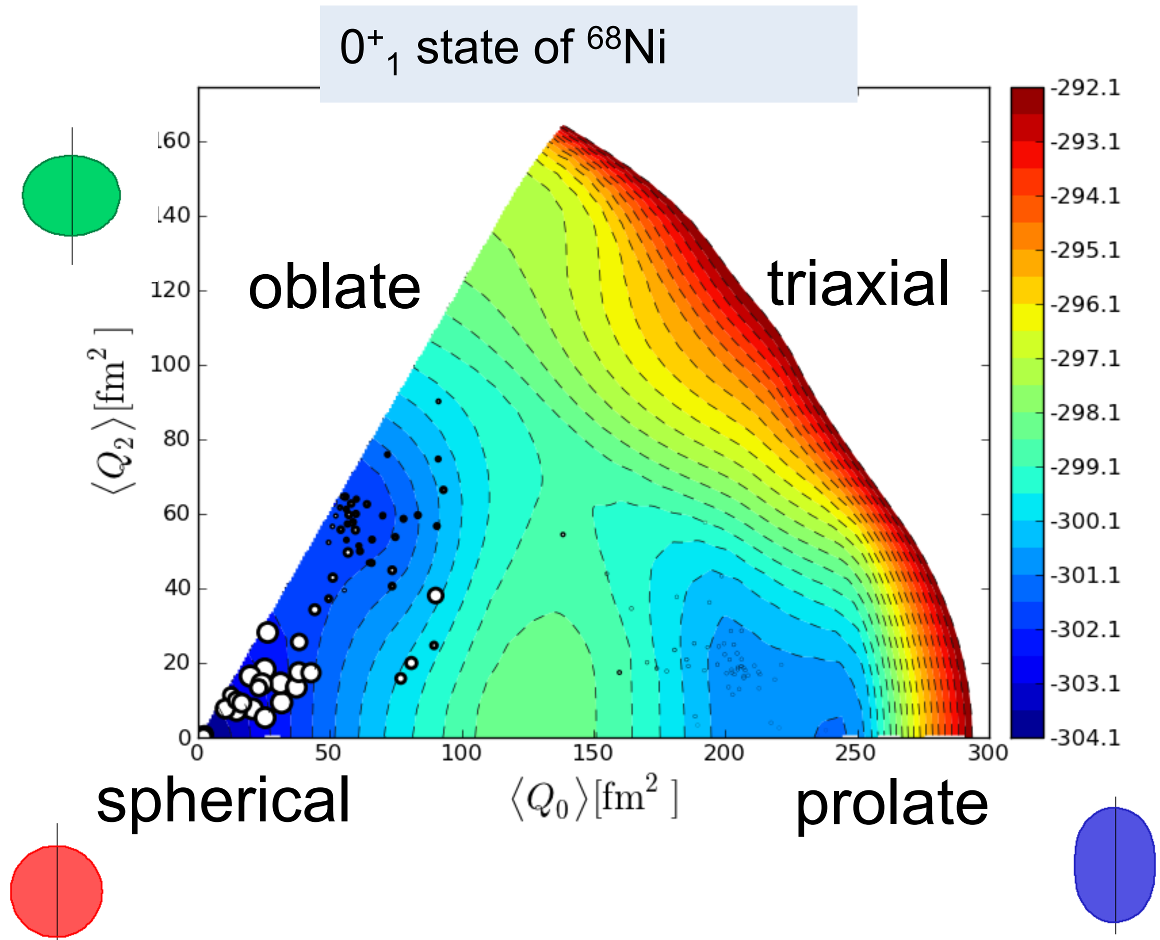
MCSM basis vectors on Potential Energy Surface (*T-plot*)

第11回（2017年）日本物理学会若手奨励賞 角田佑介

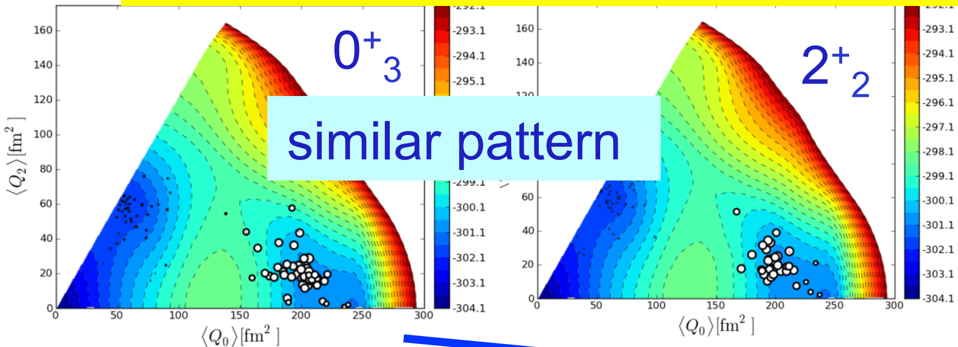
eigenstate $\Psi = \sum_i c_i P[J^\pi] \Phi_i$

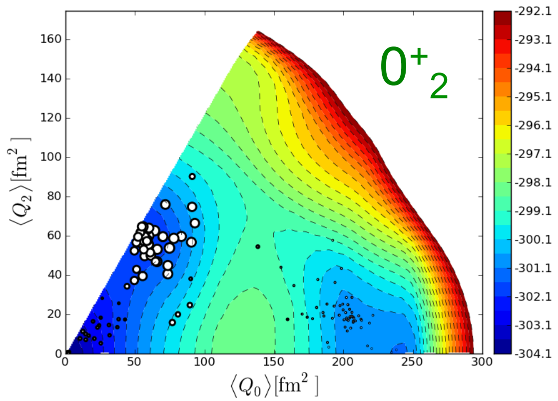
Slater determinant
→ intrinsic deformation

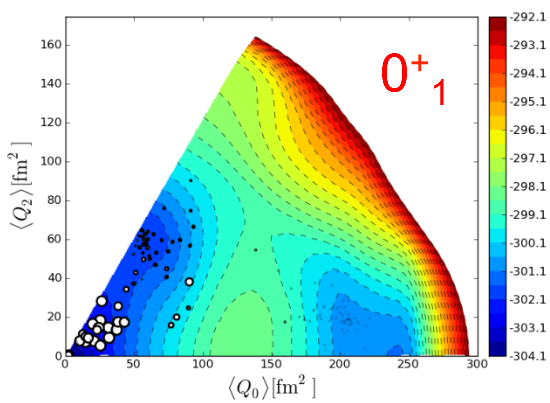
- PES is calculated by CHF
- Location of circle : quadrupole deformation of unprojected MCSM basis vectors
- Area of circle : overlap probability between each projected basis and eigen wave function

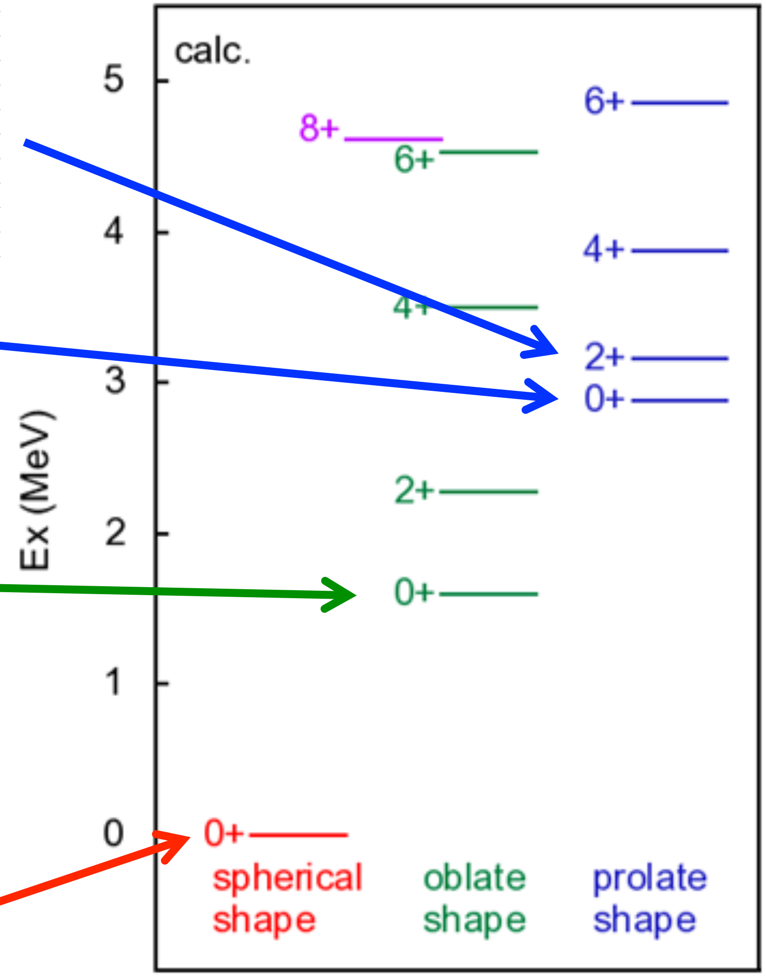


T-plot analysis of band structure of ^{68}Ni

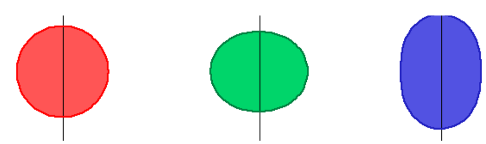








Shape coexistence



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

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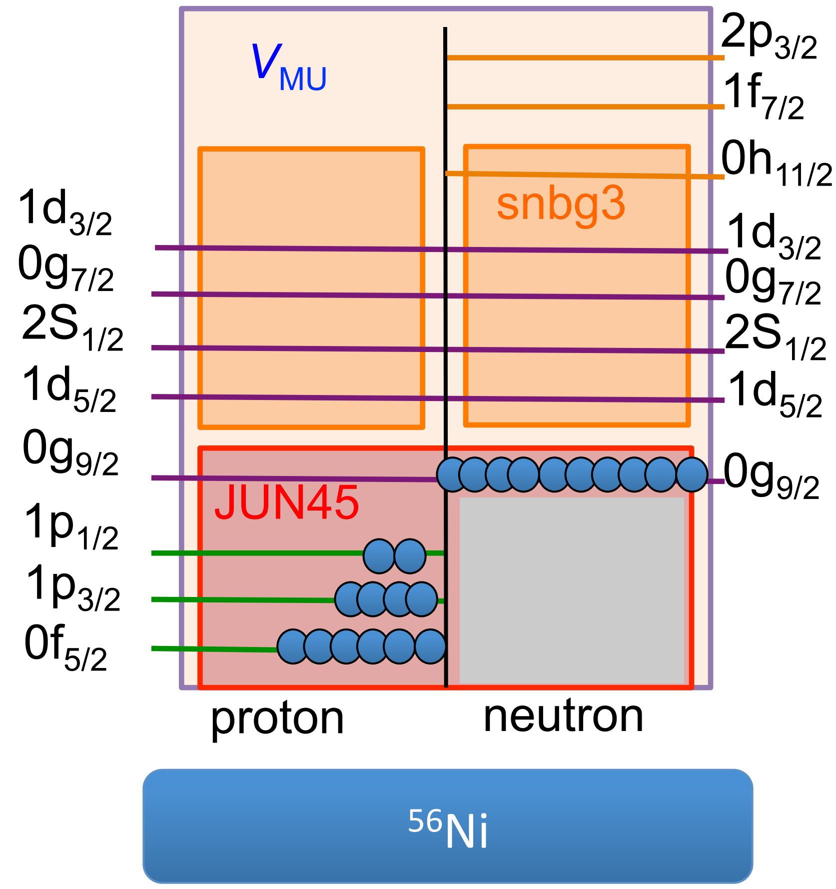
Present work : model space and effective interaction

- 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

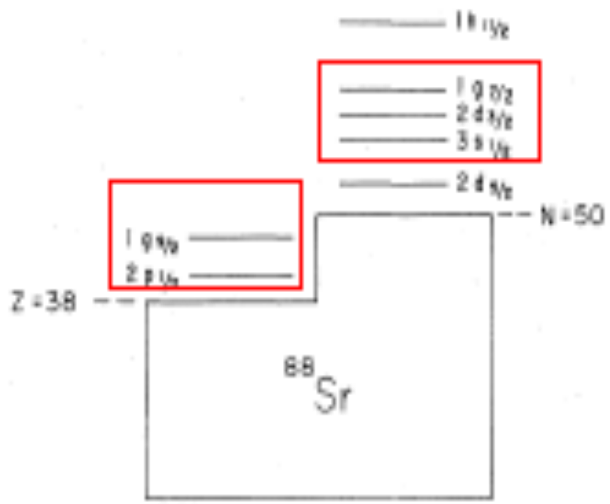


FIG. 3. Single-particle levels appropriate to a description of nuclei in the Zr-Mo region. An ^{88}Sr core is assumed.

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

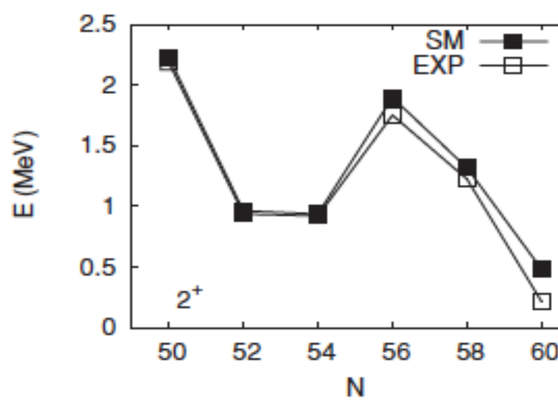
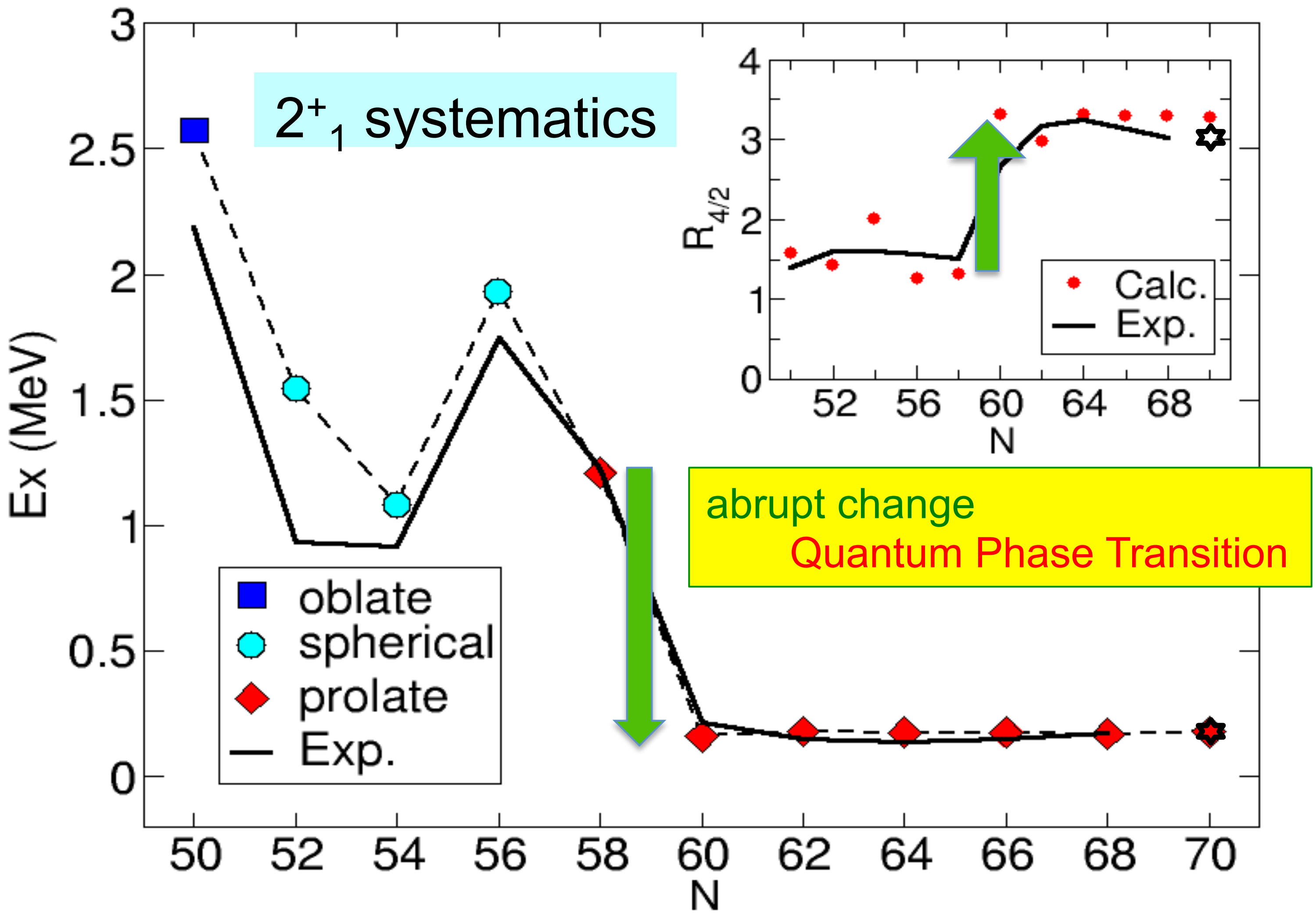


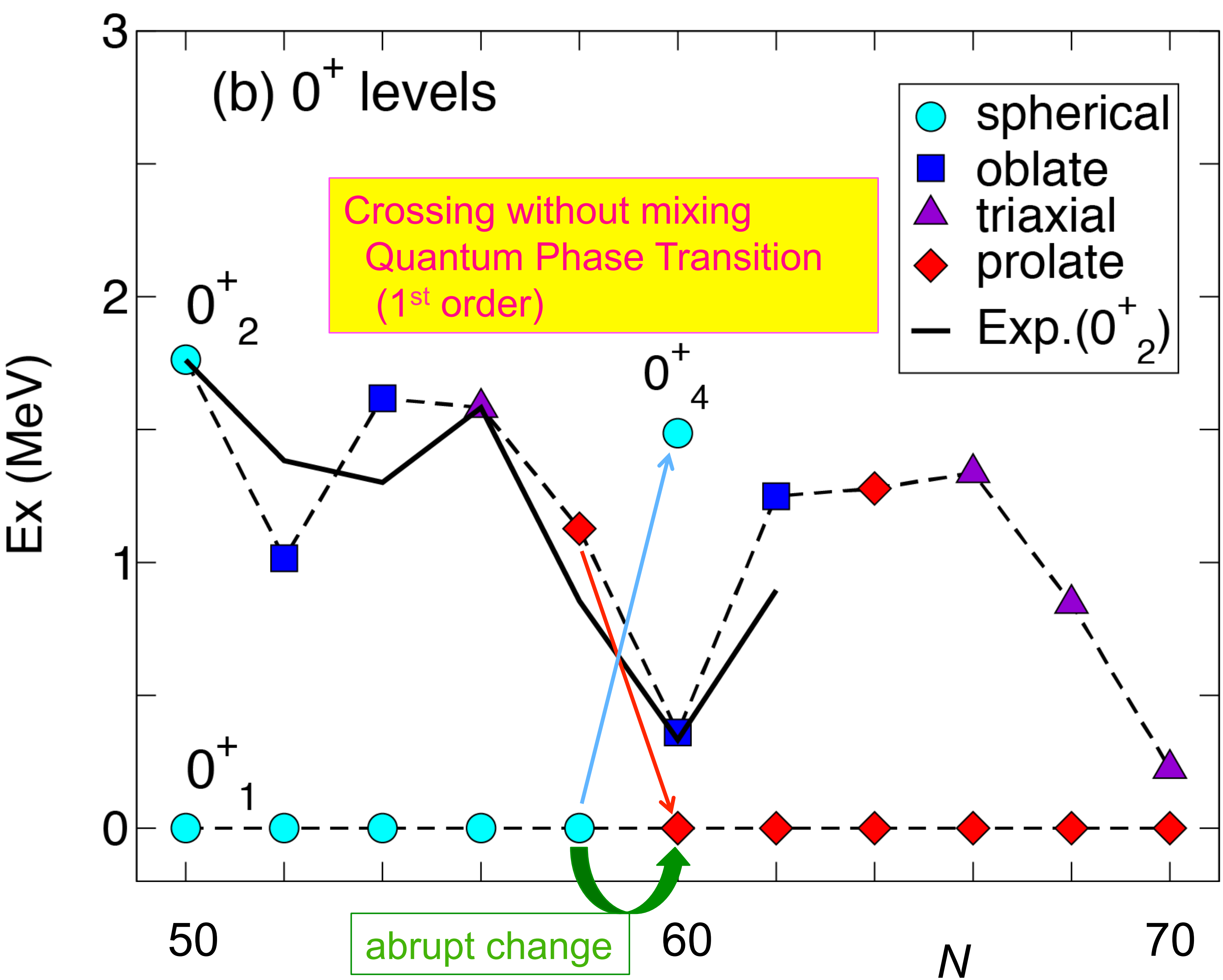
FIG. 12. Systematics of the experimental and theoretical first excited 2^+ states along the zirconium chain.

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

Quantum Phase Transition in the Shape of Zr isotopes

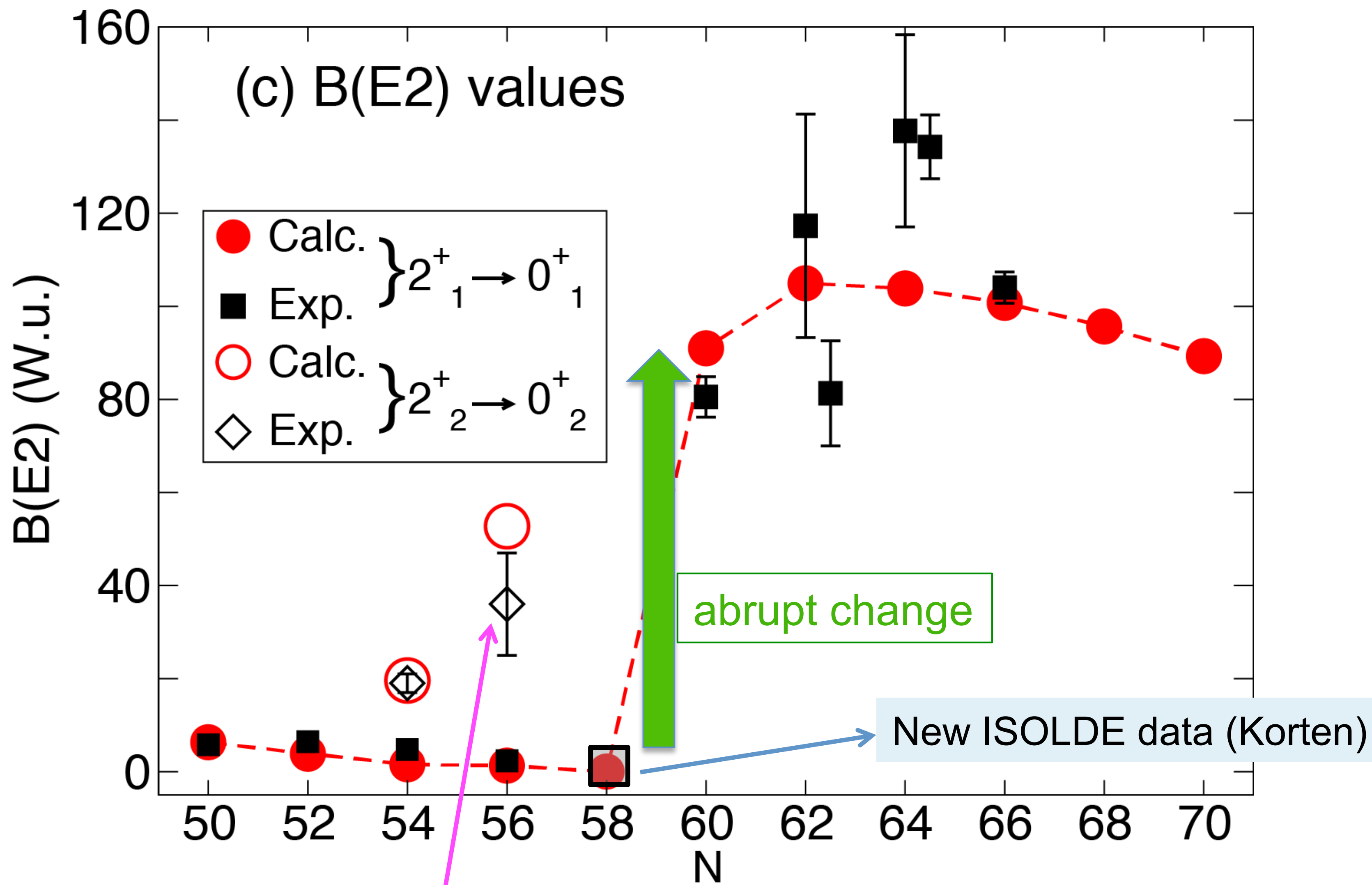
Tomoaki Togashi,[1] Yusuke Tsunoda,[1] Takaharu Otsuka,[1,2,3,4] and Noritaka Shimizu[1]



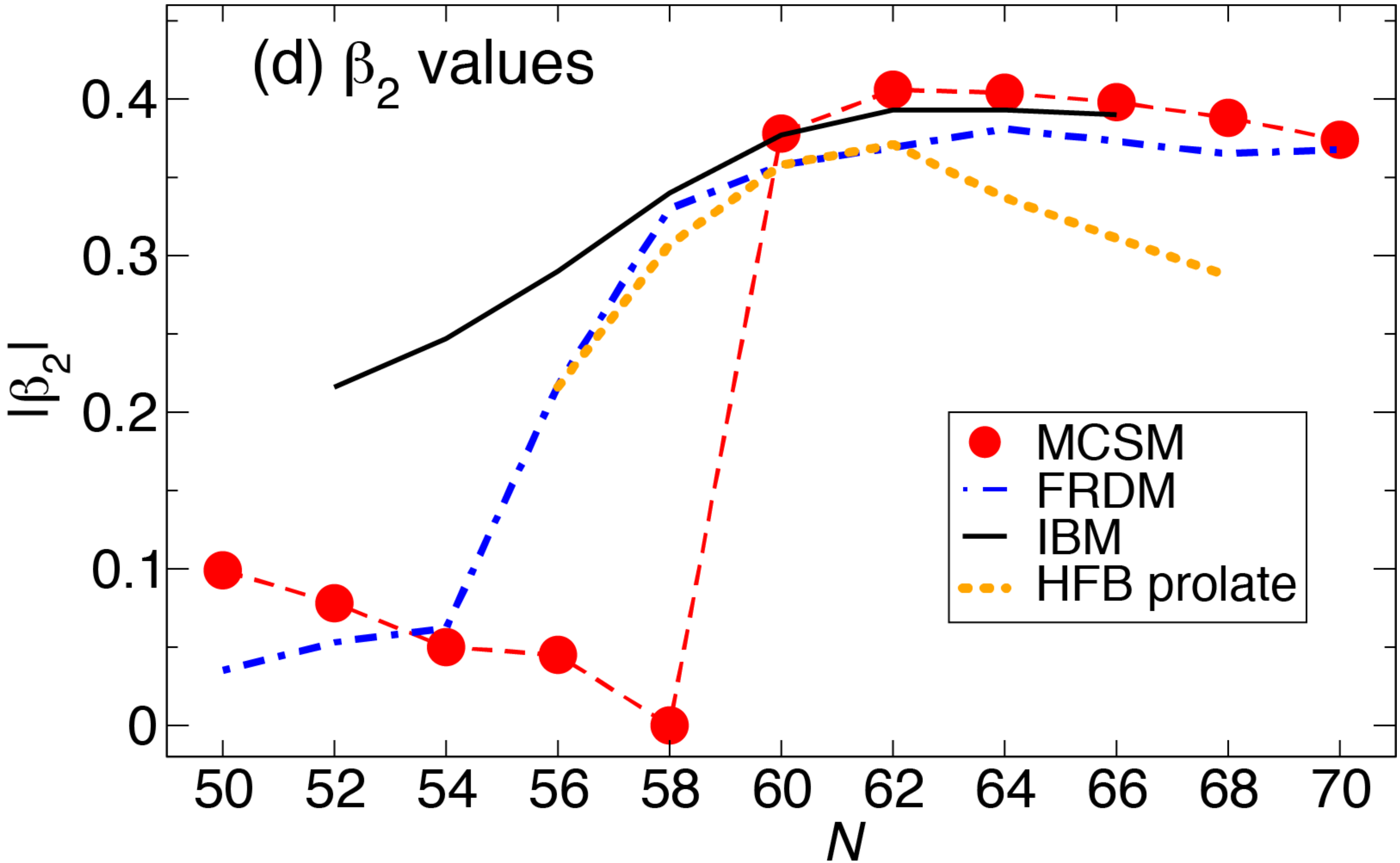


(b) 0^+ levels
Crossing without mixing
Quantum Phase Transition
(1st order)
spherical
oblate
triaxial
prolate
Exp.(0^+_2)
0^+_2
0^+_4
0^+_1
Ex (MeV)
3
2
1
0
50
60
70
N
abrupt change

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



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

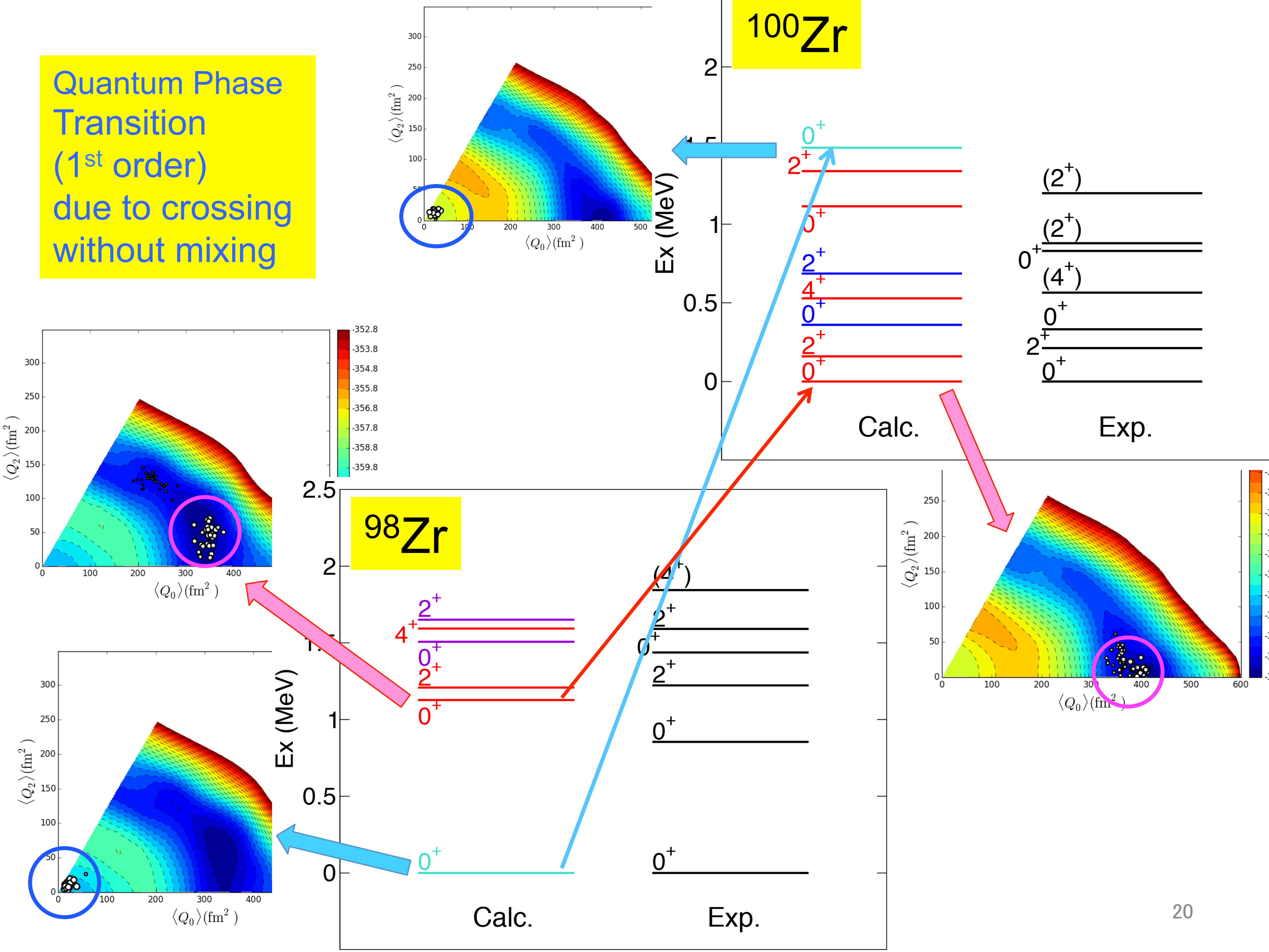


FRDM: S. Moeller et al. At. Data Nucl. Data Tables 59, 185 (1995).

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

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

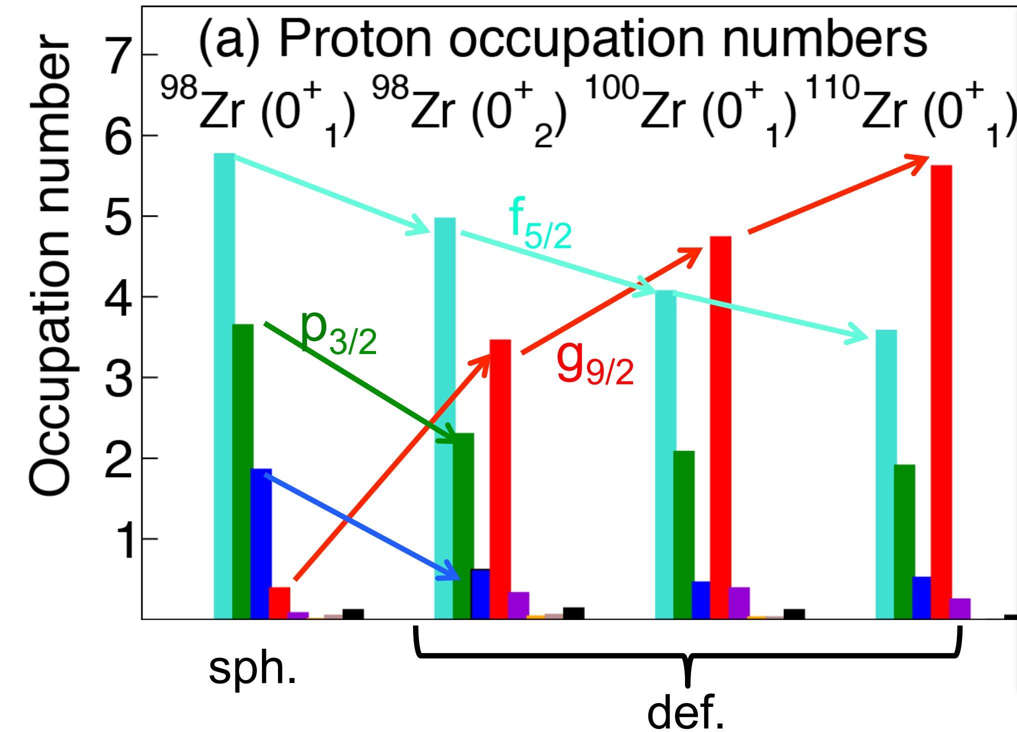
Quantum Phase Transition (1st order) due to crossing without mixing

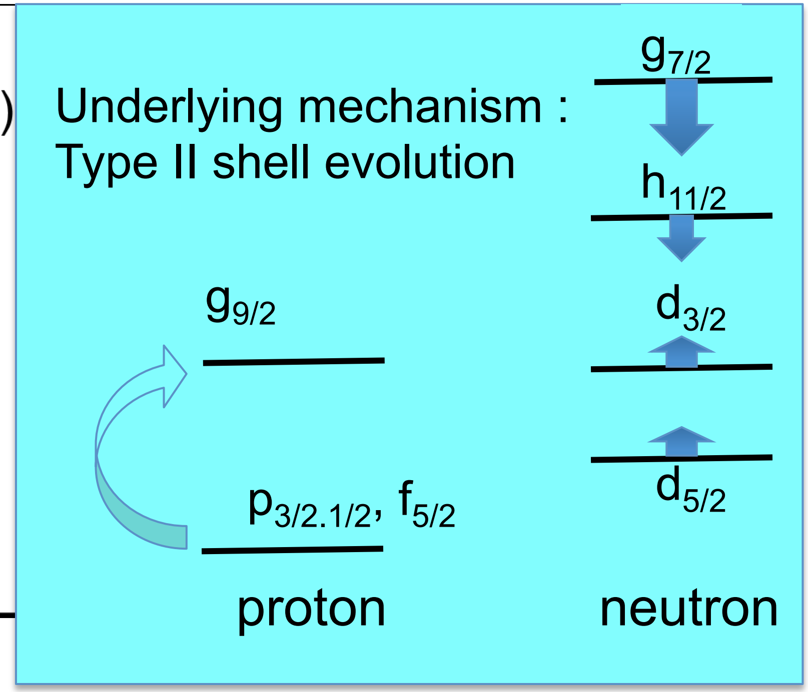


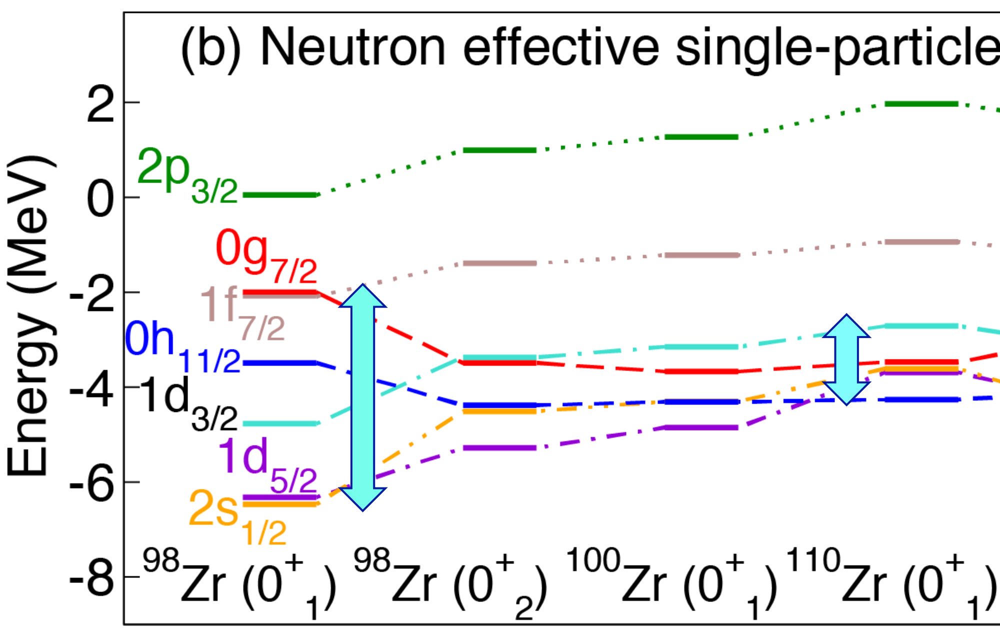
京コンピュータでの大計算で初めてジルコニウム　アイソトープでの
量子相転移が、急激な変化という定義に沿って、
実験（励起エネルギーや励起強度）で検証できる形で示された。

量子相転移が起こるには、構造の急激な変化に加えて
状態間の mixing が起こらないことも重要
（混ざってしまうと急激な変化にならない）
孤立した有限量子系では mixing は通常避けられない

状態の大きな変化と mixing の抑制を両方説明するメカニズム？







Neutron effective single-particle energies are self-reorganized by nuclear forces (tensor and central) and certain configurations, so as to reduce resistance power against deformation.

- a case of type II shell evolution -

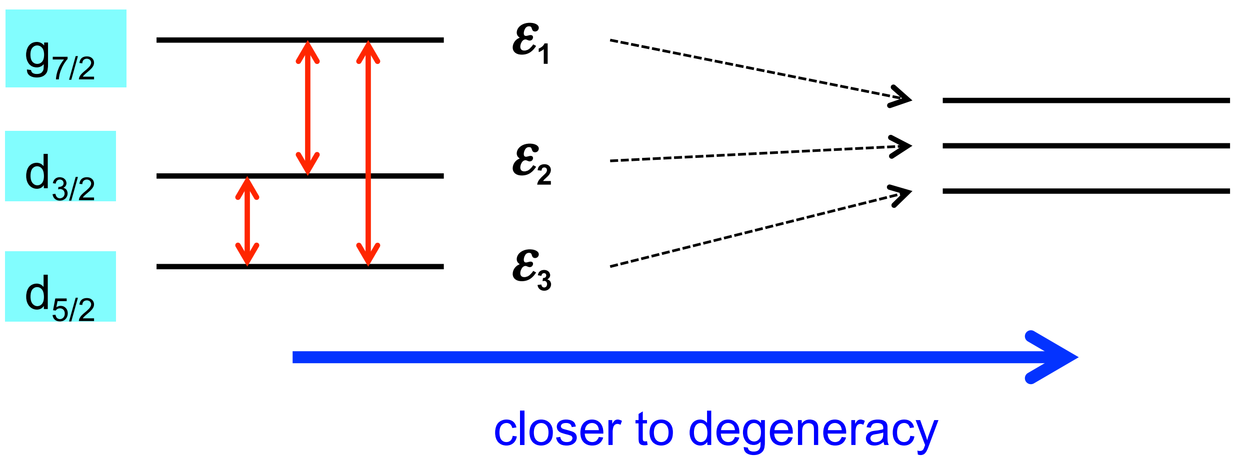
Jahn –Teller effect for nuclear deformation

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

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

stronger mixing = larger quadrupole deformation

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



larger deformation for the same deformed field

モノポール力 (Monopole interaction)

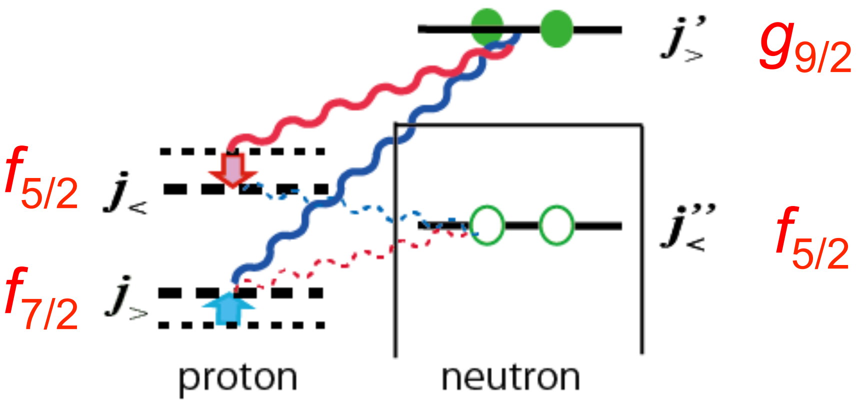
有効核力は、それがどのように導かれたにせよ、スピンテンソル分解という方法で成分に分けられる。モノポール力はその一つ。

模式的には $V = \Sigma_K \; f_K \; (U^{(K)} U^{(K)})$ の内の K=0

$U^{(K)}$: 1体のユニット演算子

軌道 j にいる陽子と軌道 j' にいる中性子の間に働くと v(j, j') $n^p_j \; n^n_{j'}$ のようになる

例:テンソル力からのモノポール力の効果



1. 粒子数に比例
（多体系で効果大）

2. 一粒子軌道エネルギーを
有効的に変化させる

3. 空孔で符号が逆
（選べば二重の効果）

4. 核力を精確に取り込む必要

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 量子自己組織化

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

Woods-Saxon potential

Parameters are constant within a given nucleus

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),

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

quadrupole deformed field

spherical field

constant within a region

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

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

A= 68 1.28

A=100 1.12 } $(\mathbf{l}\cdot\mathbf{s})$

A=186 0.91

Intuitively speaking,

特定のモードを指向
（今の場合は楕円体への変形）

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

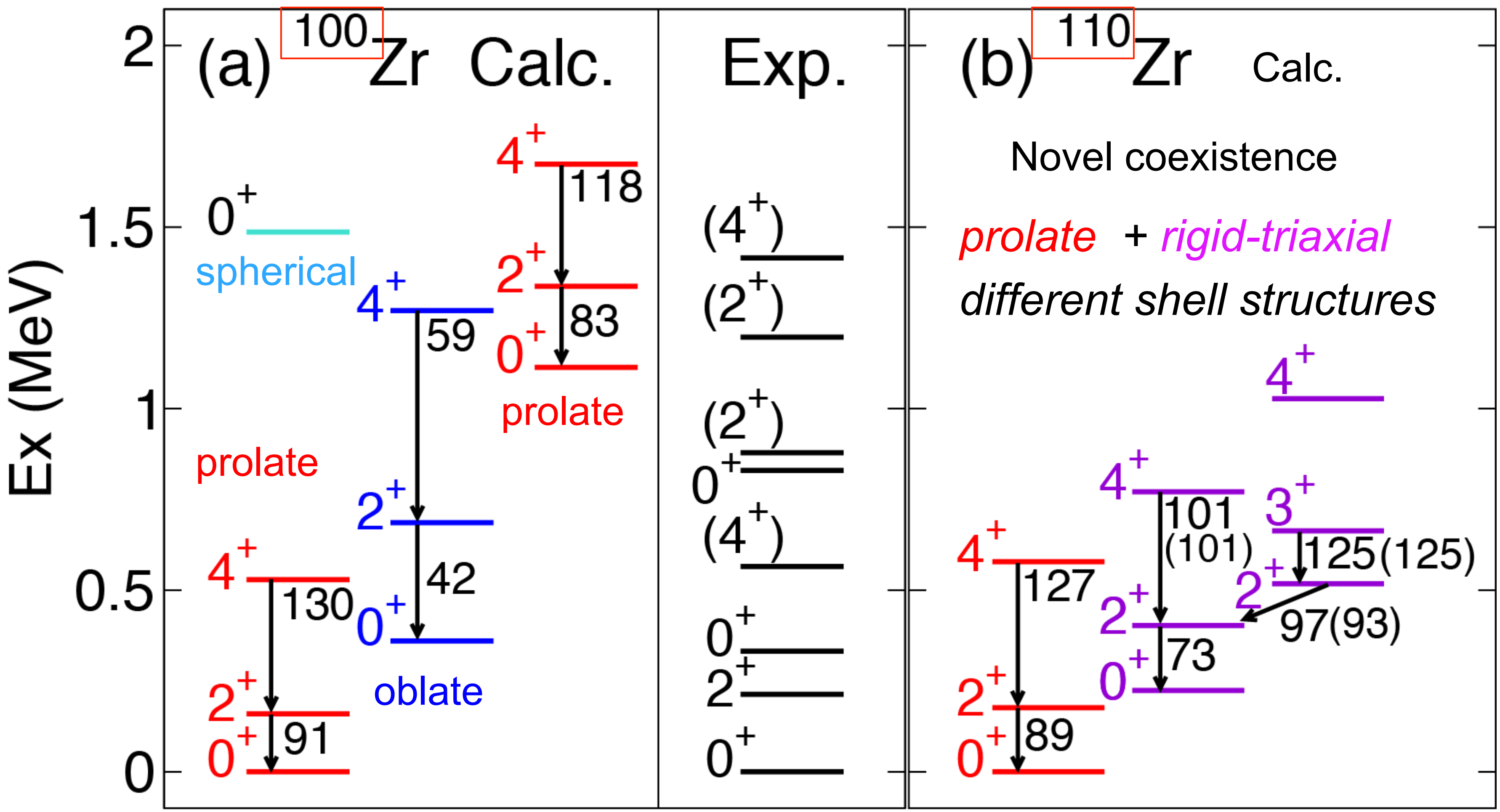
特定のモードには対応しない
（変化のしやすさのみ）

量子系の場合にはモードが稼ぐ
結合エネルギーによって
抵抗力の変化の程度が変わる

Analogy to electric current,

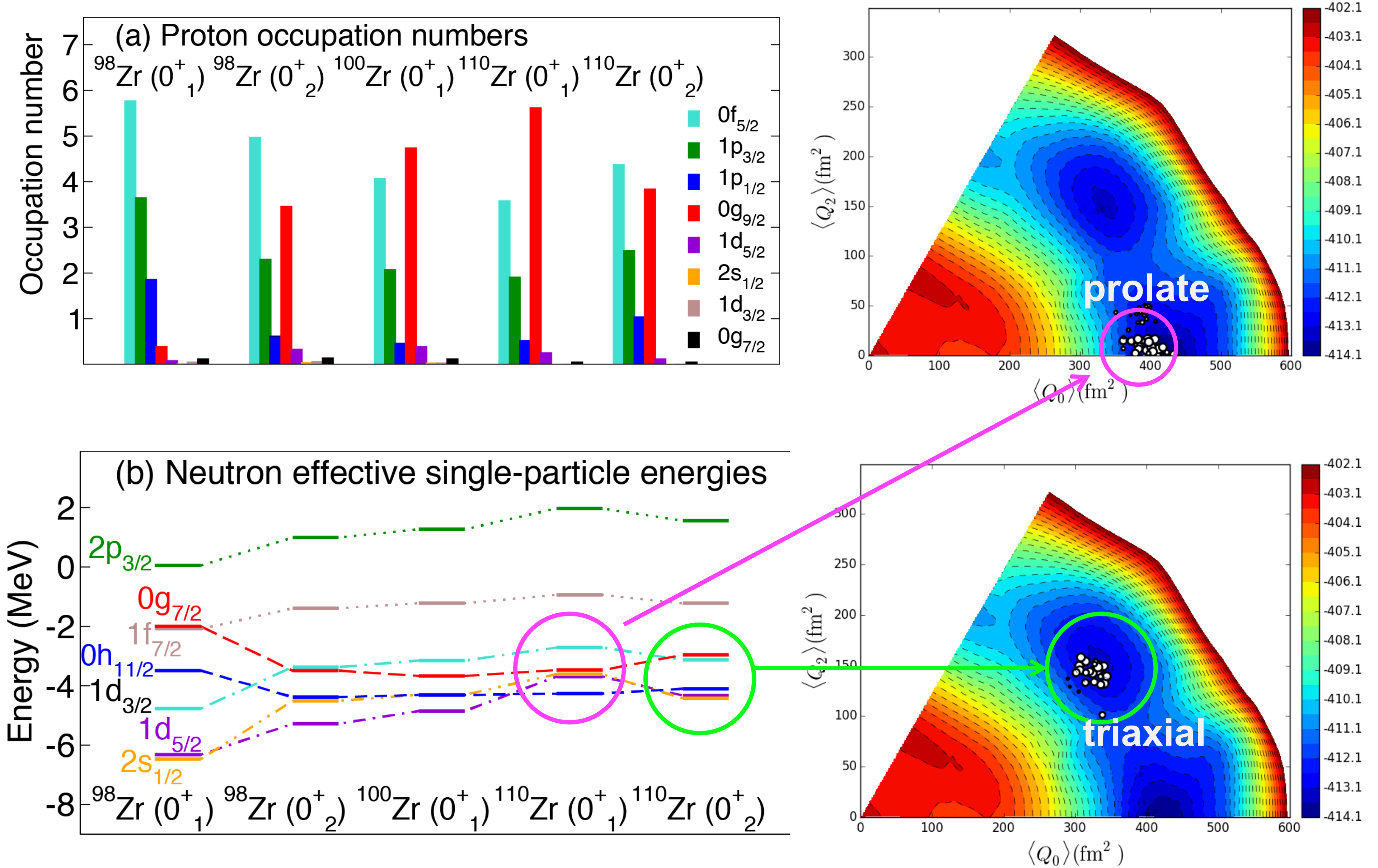
$$\text{current} = \frac{\text{voltage}}{\text{resistance}}$$

Prolate – rigid-triaxial shape coexistence



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

different shell structures ~ like “different nuclei”



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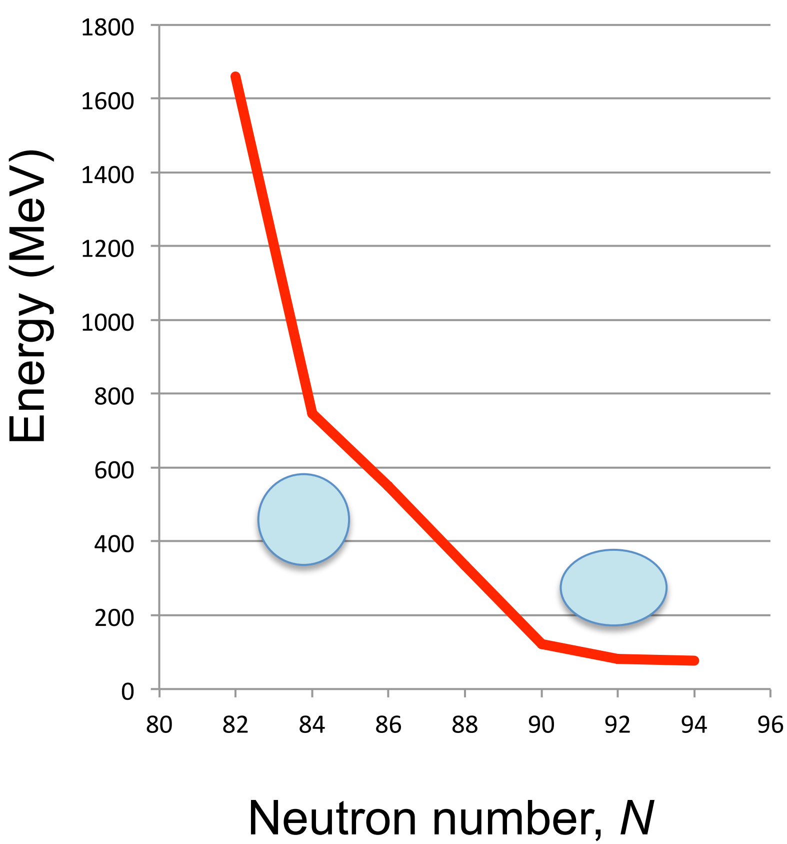
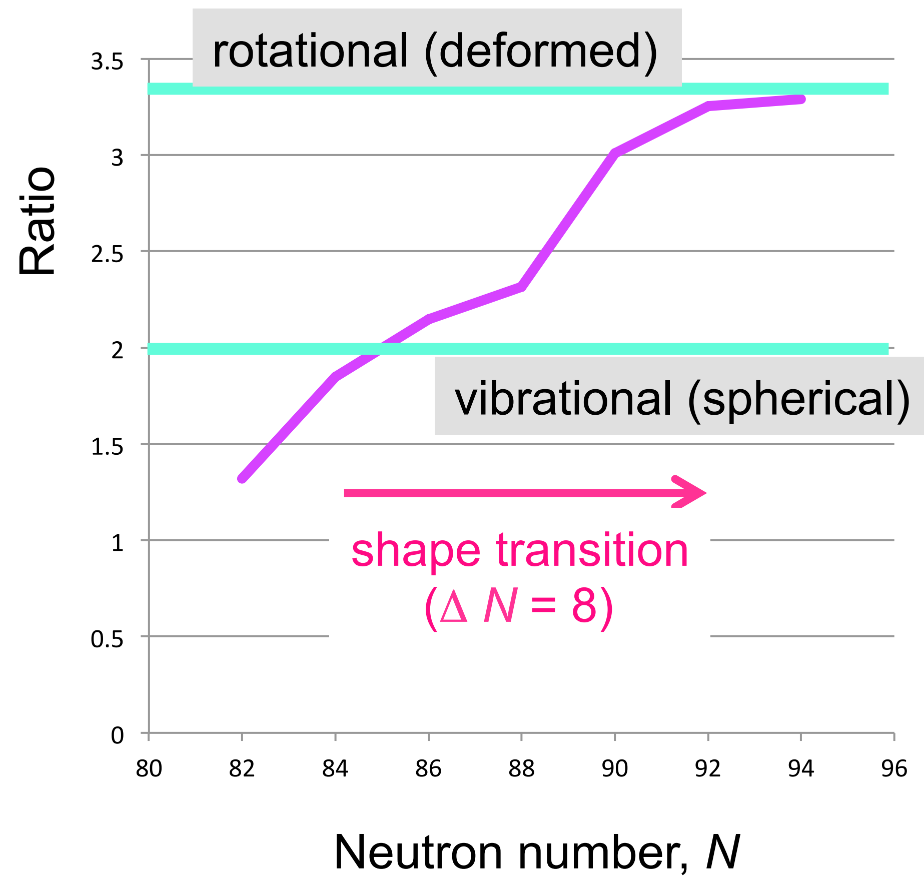
2^+ and 4^+ level properties of Sm isotopes サマリウム アイソトープ

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

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



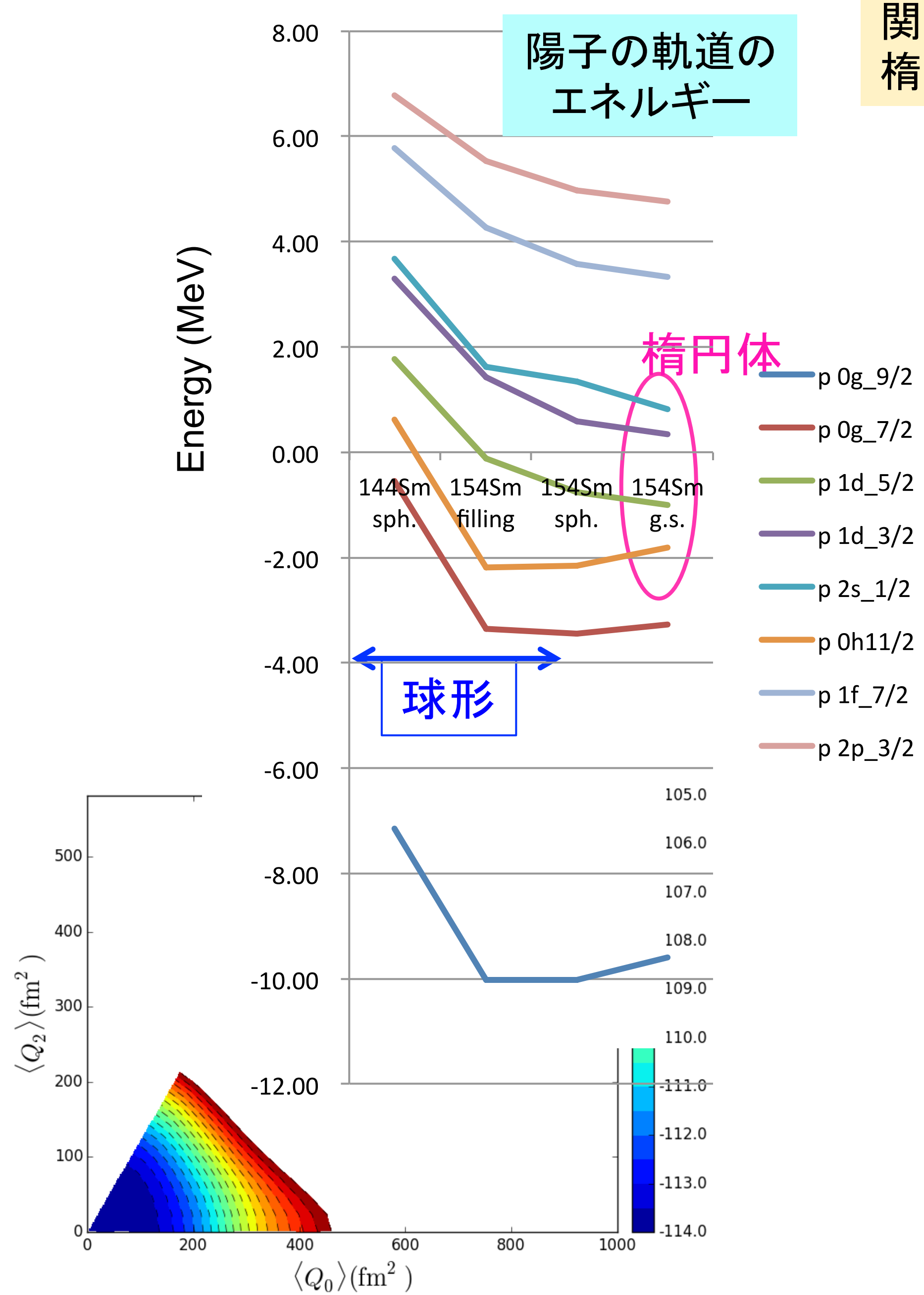


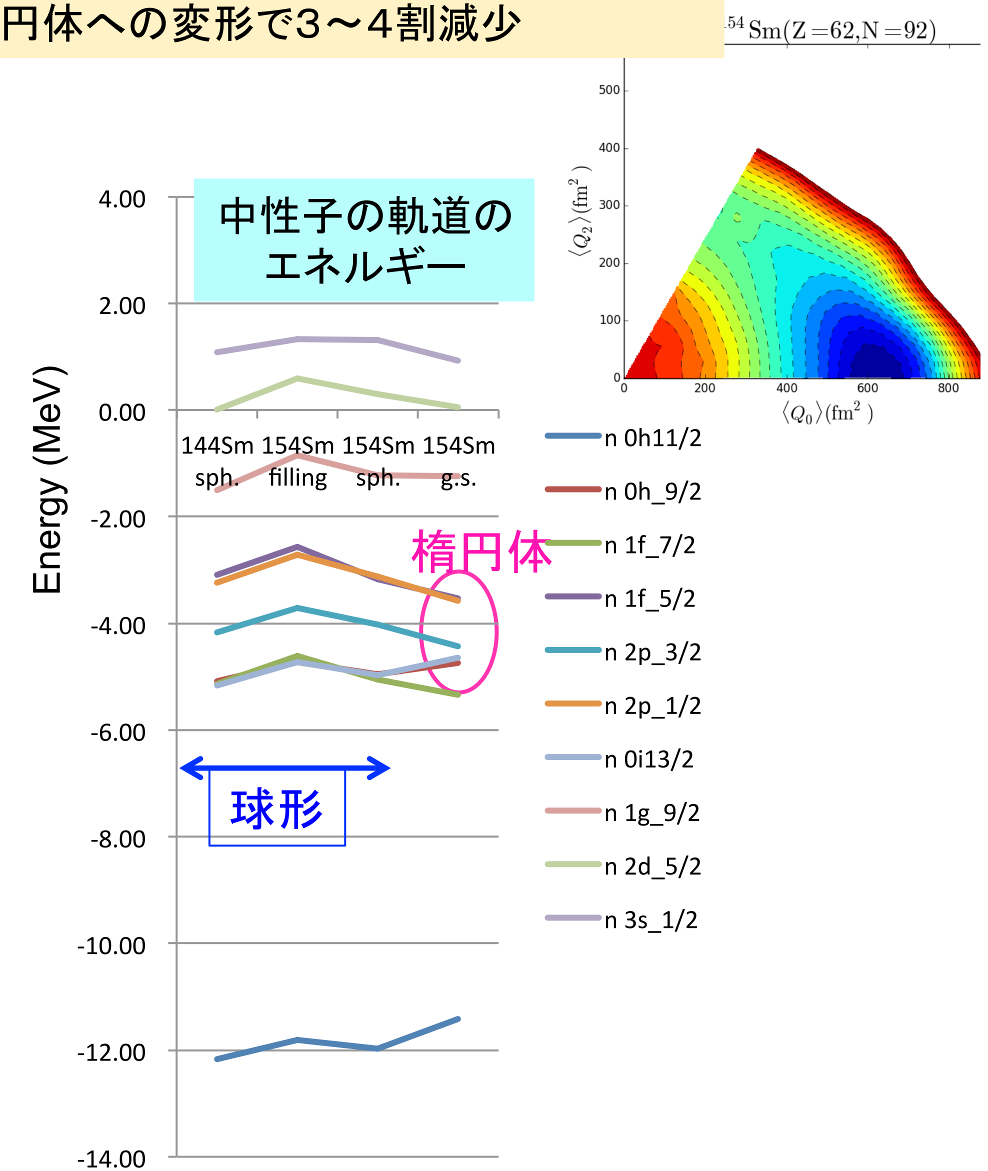
これは相転移とは言えないのではないか？

（言っている人は多いが　（岩波講座））

冒頭で議論したサマリウムのアイソトープでの形の遷移　preliminary result

関与する一粒子軌道の散らばりが球形→
楕円体への変形で3～4割減少





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

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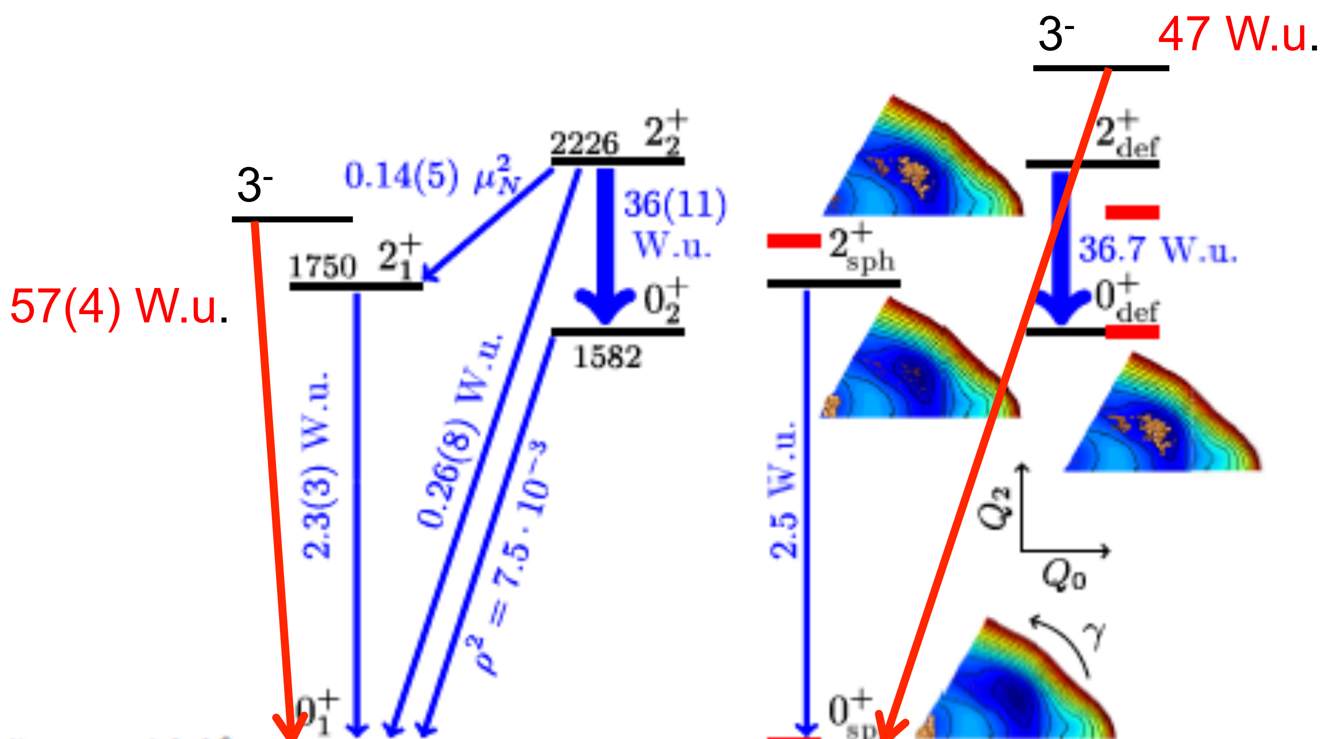

$B(E3; 3_1^- \to 0_1^+)$ [W.u.]	57(4)	46.6[a]		
$B(E1; 2_2^+ \to 3_1^-)$ [W.u.]	$28(9) \times 10^{-3}$*	0.00	···	···

[a]Effective $E3$ charges $e_p^{E3} = 1.24e$ and $e_n^{E3} = 0.82e$ are taken by applying $Z = 40$ and $N = 56$ to the estimate shown in Ref. [15].

Summary and Perspectives

- 量子相転移 （quantum phase transition (QPM)）が ^{98}Zr と ^{100}Zr の間で起きていることが、京コンピュータによる大規模計算で世界で初めて示された。核力が引き起こす様々な相関を取り込む計算が必要。1次相転移に相当。

  (abrupt qualitative change in the ground state as a function of N)

- それを起こすメカニズムとして量子自己組織化（quantum self organization）を考えることが出来る

  → 変形共存、八重極振動と変形、超変形、核分裂, などに関わる （今後の研究課題）

- 多体相関のモード（変形など）を起こす成分と、それへの抵抗力のバランスで多体状態の構造が決まる。抵抗力の状態依存性は注目されていなかった。

  力の二重性： 四重極成分 ←→ 単極（モノポール）成分

  成分の二重性： 陽子と中性子という2成分フェルミ流体

  抵抗力を少なくして、モードをより完璧に働かせる

  配位が変わるので、軌道の配位構造が異なる

  → mixing の抑制、時間発展の不可逆性 （量子多体系に於ける古典的側面）