Peking University

Probing the structure of isomers using a configuration-constrained PES model

Furong Xu

School of Physics, Peking University, China

I. Introduction

II. The configuration-constrained PES Model

III. Calculations for high-K states in

1) nuclei along proton drip line

2) neutron-rich nuclei

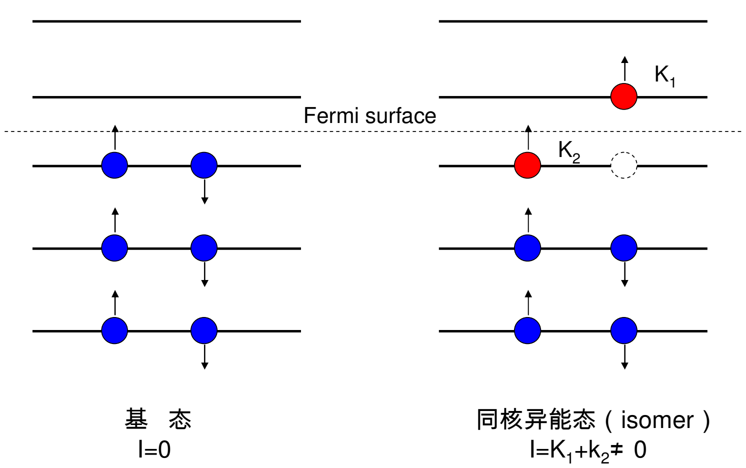
3) Superheavy nuclei

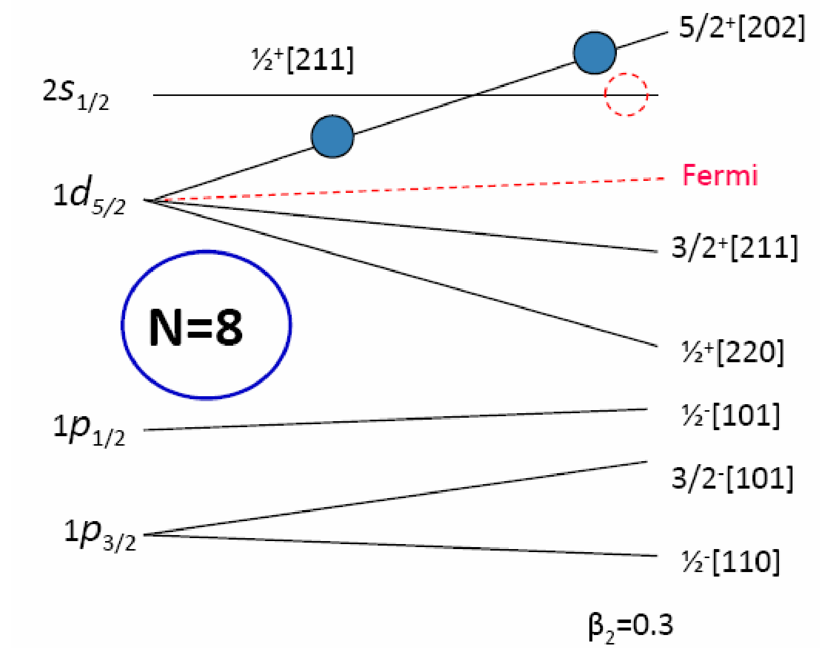
4) in superdeformation

4) K-mixing and triaxiality

IV. Summary

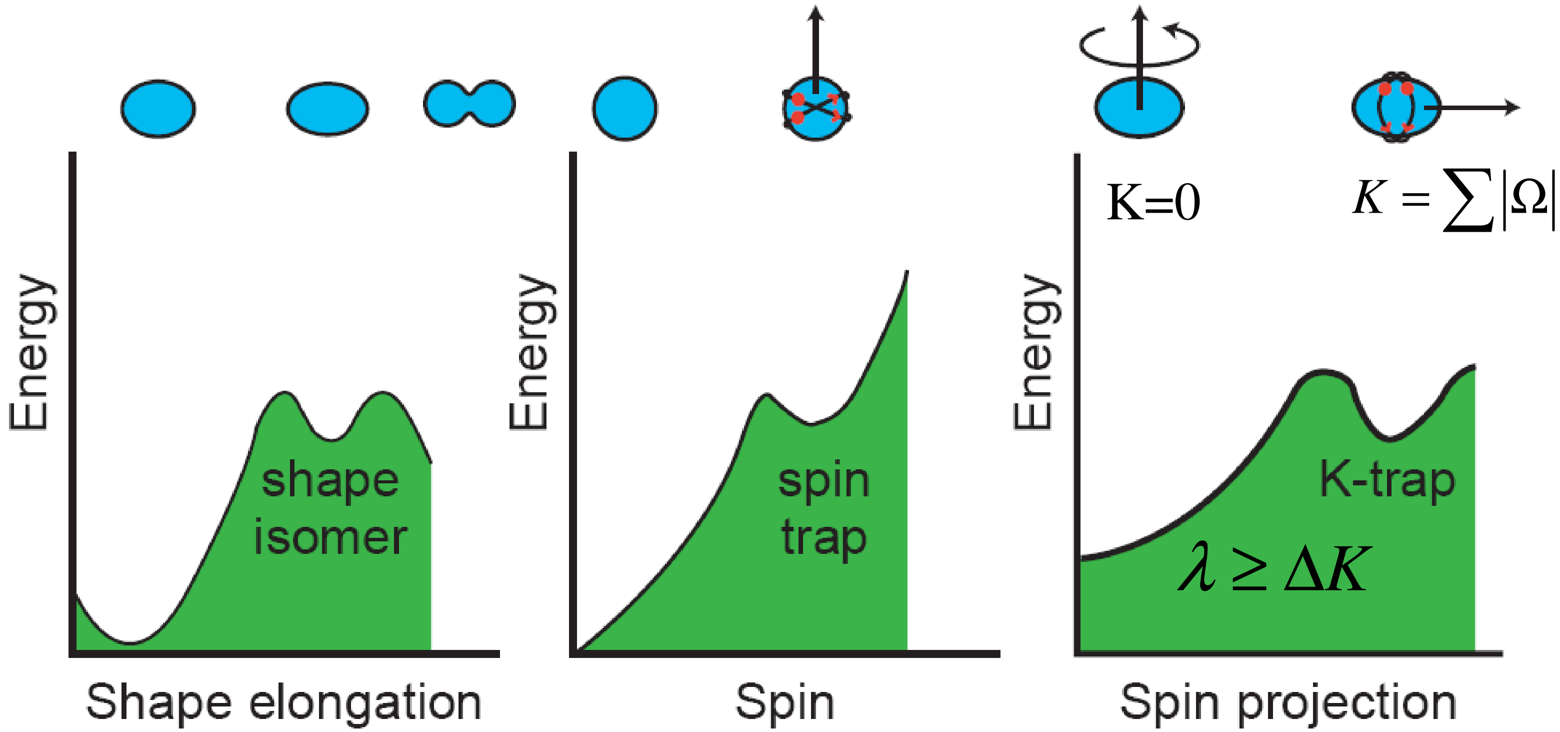
I. Introduction





Three important elements which affect the calculations of high-K states:

1. **Spacing of single-particle levels;**
2. **Effect from shape polarization;**
3. **Right pairing strength**



From: P. Walker, G. Dracoulis, Nature 399 (1999) 35

II. The configuration-constrained PES Model

Deformed Woods-Saxon Potential

$$V_{WS}(\boldsymbol{r}, \beta) = \frac{V_0}{1 + \exp\left[\text{dist}\ \Sigma_{WS}(\boldsymbol{r}, \beta)/a\right]}$$

$$V_{WS}(r; r_0) = \frac{V_0}{1 + \exp\left[(r - R_0)/a\right]}.$$

$$V_0 = V\left(1 \mp \kappa \frac{N - Z}{N + Z}\right)$$

$$R(\hat{\Omega}, \hat{\alpha}) = c(\hat{\alpha}) R_0 \left[1 + \sum_{\lambda \geqslant 2} \sum_{\mu} \alpha^*_{\lambda\mu} Y_{\lambda\mu}(\hat{\Omega})\right]$$

$$R_0 = r_0 A^{1/3}$$

$$\alpha_{20} = \beta_2 \cos\gamma$$

$$\alpha_{22} = \frac{1}{\sqrt{2}} \beta_2 \sin\gamma$$

$$\hat{V}_{\text{so}}(\boldsymbol{r},\boldsymbol{p};V_0^{\text{so}},\kappa,a_{\text{so}},r_{\text{so}})$$

$$=\lambda[\hbar/(2mc)]^2\left[\nabla\frac{V_0\left[1\pm\kappa\dfrac{N-Z}{N+Z}\right]}{\{1+\exp[\text{dist}_{\Sigma_{\text{so}}}(\boldsymbol{r};r_{\text{so}})/a_{\text{so}}]\}}\right]\times\boldsymbol{p}\cdot\boldsymbol{s}$$

$$H_{\text{ws}}=T+V+V_{\text{so}}+\tfrac{1}{2}(1+\tau_3)V_{\text{c}}$$

Parametrisation	λ (P)	λ (N)	$r_{0-\text{so}}$ (P)	$r_{0-\text{so}}$ (N)	r_0 (P)	r_0 (N)	κ	V_0	a
Blomqv.–Wahlb.	32.0	32.0	1.270	1.270	1.270	1.270	0.67	51.0	0.67
Rost	17.8	31.5	0.932	1.280	1.275	1.347	0.86	49.6	0.70
Chepurnov	calc.		1.240	1.240	1.240	1.240	0.63	53.3	0.63
"optimal"	A-dependent				1.275	1.347	0.86	49.6	0.70
"universal"	36.0	35.0	1.20	1.310	1.275	1.347	0.86	49.6	0.70
"input"				parameters read from input					
def.-dependent INCREA = 1	deformation-dependent (only for $\beta_2 > 0.325$)				depend on ICHOIC				

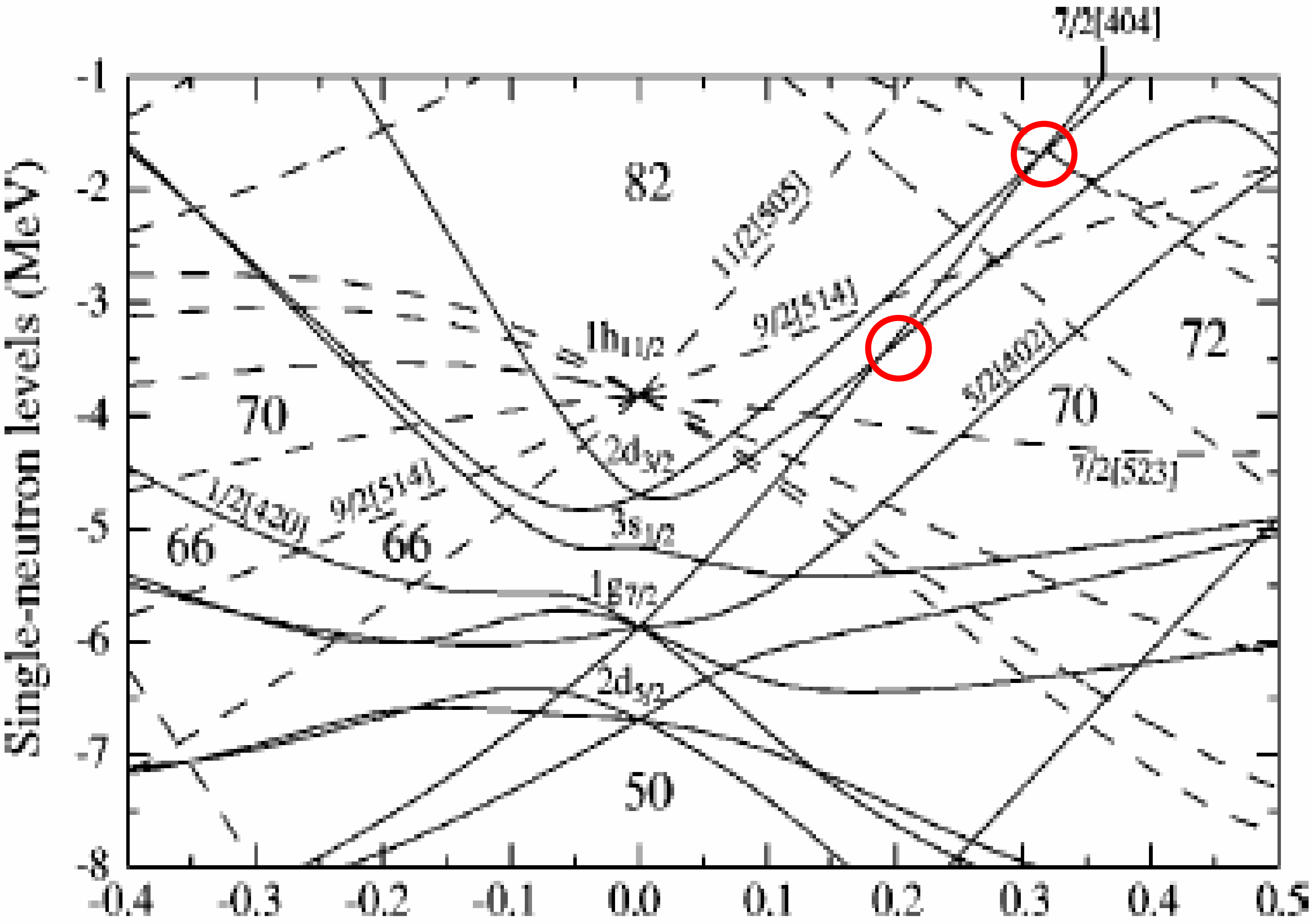
The basis:

axially symmetry harmonic oscillator in the cylindrical coordinate

$$|n_\rho n_z \Lambda \Sigma\rangle = \psi_{n_\rho}^{\Lambda}(\rho)\psi_{n_z}(z)\psi_\Lambda(\varphi)\chi(\Sigma)$$

$$[N n_z \Lambda]\Omega \qquad N = 2n_\rho + n_z + \Lambda \qquad \Omega = \Lambda + \frac{1}{2}\Sigma$$

The Nilsson numbers have been chosen for the adiabatic-blocking PES calculations.



7/2[404]
82
11/2[505]
9/2[514]
1h11/2
72
5/2[402]
70
70
7/2[523]
2d3/2
1/2[420]
9/2[514]
66
66
3s1/2
1g7/2
2d5/2
50
Single-neutron levels (MeV)
-1
-2
-3
-4
-5
-6
-7
-8
-0.4
-0.3
-0.2
-0.1
0.0
0.1
0.2
0.3
0.4
0.5

$$E = E_{LD} + \delta E_{shell}$$

E_{LD} is independent of blocking

$$\delta E_{shell} = E_{LN} - \tilde{E}_{Strut}$$

BCS calculation can be collapsed in weak pairing case.

The Lipkin-Nogami pairing can avoid this problem.

$$E_{\text{LN}} = \sum_{j=1}^{S} e_{k_j} + \sum_{k \neq k_j} 2V_k^2 e_k - \frac{\Delta^2}{G} - G \sum_{k \neq k_j} V_k^4 + G \frac{N-S}{2}$$

$$-4\lambda_2 \sum_{k \neq k_j} (U_k V_k)^2, \qquad (1)$$

with

$$N - S = \sum_{k \neq k_j} 2V_k^2, \qquad (2)$$

$$\left|BCS\right\rangle = \sum_{k>0}(U_k + V_k \alpha_k{}^{+} \alpha_{\bar{k}}{}^{+})\left|0\right\rangle$$

$$\delta\left\langle BCS\right|\hat{H}\left|BCS\right\rangle = 0$$

$$\left\langle \Psi_{LN}\right|\hat{N} - N\left|\Psi_{LN}\right\rangle = 0$$

$$\left\langle \Psi_{LN}\right|\hat{N}^2 - N^2\left|\Psi_{LN}\right\rangle = 0$$

III. Calculations for high-K states

Adjustment of pairing strength

$$D^{oe} = -\frac{1}{8}[M(N+2) - 4M(N+1) + 6M(N) - 4M(N-1) + M(N-2)], \quad (1)$$

$$\Delta_{BCS}$$

$$\Delta_{LN} + \lambda_2$$

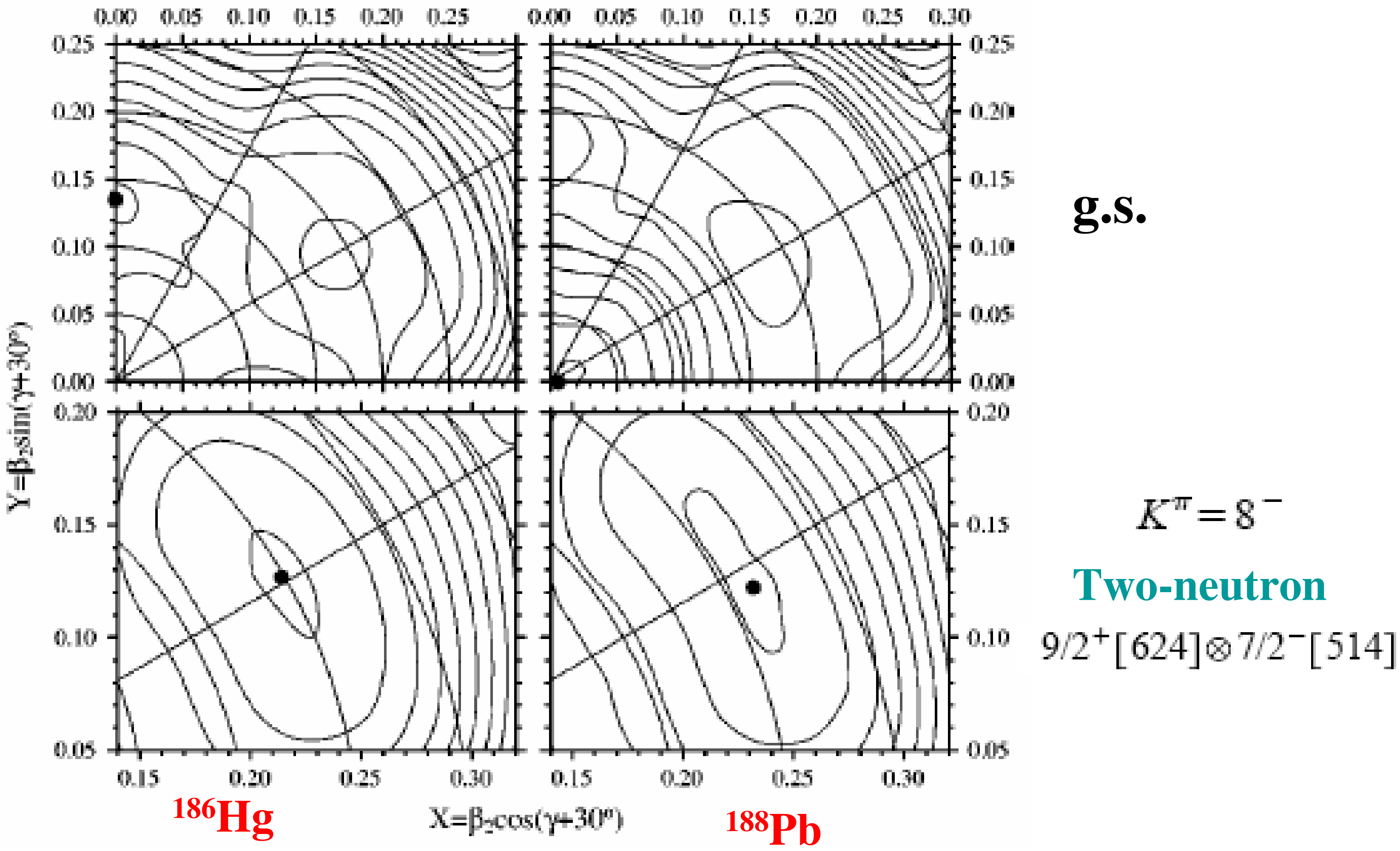
The adiabatic-blocking PES can include the effect from the shape polarization .

$$Q_0 = \sum_{j=1}^{S} q_{k_j} + \sum_{k \neq k_j} 2V_k^2 q_k$$

High-K states in:

1. **Neutron-deficient region**
2. **Neutron-rich region**
3. **Superheavy region**
4. **In the 2nd well.**

“Shape polarization in neutron-deficient nuclei” , Xu, Walker, Wyss, PRC59, 731 (1999)



E^{cal}=2230 keV; E^{expt} =2217 keV

A.M. Bruce *et al.*, PRC55, 620 (1997)

E^{cal}=2400 keV ; E^{expt}=2576 keV

Dracoulis *et al.*, PRC60, 014303(1999)

Shape polarization in neutron-deficient nuclei

N=74 isotones

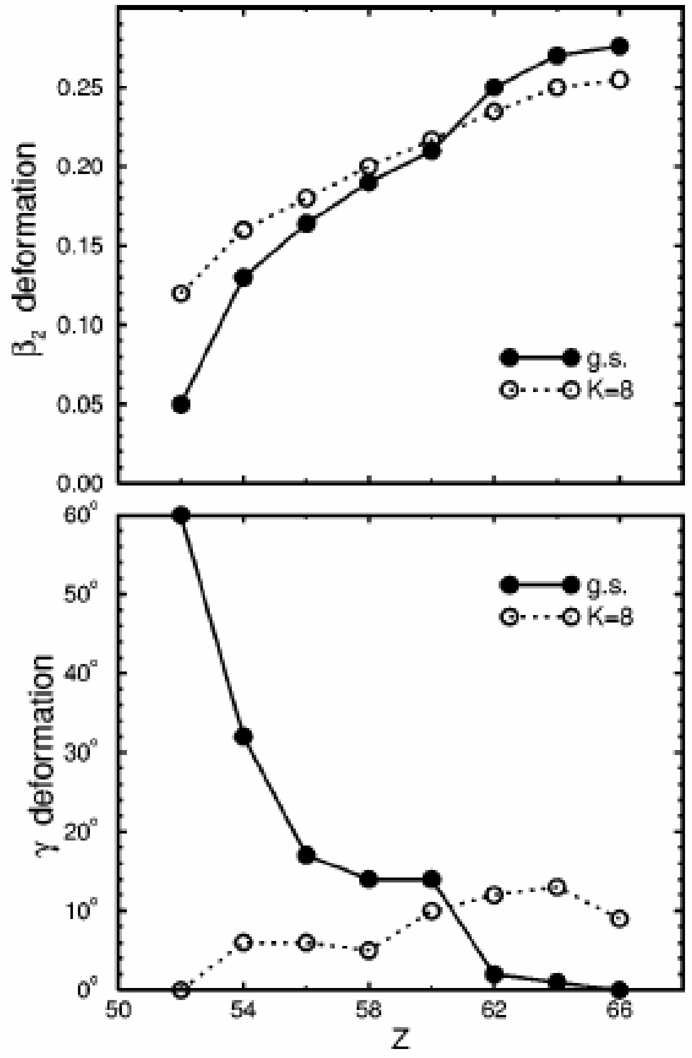


FIG. 1. The determined β_2, γ deformations for the $K^\pi=8^-$ isomers and the ground states (g.s.) in the $N=74$ isotones.

Xu, Walker, Wyss,

PRC59, 731 (1999)

$7/2^+[404]\otimes 9/2^-[514]$

PHYSICAL REVIEW C VOLUME 59, NUMBER 2 FEBRUARY 1999

Shape polarizations of two-quasiparticle $K^{\pi}=8^{-}$ isomeric configurations

F. R. Xu,[1,*] P. M. Walker,[1] and R. Wyss[2]

$K^{\pi}=8^{-}$ isomers.

Nuclei	E_{expt}	E_{cal}	β_2	β_4	$\|\gamma\|$
^{126}Te		2980	0.12	−0.005	0°
^{140}Dy		2150	0.26	−0.039	9°
^{188}Pb		2400	0.26	−0.011	2°

Proton-drop line

Physics Letters B 529 (2002) 42–49

PHYSICS LETTERS B

www.elsevier.com/locate/npe

ELSEVIER

Identification of excited states in ^{140}Dy

D.M. Cullen [a], M.P. Carpenter [b], C.N. Davids [b], A.M. Fletcher [a], S.J. Freeman [a],

Recent Woods–Saxon constrained shape polarization calculations [16] predict the existence of a $K^{\pi}=8^{-}$ isomeric state in ^{140}Dy at an excitation energy of 2150 keV with a deformation $\beta_2=0.26$. Thus, the experimental excitation energy of 2164 keV and the associated deformation of $\beta_2=0.24(3)$ are in good agreement with these theoretical expectations.

PHYSICAL REVIEW C VOLUME 59, NUMBER 2 FEBRUARY 1999

Shape polarizations of two-quasiparticle $K^\pi = 8^-$ isomeric configurations

F. R. Xu,[1,*] P. M. Walker,[1] and R. Wyss[2]

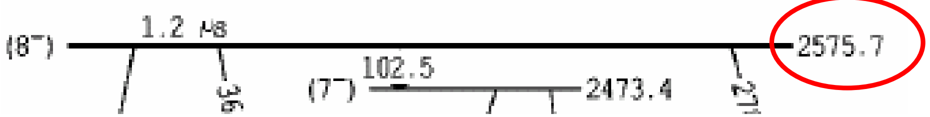
$K^\pi = 8^-$ isomers.

Nuclei	E_{expt}	E_{cal}	β_2	β_4	$\|\gamma\|$
^{126}Te		2980	0.12	−0.005	0°
^{140}Dy		2150	0.26	−0.039	9°
^{188}Pb		2400	0.26	−0.011	2°

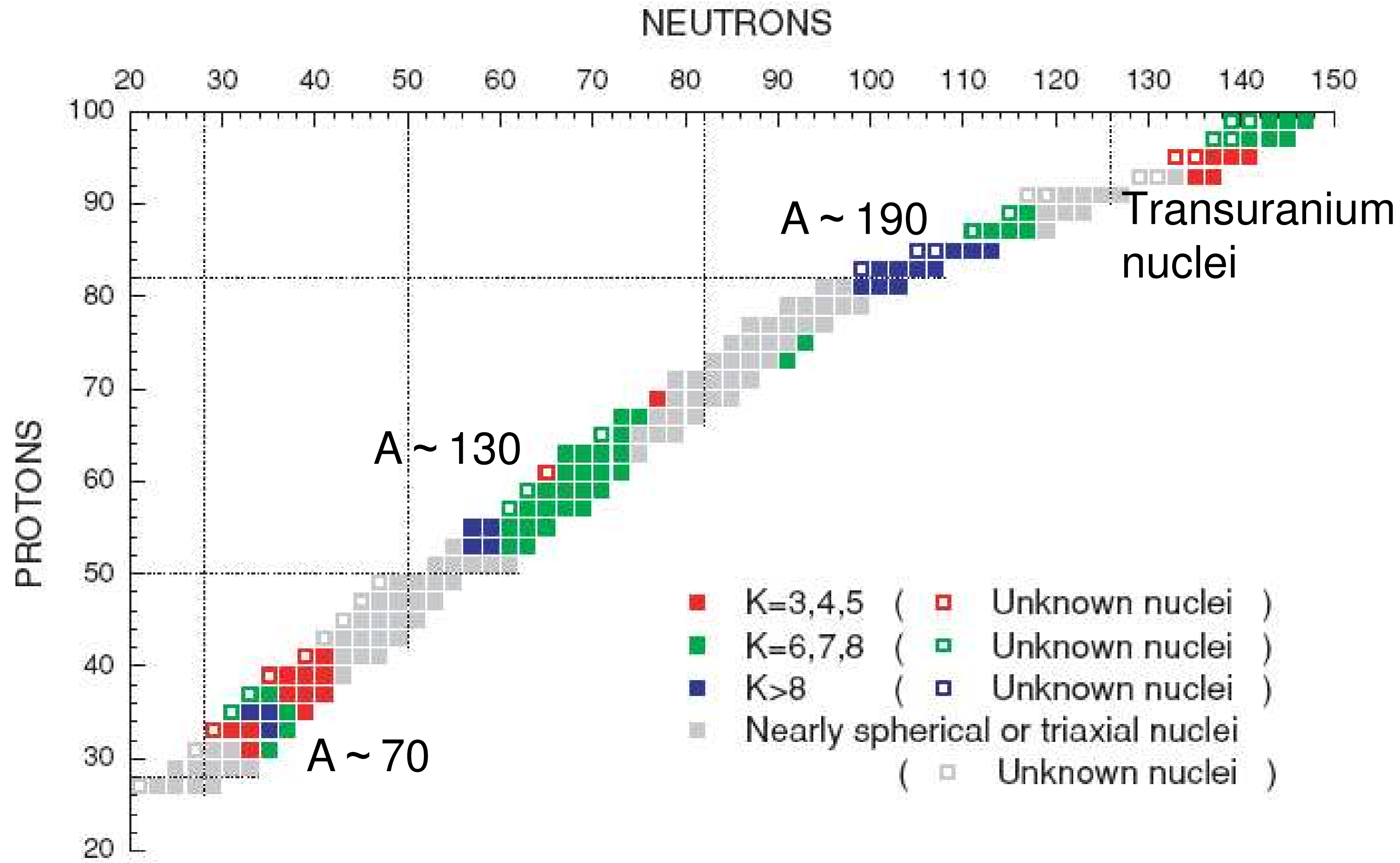
PHYSICAL REVIEW C, VOLUME 60, 014303

Spherical and deformed isomers in ^{188}Pb

G. D. Dracoulis,[1] A. P Byrne,[2] A. M Baxter,[2] P. M. Davidson,[1] T. Kibédi,[1] T. R. McGoram,[1]



Exploration of the proton drip line and beyond

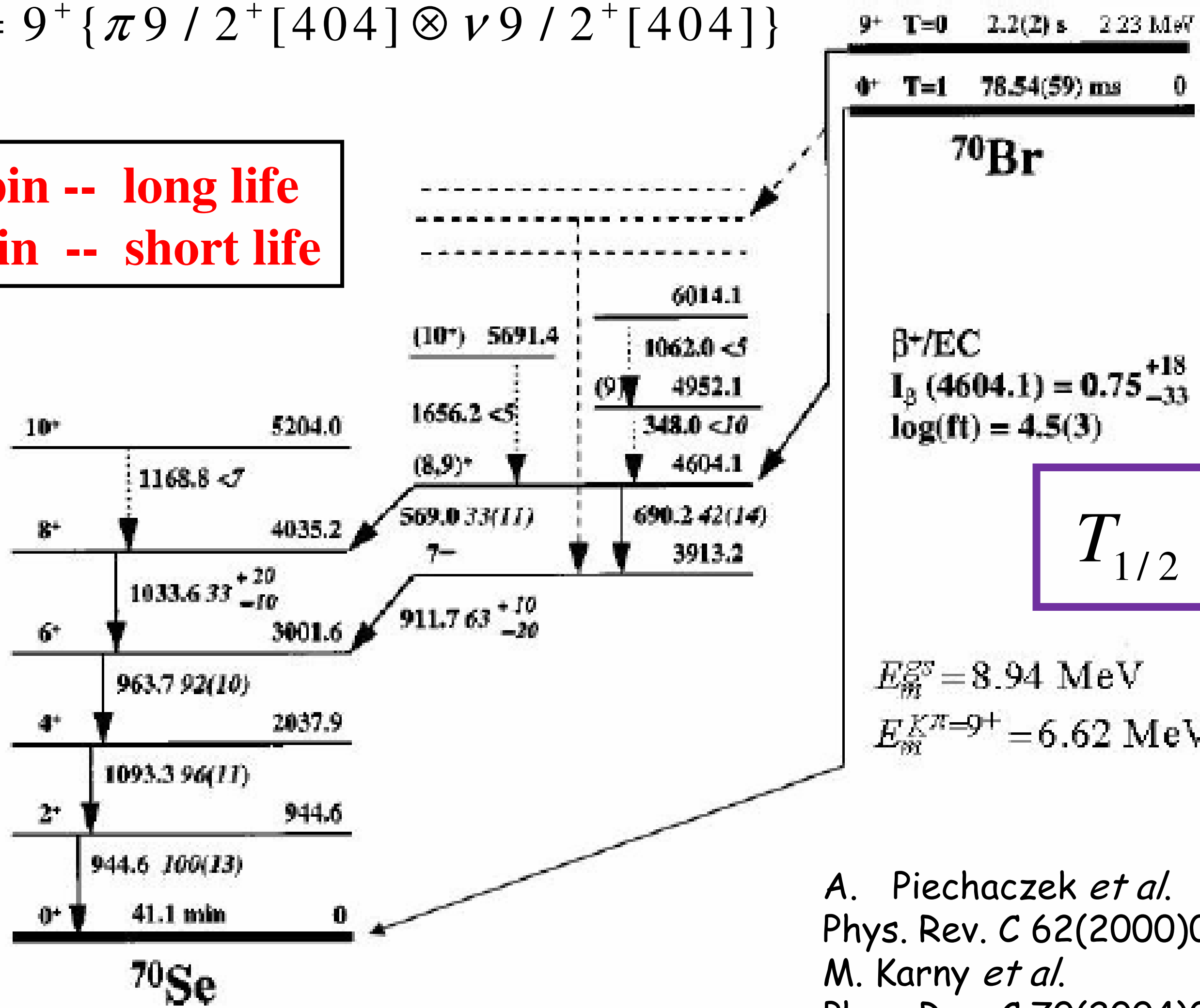


Liu *et al.*, PRC 76 (2007) 034313

$$K^{\pi} = 9^{+}\{\pi 9/2^{+}[404] \otimes \nu 9/2^{+}[404]\}$$

Calculation:
β_2 = - 0.28
$E_x \approx$ 2.56 MeV

High-spin -- long life
Low-spin -- short life



$$T_{1/2} \propto E_m^{-5}$$

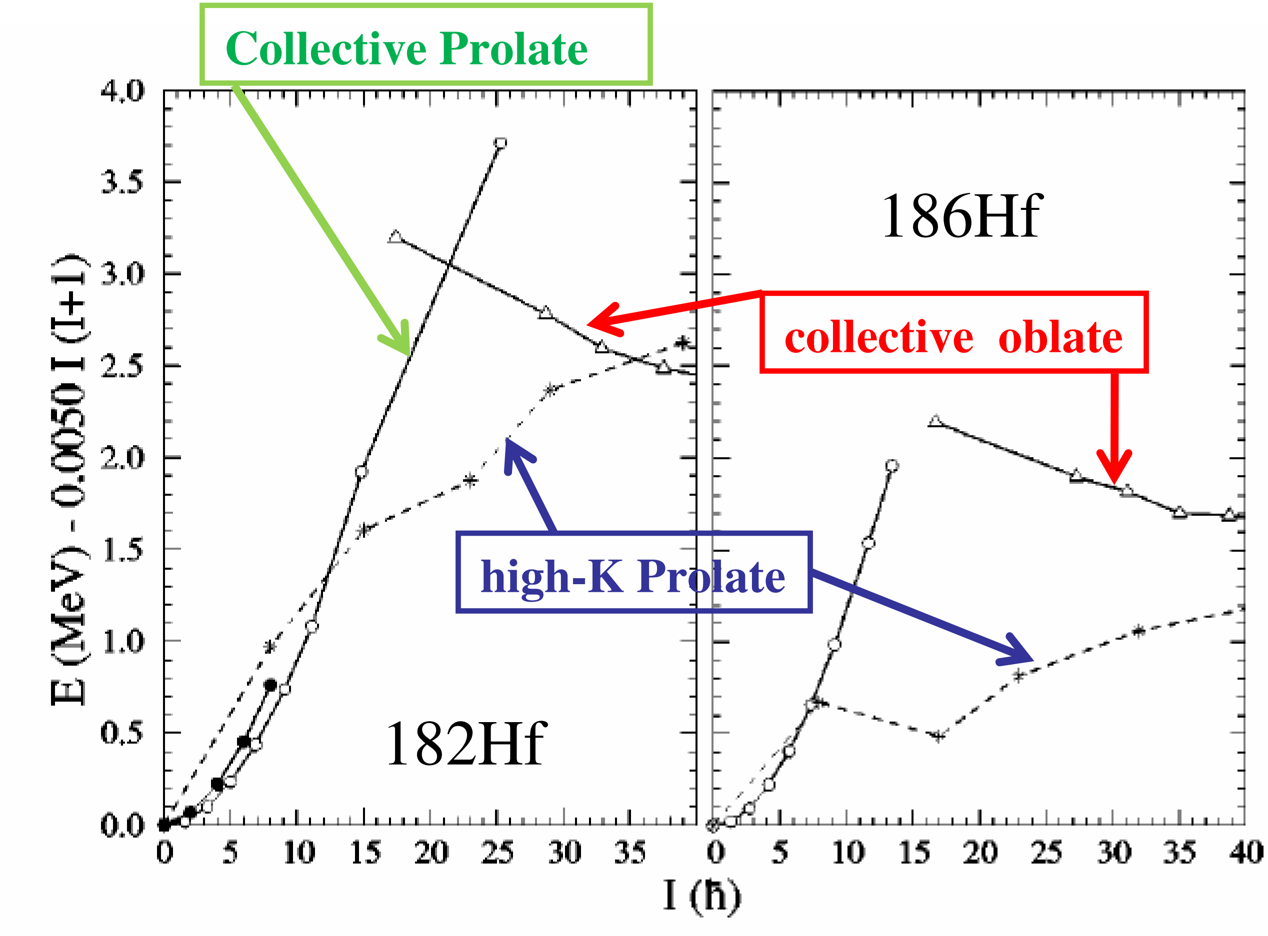
$E_m^{gs} = 8.94$ MeV

$E_m^{K\pi=9+} = 6.62$ MeV

A. Piechaczek *et al.*
Phys. Rev. C 62(2000)054317
M. Karny *et al.*
Phys. Rev. C 70(2004)014310

2. High-K states in neutron-rich nuclei

(Xu, Walker, Wyss, PRC 62 (2000) 014301)



3. High-k isomerism in SHE

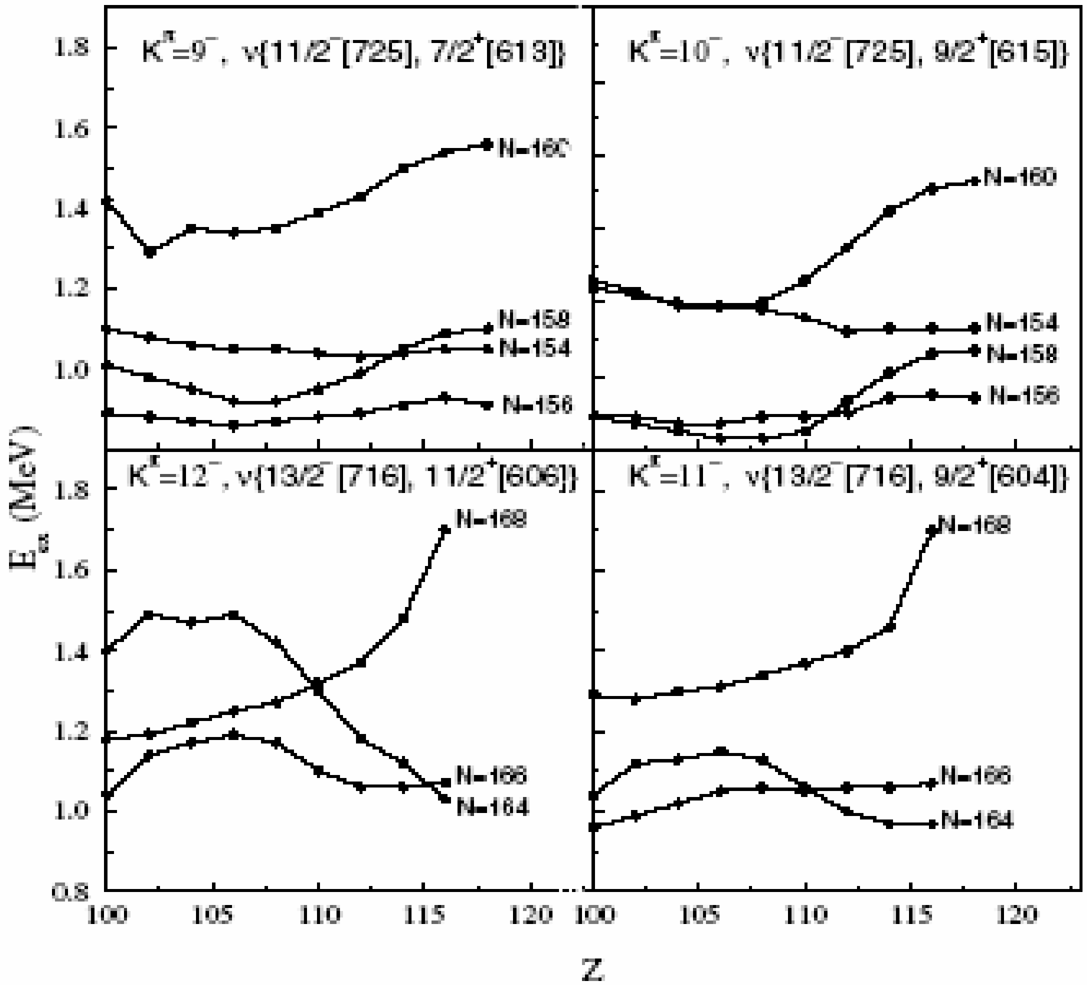
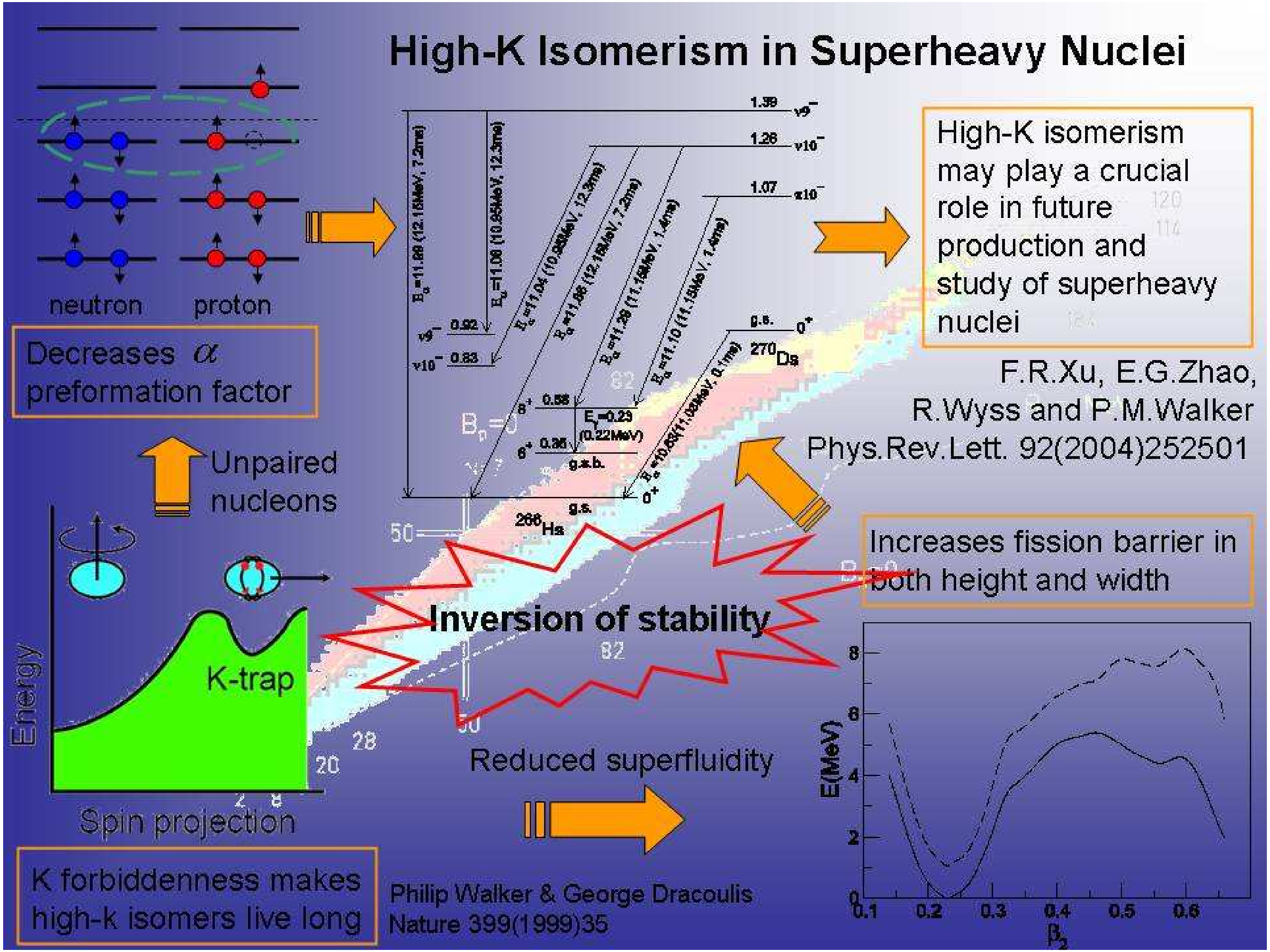
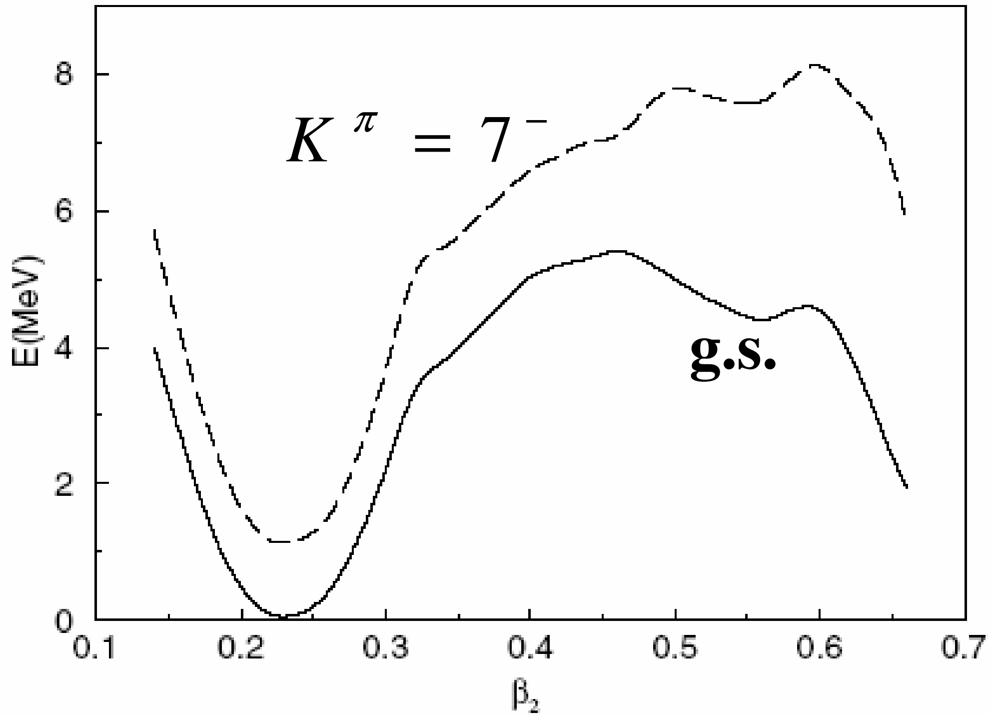


FIG. 1. Calculated excitation energies for two-quasineutron states.

F.R. Xu *et al.* , Phys. Rev. Lett. **95**, 252501 (2004)


High-K Isomerism in Superheavy Nuclei
neutron
proton
Decreases α preformation factor
Unpaired nucleons
Energy
K-trap
Spin projection
K forbiddenness makes high-k isomers live long
1.39
1.26
1.07
0.92
0.83
0.58
0.36
g.s.b.
g.s.
266Hs
270Ds
0+
8+
6+
Inversion of stability
Reduced superfluidity
Philip Walker & George Dracoulis
Nature 399(1999)35
High-K isomerism may play a crucial role in future production and study of superheavy nuclei
F.R.Xu, E.G.Zhao, R.Wyss and P.M.Walker
Phys.Rev.Lett. 92(2004)252501
Increases fission barrier in both height and width
E(MeV)
β2
0.1
0.2
0.3
0.4
0.5
0.6
0
2
4
6
8



F.R. Xu *et al.*, Phys. Rev. Lett. 95, 252501 (2004)

R.-D. Herzberg *et al.*, Nature 442 (2006) 24

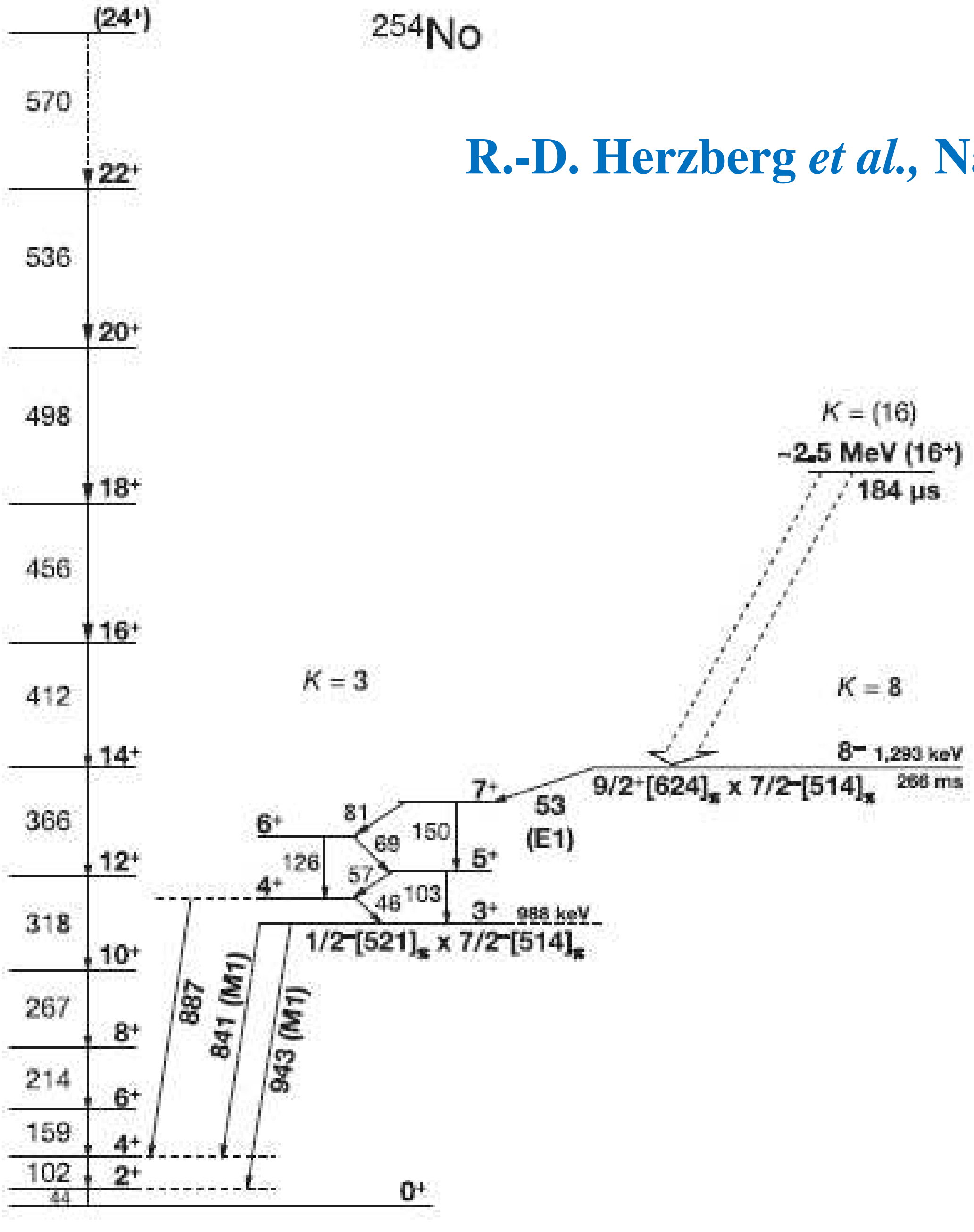
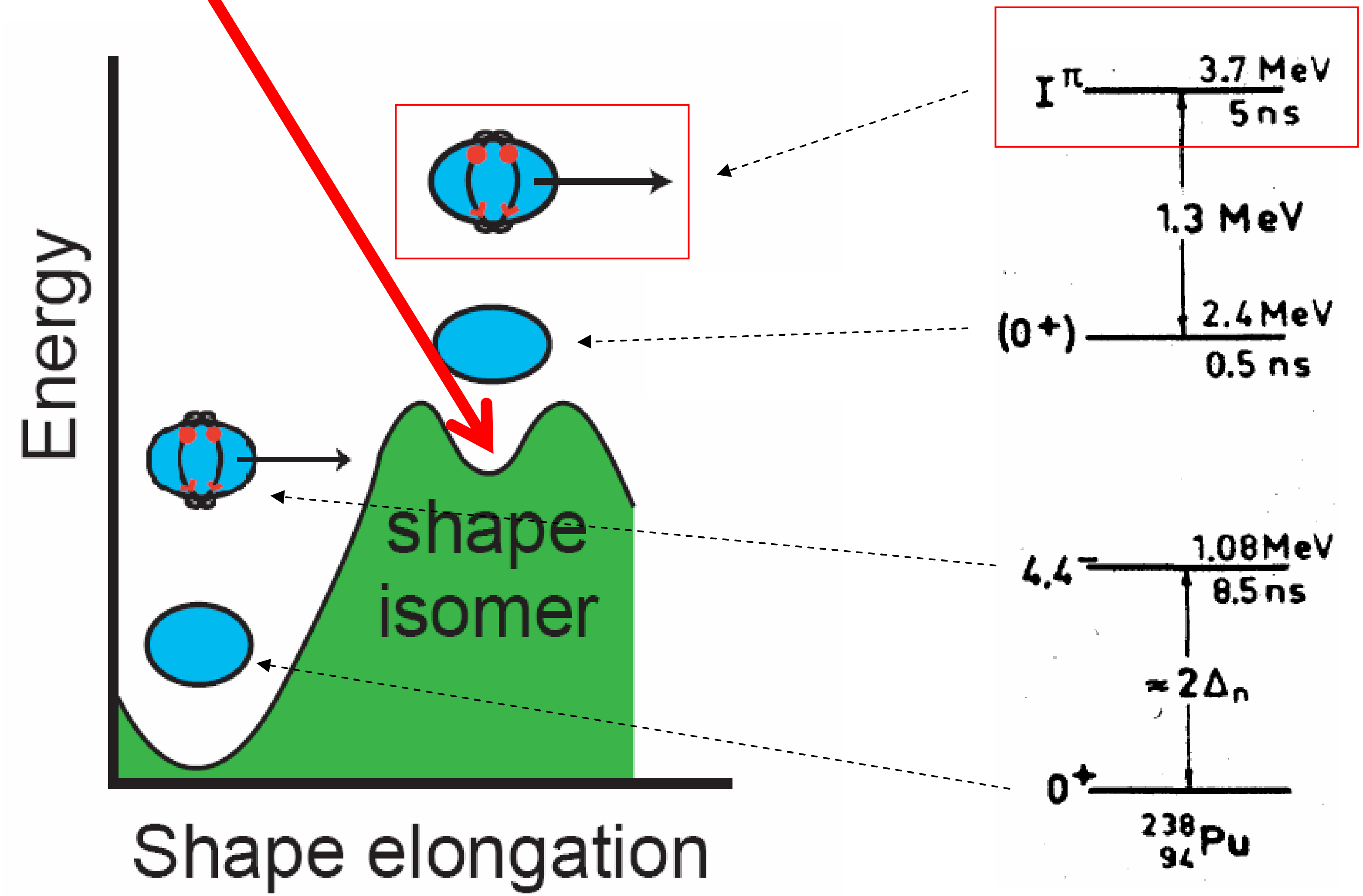


Figure 3 | Proposed level scheme of ^{254}No. The 266 ms 8^- isomer is

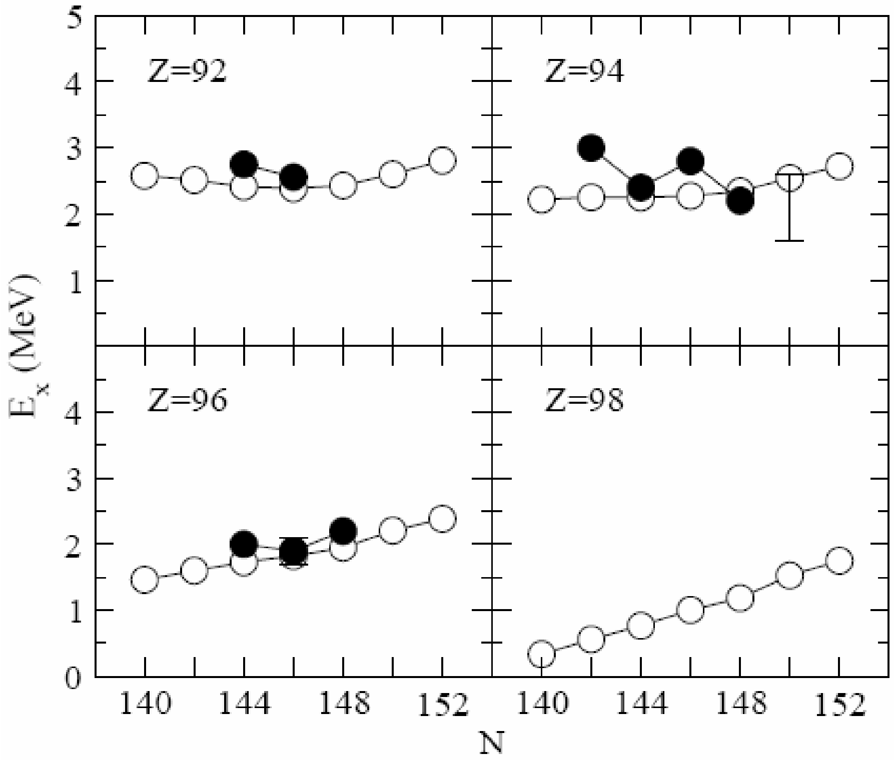
High-K in the 2nd well

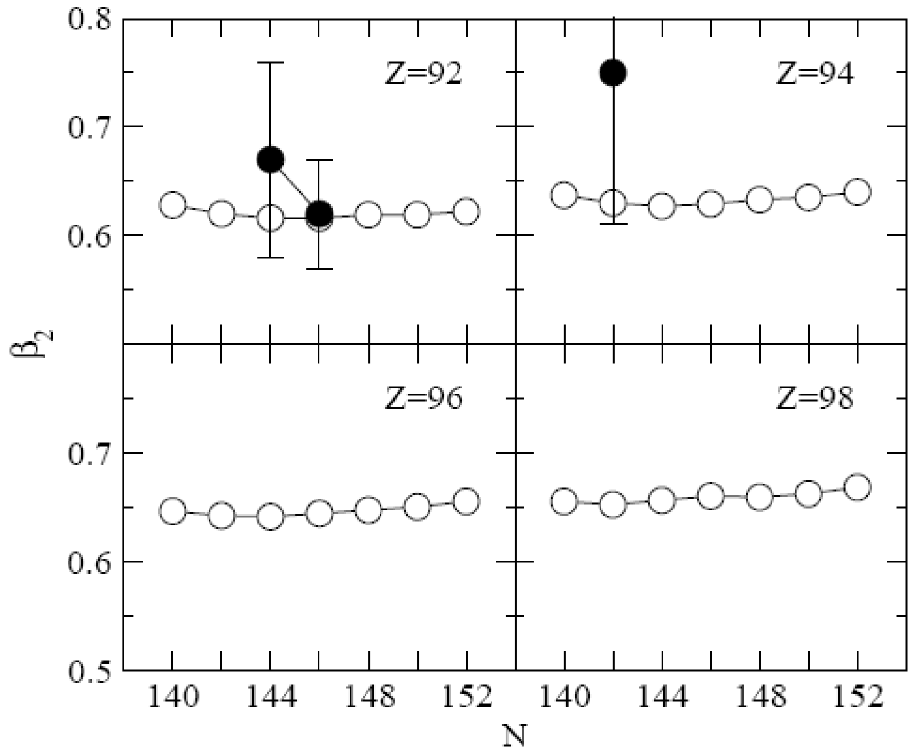
Shape isomerism + K isomerism

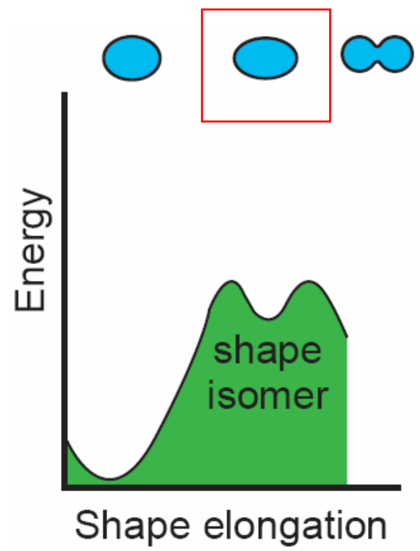


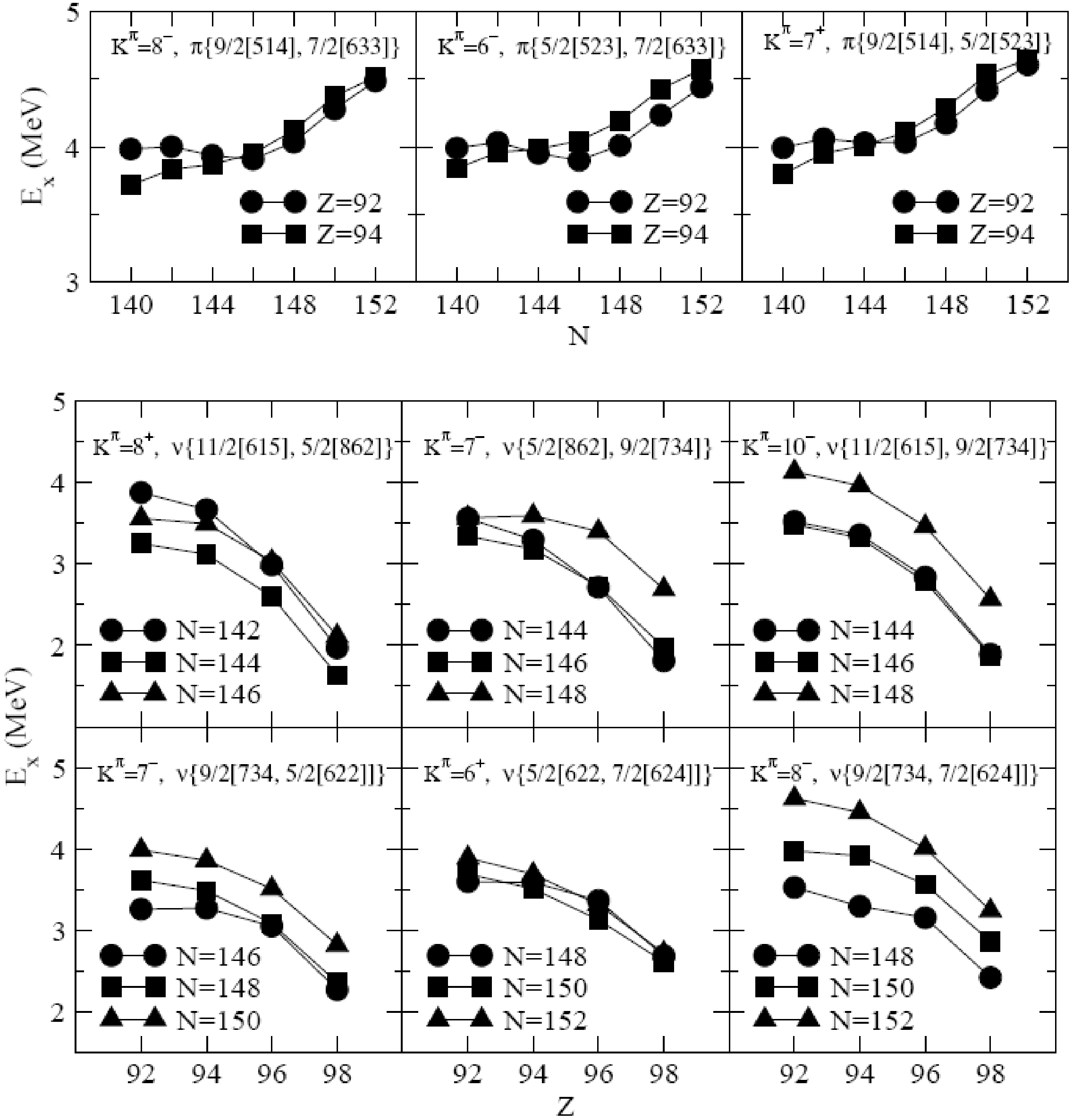
P. Limkilde & G. Sletten
Nucl. Phys. A 199(1973)504

High-K in the 2nd well

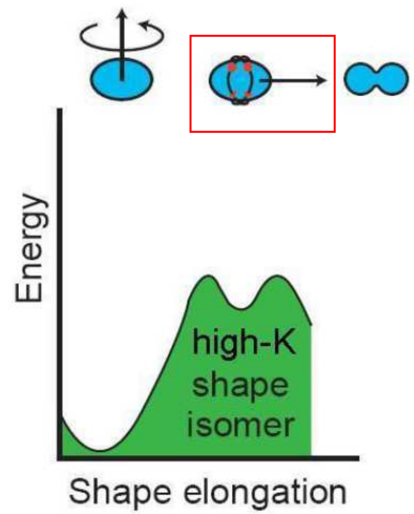








Kπ=8−, π{9/2[514], 7/2[633]}
Kπ=6−, π{5/2[523], 7/2[633]}
Kπ=7+, π{9/2[514], 5/2[523]}
Z=92
Z=94
Ex (MeV)
N
Kπ=8+, ν{11/2[615], 5/2[862]}
Kπ=7−, ν{5/2[862], 9/2[734]}
Kπ=10−, ν{11/2[615], 9/2[734]}
N=142
N=144
N=146
N=148
Kπ=7−, ν{9/2[734, 5/2[622]]}
Kπ=6+, ν{5/2[622, 7/2[624]]}
Kπ=8−, ν{9/2[734, 7/2[624]]}
N=150
N=152
Ex (MeV)
Z



Energy
high-K
shape
isomer
Shape elongation

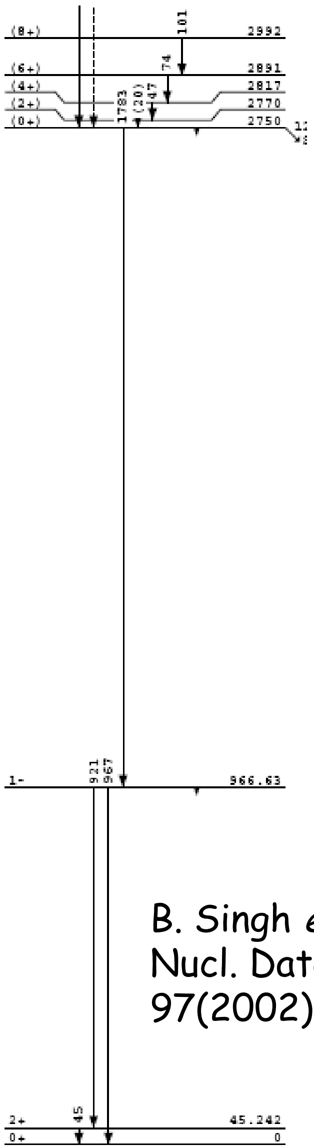
Experimental spins and parities have not been known

Calculations can predict configurations (spins and parities) and energies.

Longer lifetimes for shape+K isomers

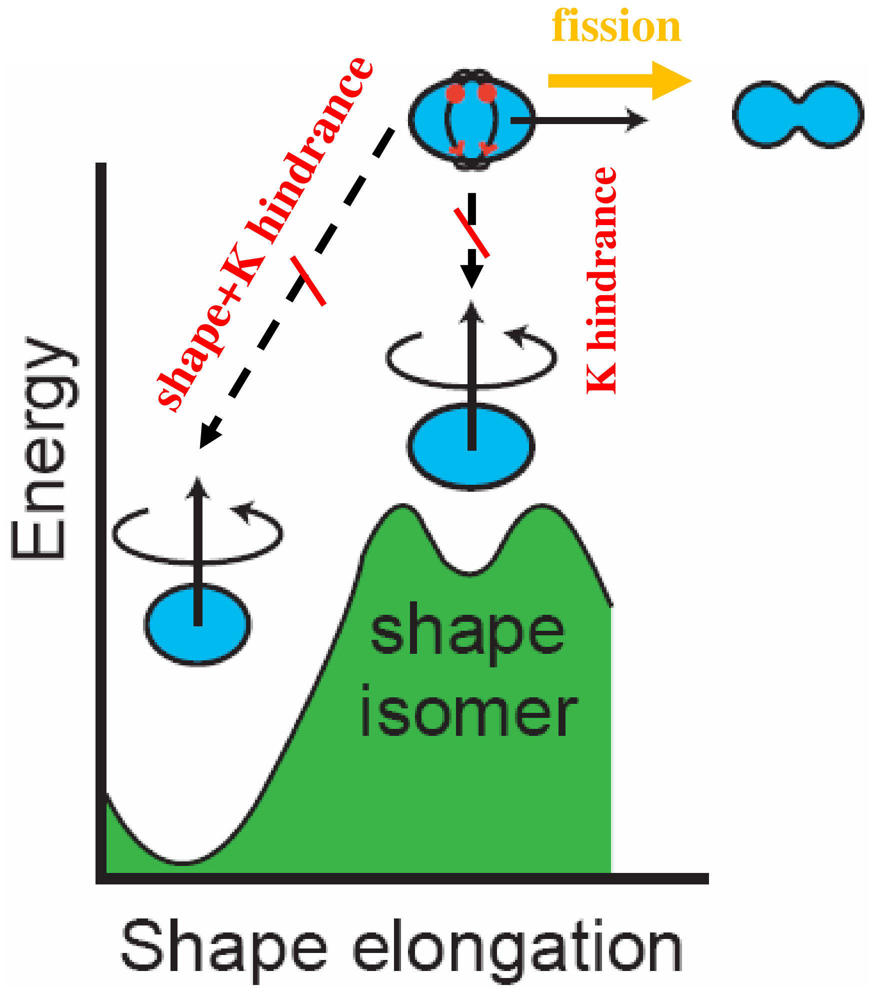
Nuclei	K^π	Configurations	β_2	β_4	Δ_n(keV)	Δ_p(keV)	$E_x^{\mathrm{cal.}}$(keV)	$E_x^{\mathrm{expt.}}$(keV)	$T_{1/2}$
^{238}U	0^+	Shape Isomer	0.62	0.029	610	840	2383	2557.9	298 ns
	7^-	$\nu\{9/2[734],5/2[622]\}$	0.61	0.022	428	840	3258	< 3558	> 1 ns
	7^-	$\nu\{5/2[862],9/2[734]\}$	0.63	0.037	417	853	3344		
	10^-	$\nu\{11/2[615],9/2[734]\}$	0.62	0.036	423	851	3486		
	8^+	$\nu\{11/2[615],5/2[862]\}$	0.62	0.043	430	852	3563		
	6^-	$\pi\{5/2[523],7/2[633]\}$	0.62	0.033	574	630	3899		
	8^-	$\pi\{9/2[514],7/2[633]\}$	0.62	0.037	573	630	3907		
	7^+	$\pi\{9/2[514],5/2[523]\}$	0.63	0.042	574	638	4032		
^{236}Pu	0^+	Shape Isomer	0.63	0.045	600	830	2252	≈ 3000	37 ps
	8^+	$\nu\{11/2[615],5/2[862]\}$	0.63	0.053	459	841	3671	4000	34 ns
	8^-	$\pi\{9/2[514],7/2[633]\}$	0.64	0.056	596	621	3833		
	7^+	$\pi\{9/2[514],5/2[523]\}$	0.64	0.060	596	627	3951		
	6^-	$\pi\{5/2[523],7/2[633]\}$	0.64	0.055	597	628	3958		
^{238}Pu	0^+	Shape Isomer	0.63	0.038	610	830	2249	≈ 2400	0.6 ns
	8^+	$\nu\{11/2[615],5/2[862]\}$	0.62	0.048	425	839	3120	≈ 3500	6.0 ns
	7^-	$\nu\{5/2[862],9/2[734]\}$	0.64	0.042	528	833	3299		
	10^-	$\nu\{11/2[615],9/2[734]\}$	0.62	0.034	448	831	3363		
	8^-	$\pi\{9/2[514],7/2[633]\}$	0.64	0.048	584	620	3868		
	6^-	$\pi\{5/2[523],7/2[633]\}$	0.64	0.045	582	626	3982		
	7^+	$\pi\{9/2[514],5/2[523]\}$	0.64	0.051	586	627	4010		
^{242}Pu	0^+	Shape Isomer	0.63	0.016	570	820	2341	≈ 2200	3.5 ns
	8^-	$\nu\{9/2[734],7/2[624]\}$	0.62	0.013	420	813	3473	< 3200	28 ns
	7^-	$\nu\{9/2[734],5/2[622]\}$	0.63	0.026	417	826	3484		
	6^+	$\nu\{5/2[622],7/2[624]\}$	0.62	0.013	427	812	3587		
	7^-	$\nu\{5/2[862],9/2[734]\}$	0.61	0.025	427	823	3595		
	10^-	$\nu\{11/2[615],9/2[734]\}$	0.65	0.037	453	831	[illegible]		
	8^-	$\pi\{9/2[514],7/2[633]\}$	0.64	0.033	579	618	4120		
	6^-	$\pi\{5/2[523],7/2[633]\}$	0.64	0.027	576	621	4188		
	7^+	$\pi\{9/2[514],5/2[523]\}$	0.65	0.036	583	626	4288		
^{240}Cm	0^+	Shape Isomer	0.64	0.036	630	790	1729	≈ 2000	10 ps
	8^+	$\nu\{11/2[615],5/2[862]\}$	0.64	0.046	423	801	2602	≈ 3000	55 ns
	7^-	$\nu\{5/2[862],9/2[734]\}$	0.64	0.042	524	797	2714		
	10^-	$\nu\{11/2[615],9/2[734]\}$	0.64	0.032	445	791	2841		
^{242}Cm	0^+	Shape Isomer	0.64	0.025	630	780	1822	1900	40 ps
	7^-	$\nu\{5/2[862],9/2[734]\}$	0.64	0.035	418	794	2728	≈ 2800	0.18 ms
	10^-	$\nu\{11/2[615],9/2[734]\}$	0.65	0.030	421	787	2786		
	8^+	$\nu\{11/2[615],5/2[862]\}$	0.64	0.038	431	794	3034		
	7^-	$\nu\{9/2[734],5/2[622]\}$	0.61	0.024	426	797	3049		
^{244}Cm	0^+	Shape Isomer	0.65	0.016	570	770	1947	≈ 2200	< 5 ps
	7^-	$\nu\{9/2[734],5/2[622]\}$	0.64	0.025	419	786	3082	≈ 3500	> 100 ns
	8^-	$\nu\{9/2[734],7/2[624]\}$	0.64	0.013	419	778	3153		
	6^+	$\nu\{5/2[622],7/2[624]\}$	0.62	0.015	426	784	3364		
	7^-	$\nu\{5/2[862],9/2[734]\}$	0.62	0.026	430	797	3404		
	10^-	$\nu\{11/2[615],9/2[734]\}$	0.66	0.034	453	789	3462		

Experimentally, only fission observed, no γ transition observed



$^{236}_{92}U_{144}$

B. Singh *et al.*
Nucl. Data Sheets
97(2002)241



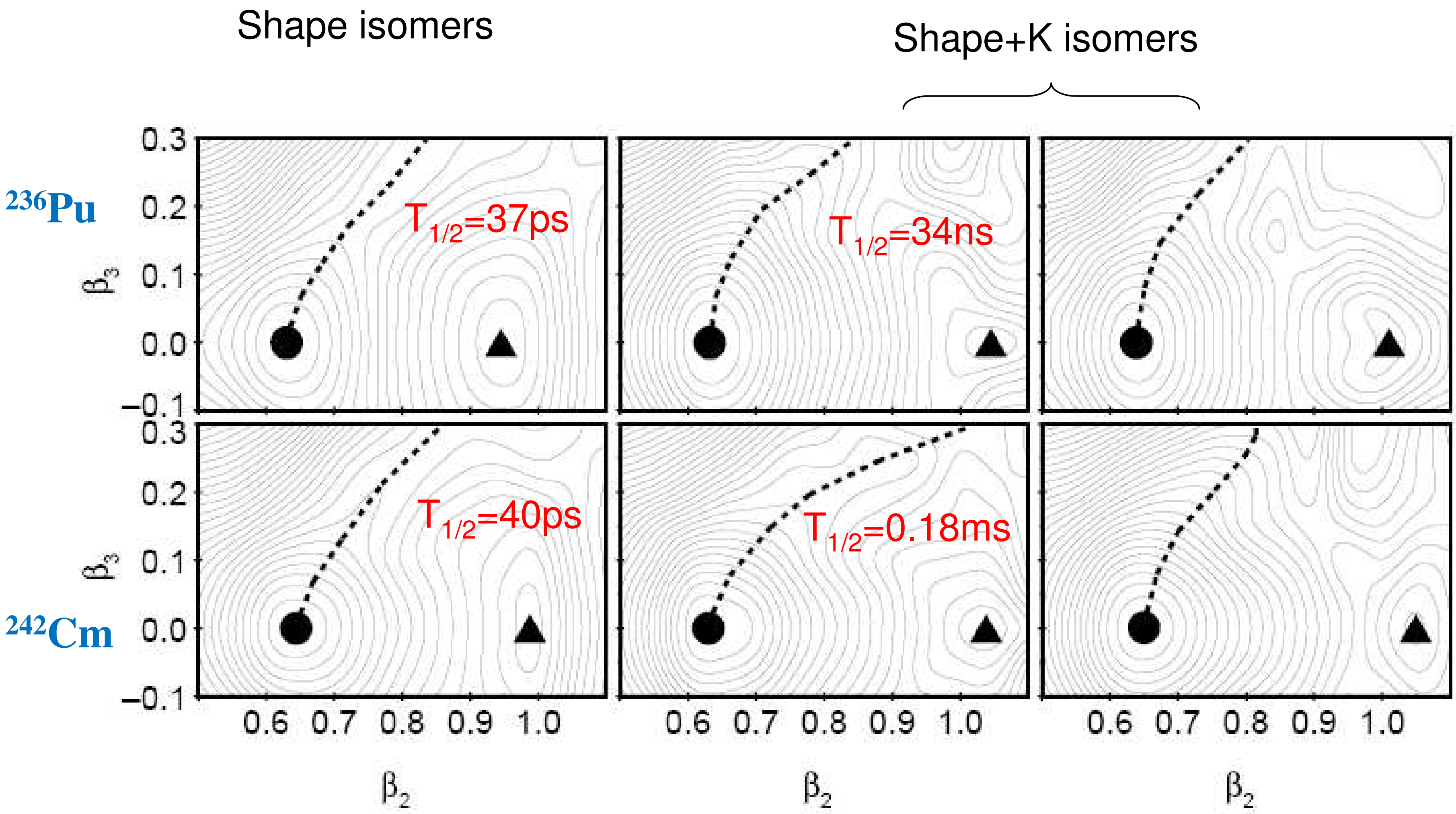
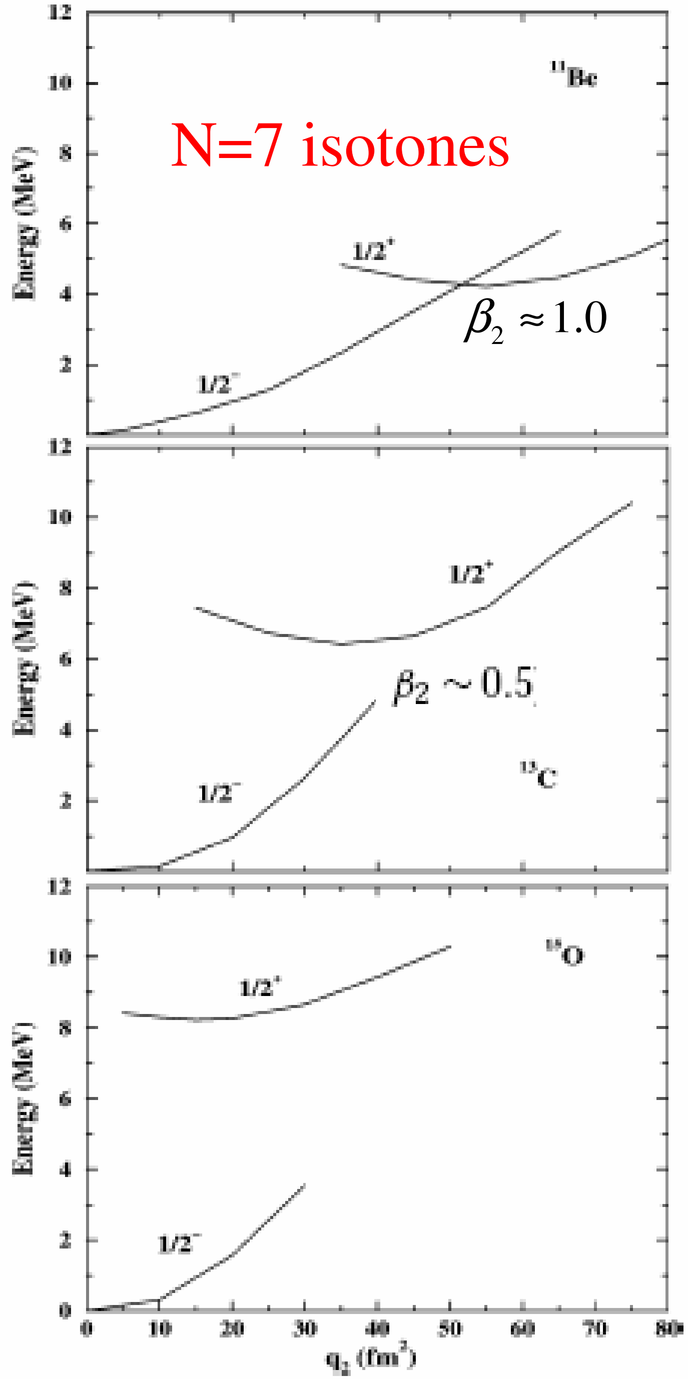


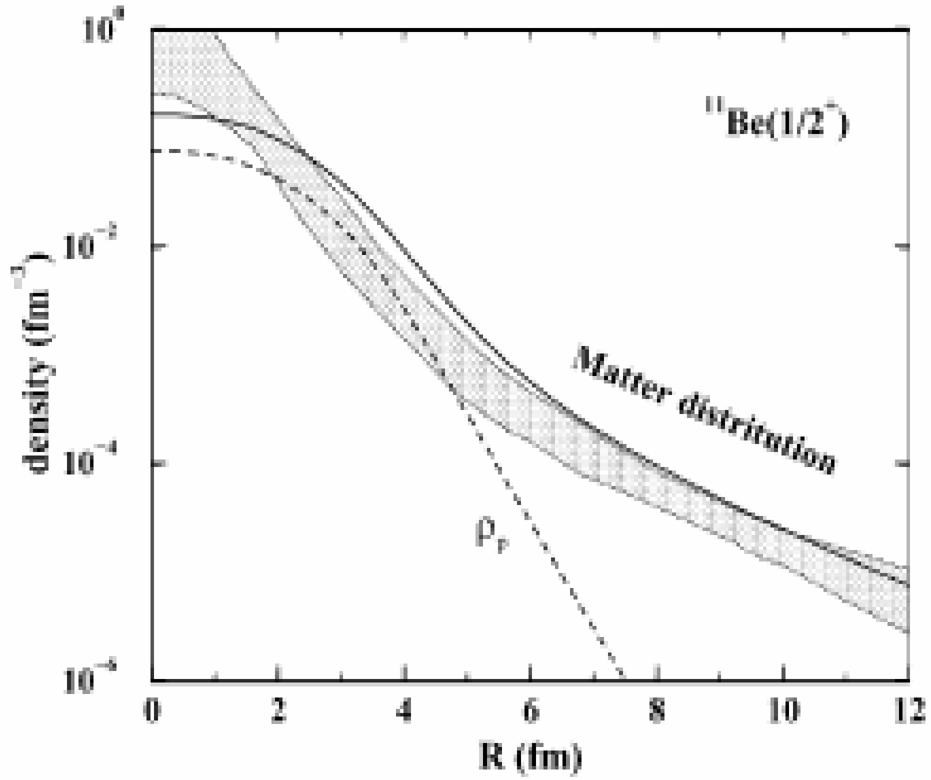
FIG. 4: Representative PESs for the shape isomeric (top left), $K^\pi = 8^+\{\nu 11/2[615] \otimes 5/2[862]\}$ (top middle) and $K^\pi = 8^-\{\pi\ 9/2[514] \otimes 7/2[633]\}$ (top right) states of ^{236}Pu as well as shape isomeric (bottom left), $K^\pi = 7^-\{\nu\ 5/2[862] \otimes 9/2[734]\}$ (bottom middle) and $K^\pi = 10^-\{\nu 11/2[615] \otimes 9/2[734]\}$ (bottom right) states of ^{242}Cm.

Exploration of the adiabatic-blocking calculation



SHF+BCS with SkI4

Pei, Xu, Stevenson, NPA 765 (2006) 29



130Ce

$\nu\frac{7}{2}^{-}[523] \otimes \nu\frac{7}{2}^{+}[404]$

M.Ionescu-Bujor *et.al*
PRC 60, 024316(1999)

- Measured Q, K=7 } ⟶ Q_0 ⟶ β_2=0.16 << $\beta_2^{g.s} \approx 0.26$

  ⇧ Shape polarization ?

- Assume $\beta_2^{isomer}=\beta_2^{g.s.} \approx 0.26$ ⟶ Q_0, Measured Q } ⟶(1) K=6.0(2)

  ⇧ K mixing ?

$$Q = \frac{3K^2 - J(J+1)}{(J+1)(2J+3)} Q_0 \quad (1)$$

$$Q_0 = 0.0109 Z A^{2/3} \beta_2 (1 + 0.36\beta_2) \quad (2)$$

PES calculations

Configuration	β_2	β_4	$\lvert\gamma\rvert$	γ-soft[†] -ness	$Q_0(eb)$ cal.	$Q_0(eb)$ expt.[‡]	$E_x(KeV)$ cal.	$E_x(KeV)$ expt.[‡]
g.s.	0.23	-0.008	0°	13°	4.53			
$7_a^-\{\nu 7/2^-[523] \otimes \nu \ \ 7/2^+[404]\}$	0.22	-0.005	2°	16°	4.22	2.65	2503	2454
$7_b^-\{\nu 5/2^+[402] \otimes \nu \ \ 9/2^-[514]\}$	0.24	-0.025	0°	8°	4.85		2407	

† 定义为沿势能面的 γ 自由度从极小值点到极小值点上 100KeV 的距离。
‡ 取自 M. Ionescu-Bujor *et al.*, Phys. Rev. C **60**, 024316 (1999)。

Good agreement

The ground state

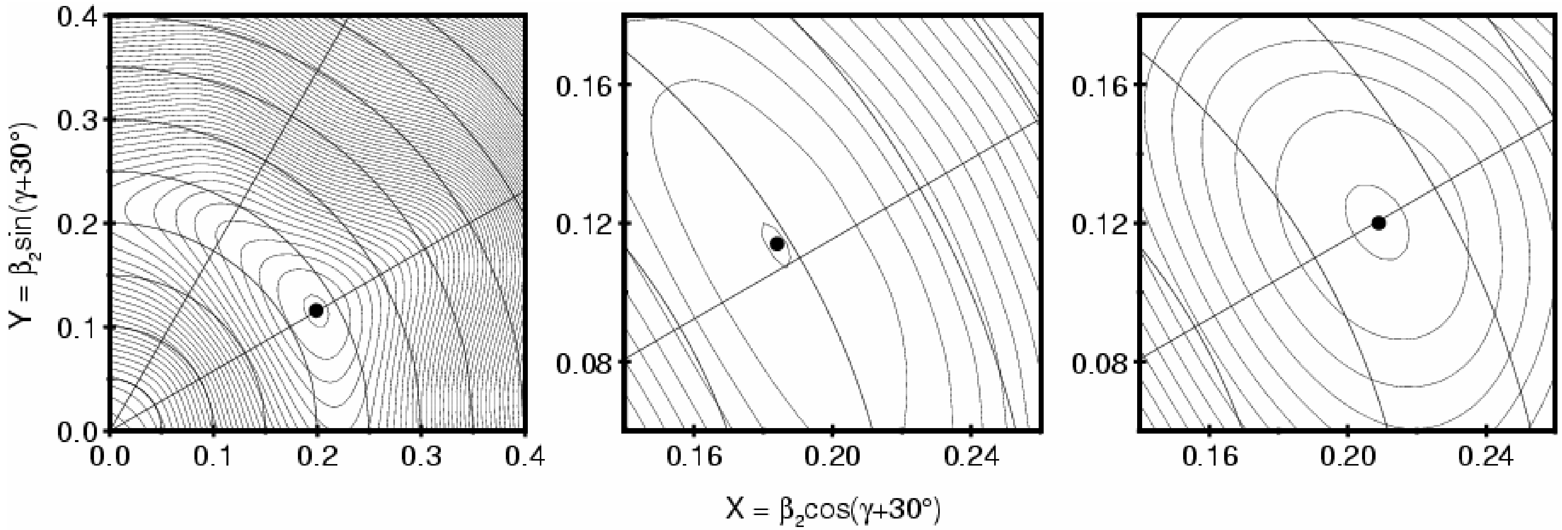
Table 8. Mean lifetime measurements, transition strengths and deduced β and γ deformations.

J_i^π	E_γ (keV)	τ(ps)	B(E2) (Wu)	$B(E2)_{norm}$ †	$\gamma(\beta=0.25)$ (deg)	$\beta(\gamma=0°)$
2^+	254	180 ± 15	107 ± 9	1.00 ± 0.08	0	0.25
4^+	456	7.3 ± 0.8	144 ± 15	0.95 ± 0.10	3 ± 5	0.243 ± 0.011

D.M. Todd *et.al* JPG 10,1407(1984)

Configuration	β_2	β_4	$\lvert\gamma\rvert$	γ-soft[†] -ness	$Q_0(eb)$ cal.	$Q_0(eb)$ expt.[‡]	$E_x(KeV)$ cal.	$E_x(KeV)$ expt.[‡]
g.s.	0.23	-0.008	0°	13°	4.53			
$7_a^-\{\nu 7/2^-[523] \otimes \nu \ \ 7/2^+[404]\}$	0.22	-0.005	2°	16°	4.22	2.65	2503	2454
$7_b^-\{\nu 5/2^+[402] \otimes \nu \ \ 9/2^-[514]\}$	0.24	-0.025	0°	8°	4.85		2407	

[†] 定义为沿势能面的 γ 自由度从极小值点到极小值点上 100KeV 的距离。
[‡] 取自 M. Ionescu-Bujor *et al.*, Phys. Rev. C **60**, 024316 (1999)。



g.s. $\quad 7_a^- \quad 7_b^-$

γ_{eff} □ 21°

Rigid triaxial rotor model , by J. Yan *et al*. PRC 48, 1046 (1993)

Interacting Boson Model , by O. Vogel *et al*. PRC 53, 1660 (1996)

A candidate for critical-point nuclei

R.M. Clark et al. PRC 68, 037301 (2003)

The $K^{\pi} = 7^{-}$ isomer:

γ-soft prolate shape as large as the g.s.

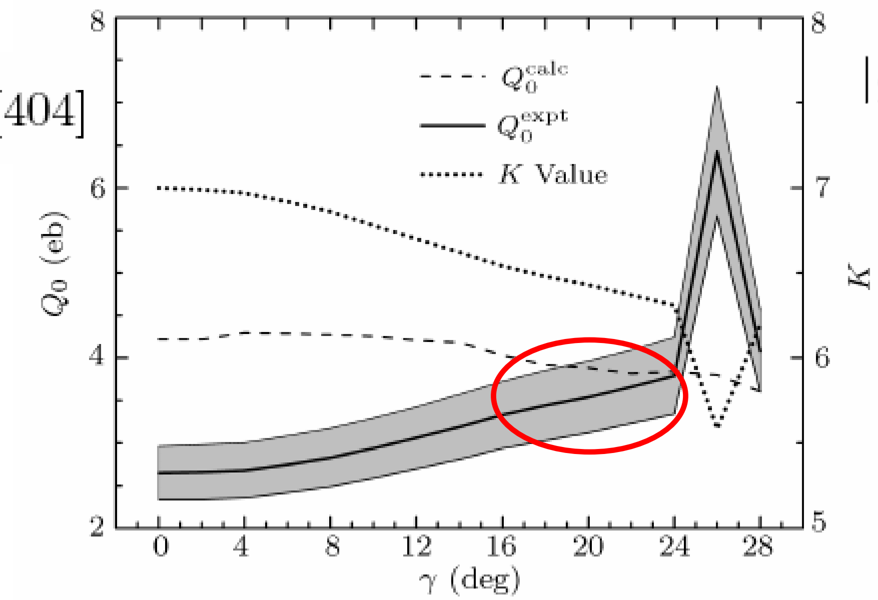
Measured Q

K mixing ⇒ K < 7

K-mixing or decay via gateway states ?

$$\nu\frac{7}{2}^{-}[523]\otimes\nu\frac{7}{2}^{+}[404]$$

130Ce



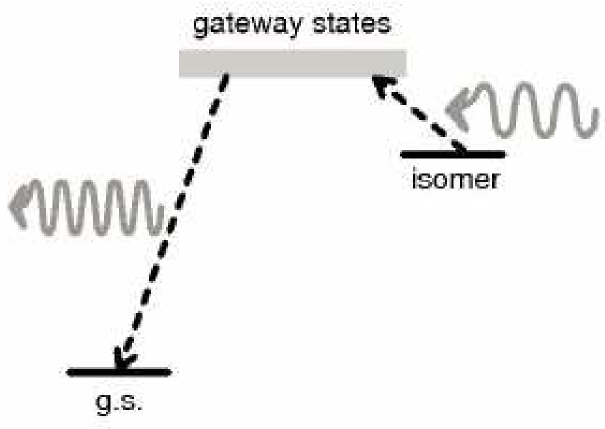
$$|Q|(7^-,{}^{130}\mathrm{Ce}) = 1.77(21)\quad e\,\mathrm{b}$$

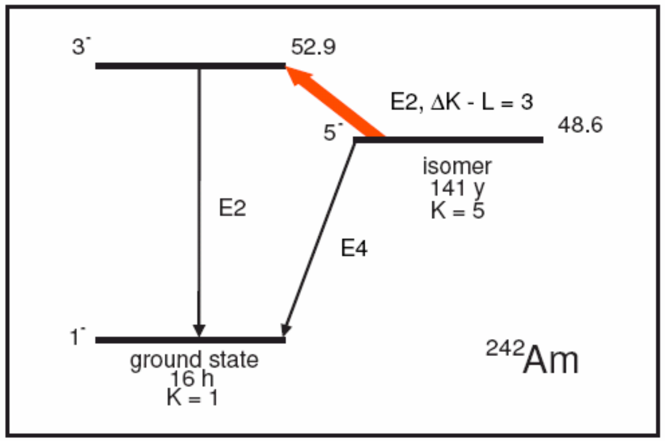
$$Q_0 = Q_s\frac{(2I+3)(I+1)}{3K^2 - I(I+1)}.$$

M.Ionescu-Bujor *et.al*

PRC 60, 024316(1999)

[Y. Sun et al., Phys. Lett. B589 (2004) 83]





IV. Sumary

The configuration-constrained PES calculations predict the properties of nuclear states, including:

1) Deformations

2) Configurations (then spin and parity)

3) Hardness or softness (triaxiality, K mixing)

4) Fission barrier, and then stability (lifetime)

Special thanks to:

Phil Walker

Ramon Wyss

All my students

……

Thank You !