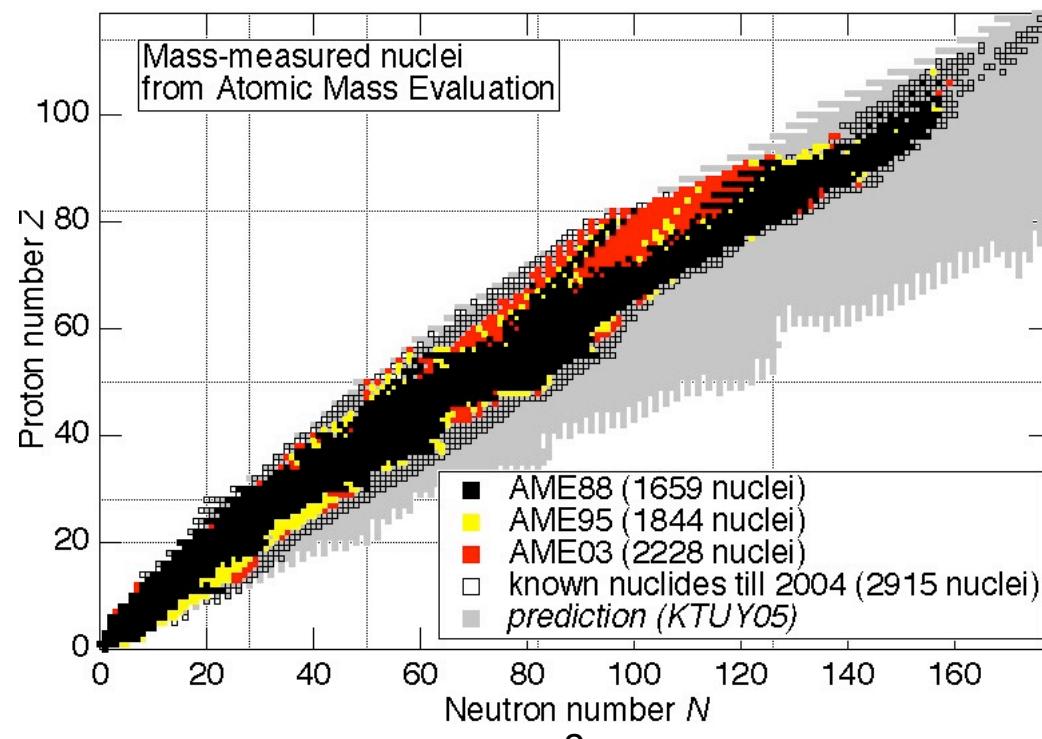
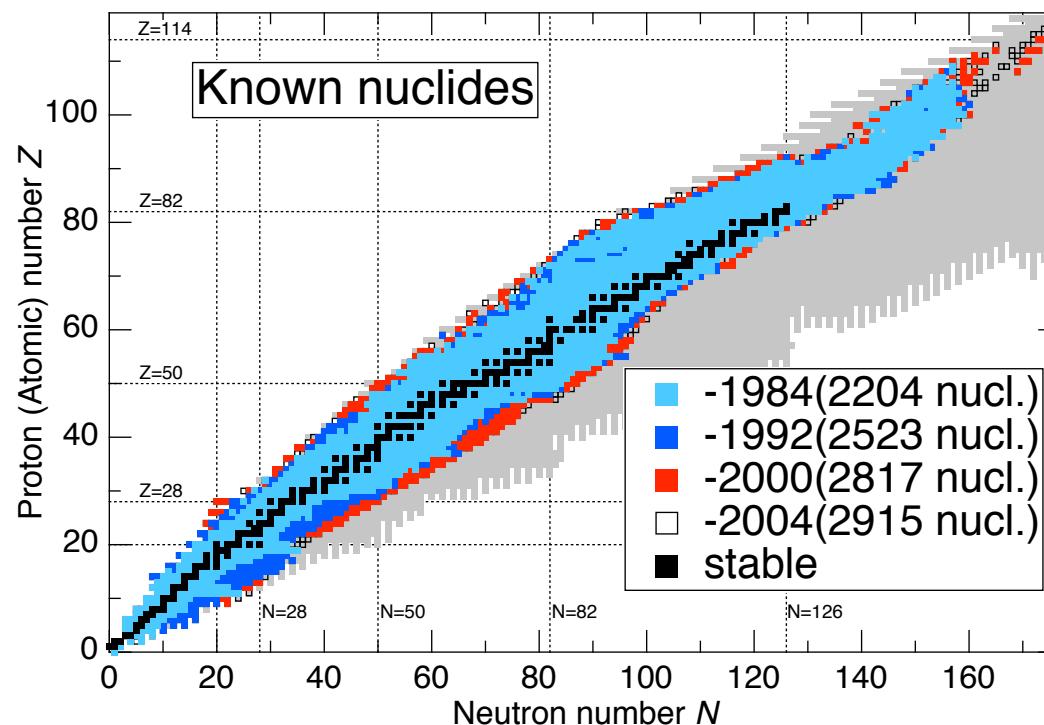


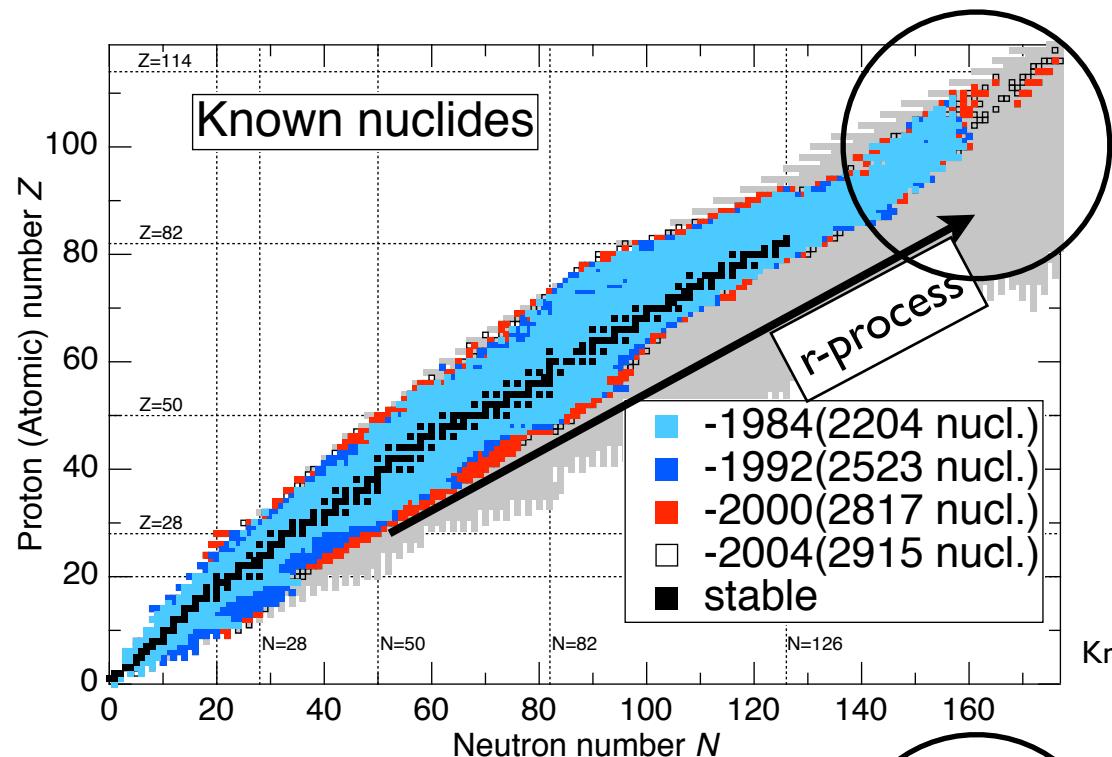
# 原子核質量公式とr-過程元素合成

## Nuclear mass formulae and the r-process nucleosynthesis

Hiroyuki KOURA  
Japan Atomic Energy Agency (JAEA)

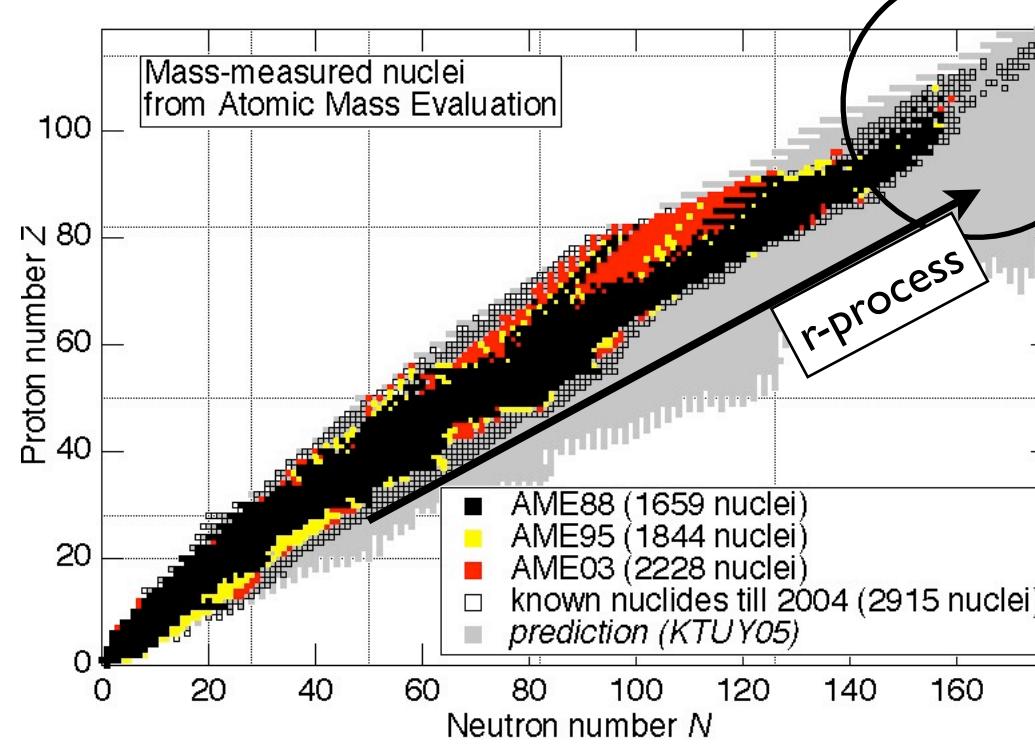
1. Bulk properties of nuclear mass formulae
2. r-process nucleosynthesis
- (3. Effect of  $\beta$ -delayed fission to r-process abundance)





SHE

Known nuclides: taken from Chart of the nuclides by JAERI



SHE

# Importance of nuclear masses for the r-process nucleosynthesis

Neutron-rich nuclei( $A \gtrsim 80$ )=>quite difficult to measure so far.

- $Q_\beta, S_n, \dots \Rightarrow$  require to estimate  $\lambda_\beta, \lambda_n, \dots$
- Estimations of decay modes of  $\alpha, \beta$  and SF =>important in the SHE region
- Nuclear structure (magicity, isomer)=>gives abundance pattern
- mass curvature=> reach 3rd peak (+U,Th) or not
- . . .

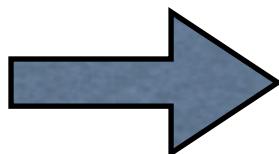
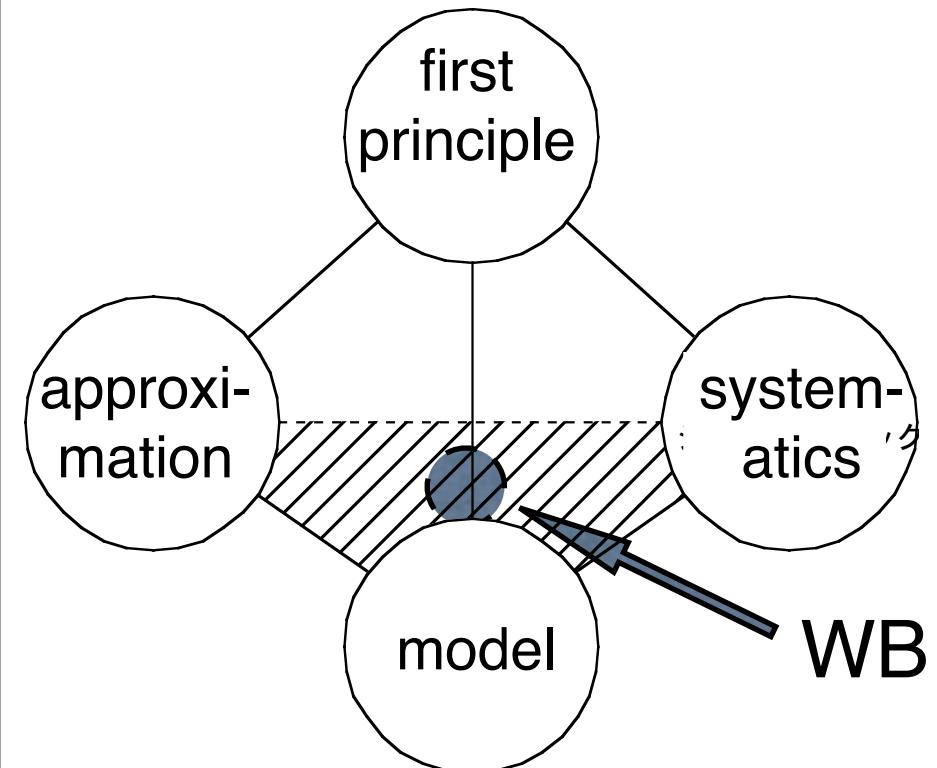
## II. Phenomenological Mass Formulas

- First-principle calculation

(calculation from the realistic nuclear force)

To treat nuclear masses with the first principle is not appropriate way from consideration on properties of nuclear force, many-body force, computational time, and accuracy for the present and in the near future.

Theoretical approaches  
on nuclear masses



Nuclear masses are estimated from various viewpoints for various purposes.

# Systematics • Phenomenology

- **Garvey-Kelson-like mass systematics**

focusing on relation between mass values and  $Z, N$

**Comay-Kelson-Zidon, Jänecke-Masson (1988)**

- **Empirical shell term**

focusing on Bulk part (WB-like)+deviation (Shell term)

**Tachibana-Uno-Yamada-Yamada (1988)**

- **Phenomenological shell model calculation**

Polynomials of particle and hole numbers,  
obliged to assume magic numbers in advance.

**Liran-Zeldes (1976)**

- ...

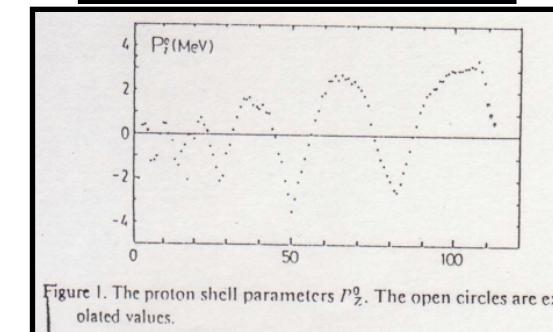
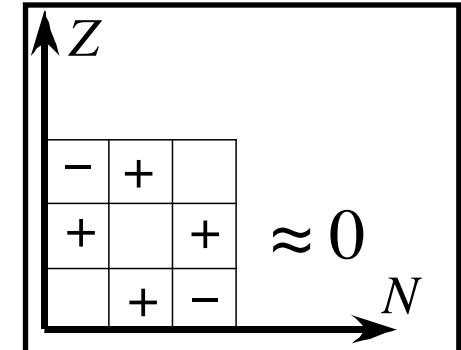
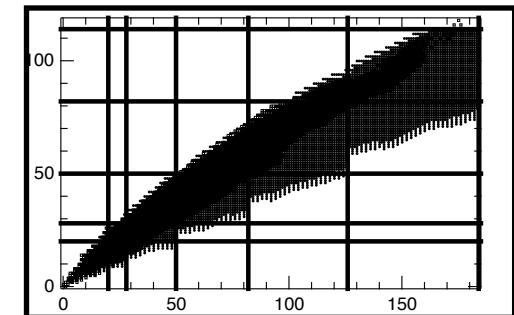


Figure I. The proton shell parameters  $P_z^0$ . The open circles are extrapolated values.



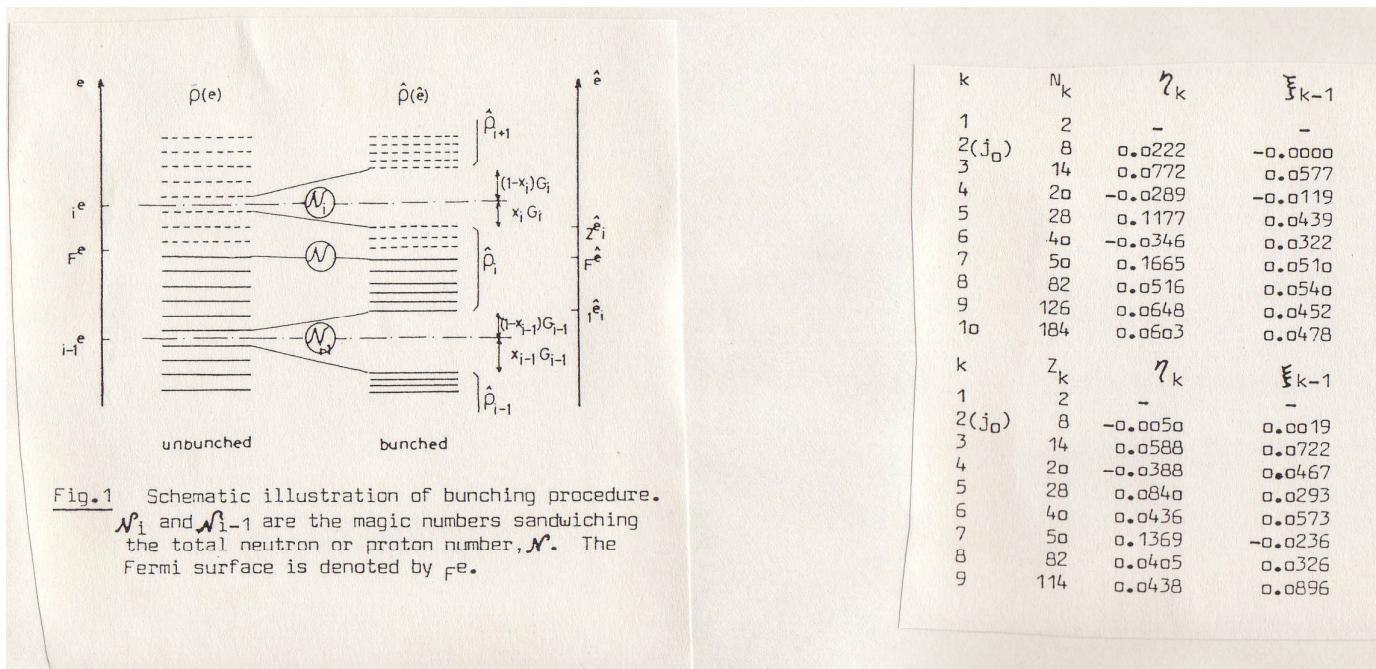
## Properties

- Good reproduction of masses for known nuclei + good prediction for unknown nuclei (quite) near mass-measured nuclides. (300-600 keV)
- No predictable power for superheavy nuclei (next magic number, etc.)
- No deformation is obtained.

# Hilf-Groote-Takahashi(HGT,1976)

## Macroscopic part: deformed liquid-drop (Myers-Swiatecki-type)

## Microscopic part



For the nucleus with  $N_{i-1} < N \leq N_i$  with  $N_i$  and  $N_{i-1}$  being the neutron magic numbers, we have

$$\tilde{M}_n(N, I) = C_n A^{-2/3} [(1-3\bar{\epsilon})(1+\bar{\delta})/(1+I)]^{2/3} \times \\ \times \left[ \tilde{S}_i(N) + \sum_{j=j_0}^{i-1} \tilde{S}_j(N_j) + c_n \right]$$

where

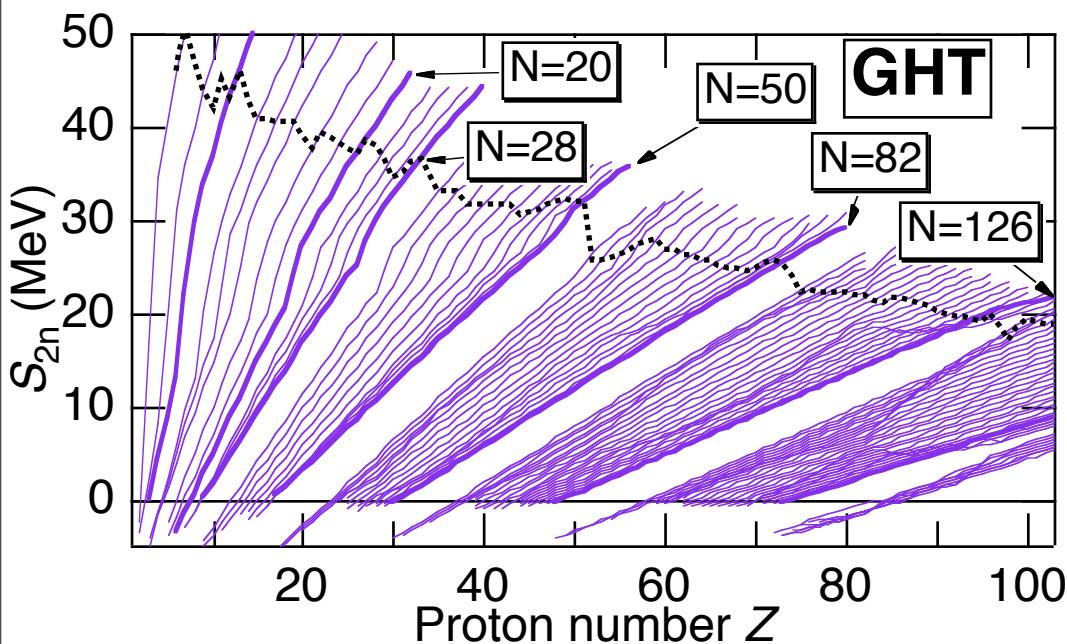
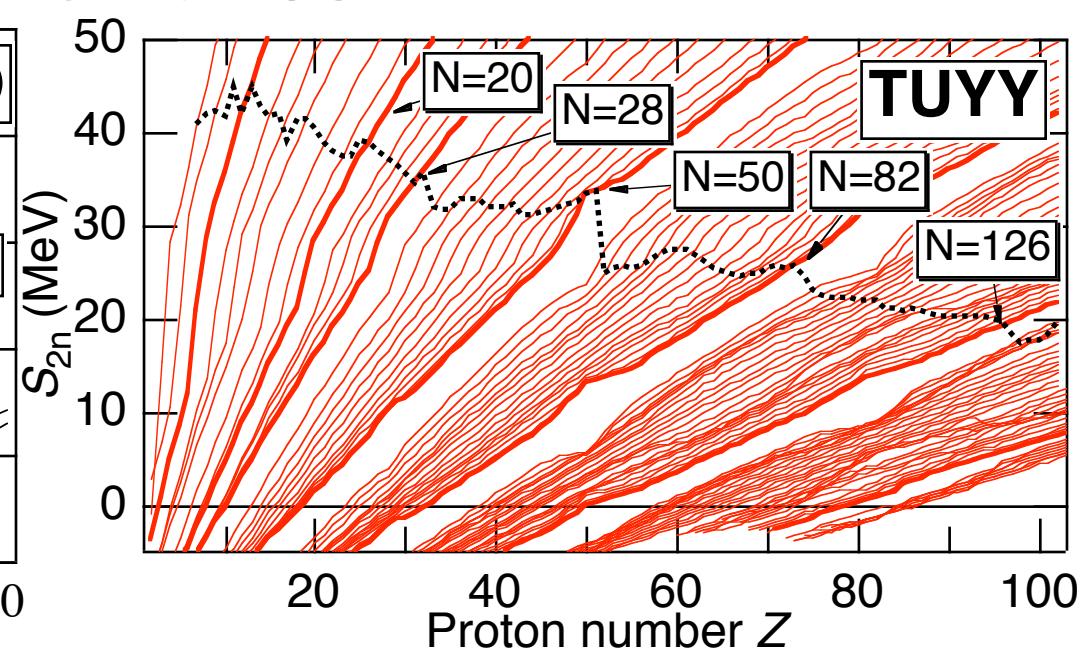
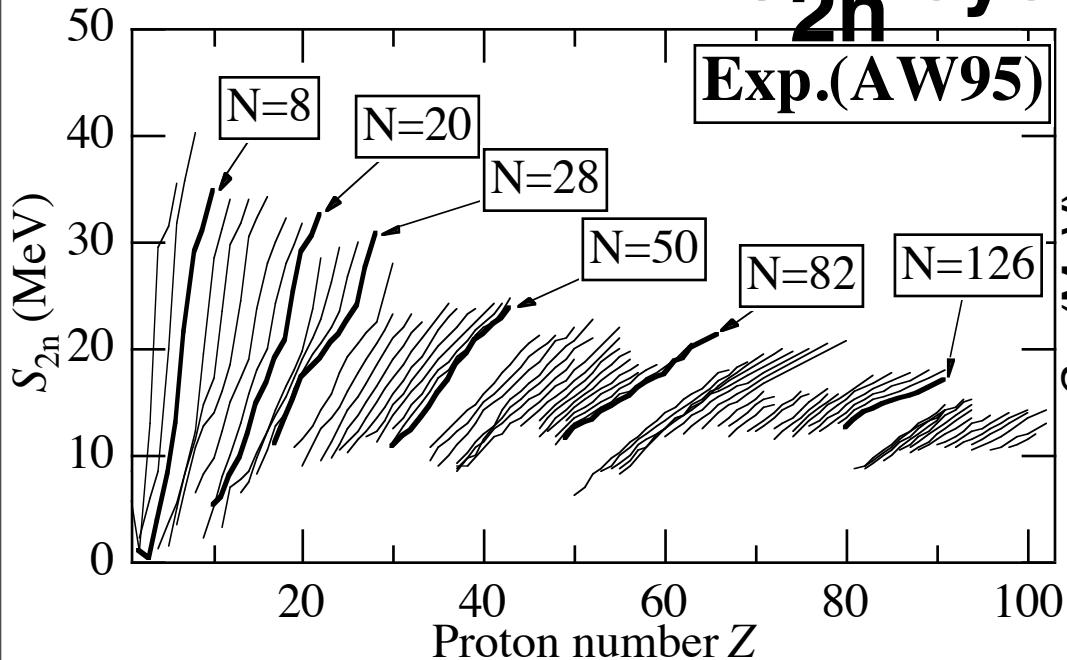
$$\tilde{S}_k(N) = [S_{k-1}^{(-)}(N) \xi_{k-1} - S_k^{(+)}(N) \gamma_k] / (1 - \xi_{k-1} \gamma_k)$$

with

$$S_{k-1}^{(+)}(N) = \frac{2}{5} N^{2/3} (N - N_{k-1}) - \frac{3}{5} N_{k-1} (N^{2/3} - N_{k-1}^{2/3}),$$

$$S_k^{(-)}(N) = \frac{2}{5} N^{2/3} (N_k - N) + \frac{3}{5} N_k (N^{2/3} - N_{k-1}^{2/3}) \\ - \frac{2}{5} N_{k-1} (N_k - N_{k-1}).$$

# $S_{2n}$ systematics



# Mass Model, Approximation

Recent mass formulas:

- are designed for nuclei **with  $Z, N=8$  to  $^{310}\text{[126]}_{184}$  or more**
- have the RMS dev. from exp. masses. **of 600-800 keV**
- give **deformation parameters  $\beta_2, \beta_4\dots$**  and **fission barriers**

- **Density functional theory** <- recent project

- **Hartree-Fock method with Skyrme force**

by M.Stoitsov, etc.

Strong short-range force =>  $\delta$ -function => HF calc.  
[ETFSI](#) (1995), [HFBCS](#) (2001), [HFB](#) (2002-)

- **Liquid-drop model**

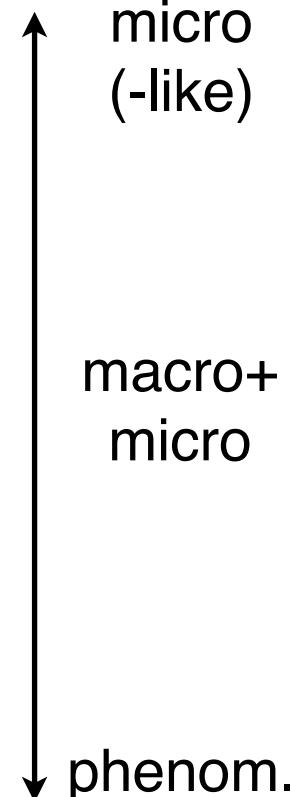
by S.Goriely

Deformed liquid-drop part+Micro. (folded Yukawa)  
[FRDM](#) (1995), [FRLDM](#) (2002),

- **Mass formula with spherical-basis shell term**

by P.Möller

Phenom. gross (WB-like)+spherical-basis shell part  
[KUTY](#) (2000), [KTUY](#) (2005) Koura, Uno, Tachibana, Yamada



### III. KTUY (KUTY) mass formula

(Koura, Uno, Tachibana, Yamada, NPA674, 2000)  
 (Koura, Tachibana, Uno, Yamada, PTP113, 2005)

$$M(Z, N) = M_{\text{gross}}(Z, N) + M_{\text{eo}}(Z, N) + M_{\text{shell}}(Z, N)$$

$M_{\text{gross}}(Z, N)$ : gross term

$$M_{\text{gross}}(Z, N) = M_H Z + M_n N + a(A) A + b(A) |N - Z| + c(A)(N - Z)^2/A + E_C(Z, N) - k_{\text{el}} Z^{2.39}$$

$$\left\{ \begin{array}{l} a(A) = a_1 + a_2 A^{-1/3} + a_3 A^{-2/3} + a_4 (A + \alpha_a)^{-1} \\ b(A) = \qquad \qquad \qquad + b_4 (A + \alpha_b)^{-1} \\ c(A) = c_1 + c_2 A^{-1/3} + c_3 A^{-2/3} + c_4 (A + \alpha_c)^{-1} \\ E_C = a_C(Z, N) \frac{Z^2}{A^{1/3}} \left[ 1 - 0.76 C_x \frac{1}{Z^{2/3}} \right] \end{array} \right.$$

← Volume, Surface, etc...  
 ← Wigner term  
 ← Asymmetry term  
 ← Coulomb with an exchange term

$M_{\text{shell}}(Z, N)$ : shell term

Spherical nuclei

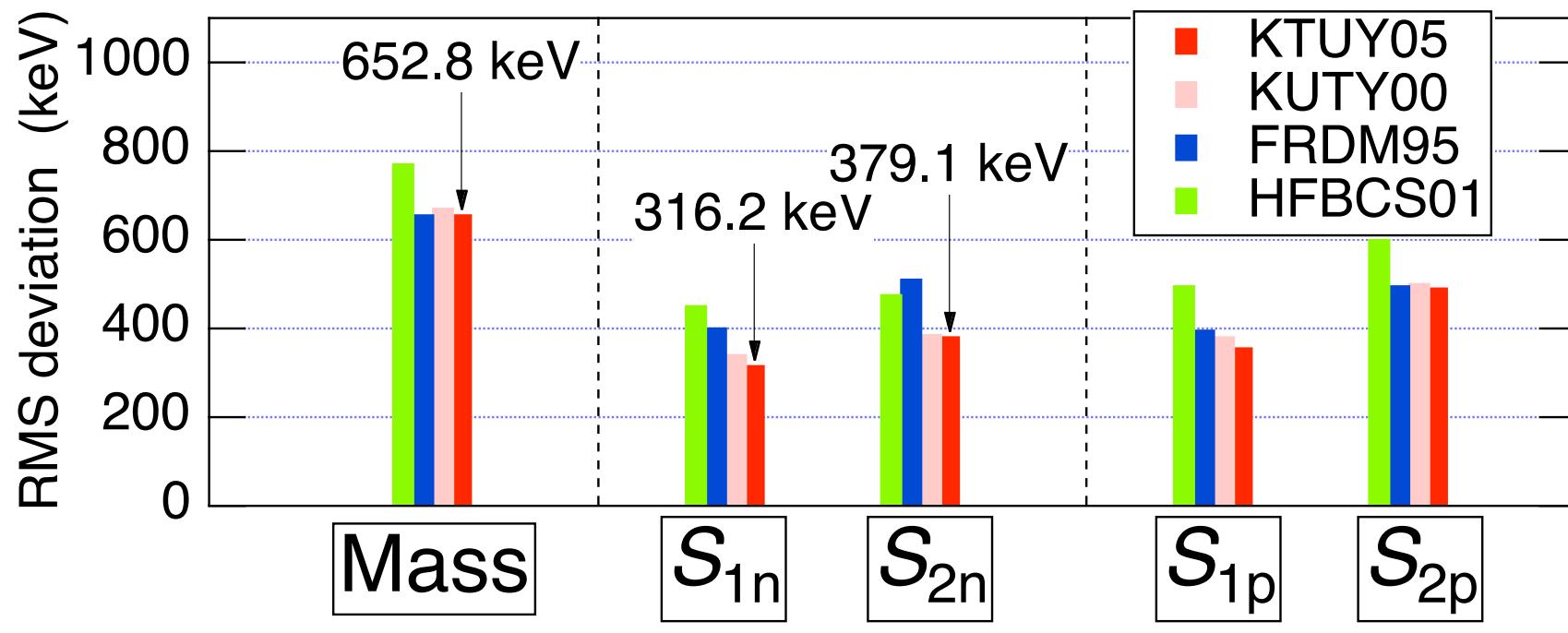
Calculated from **Spherical single-particle potential** for any nuclei (includes the BCS paring, reduction)

Deformed nuclei (Spherical-basis condieration)

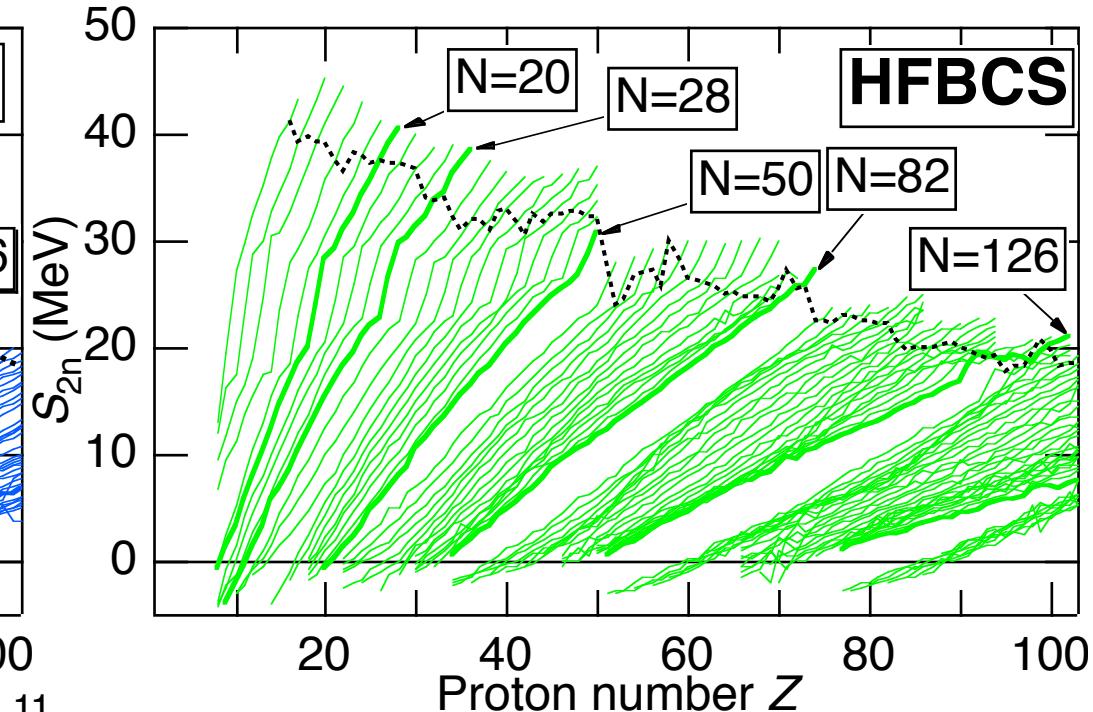
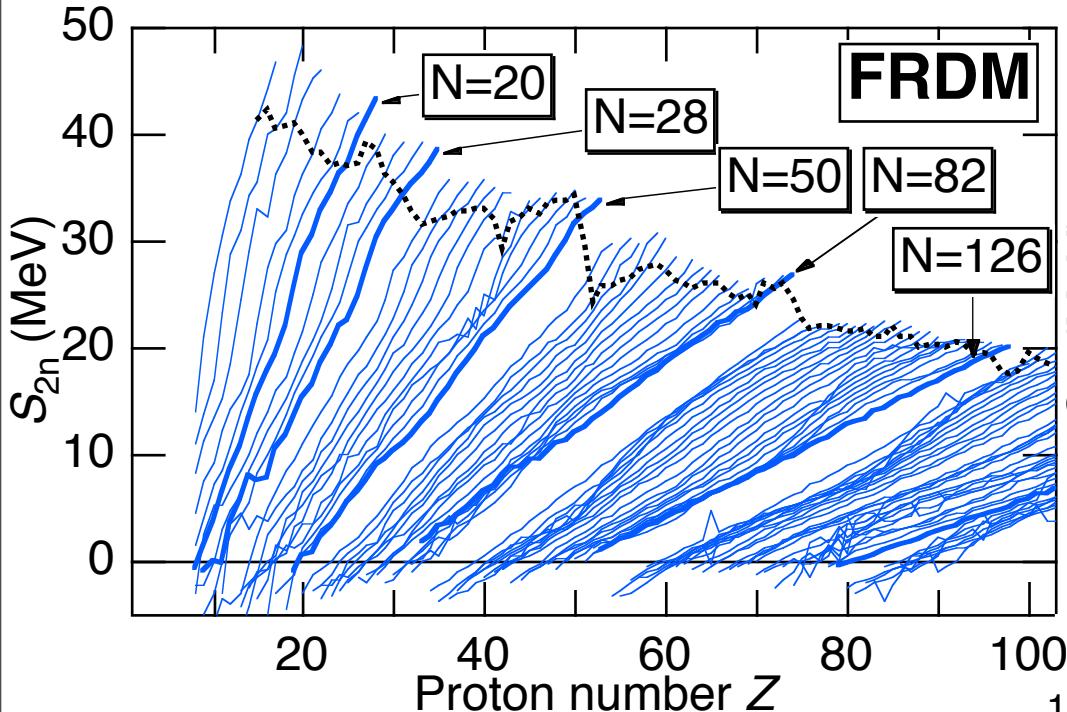
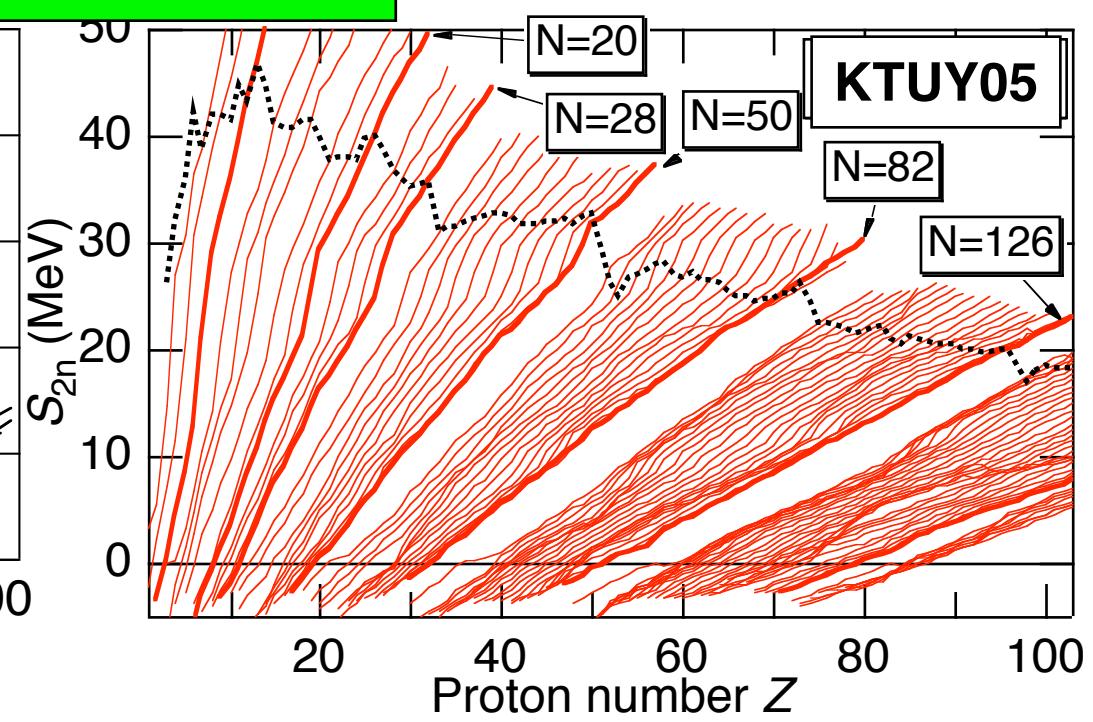
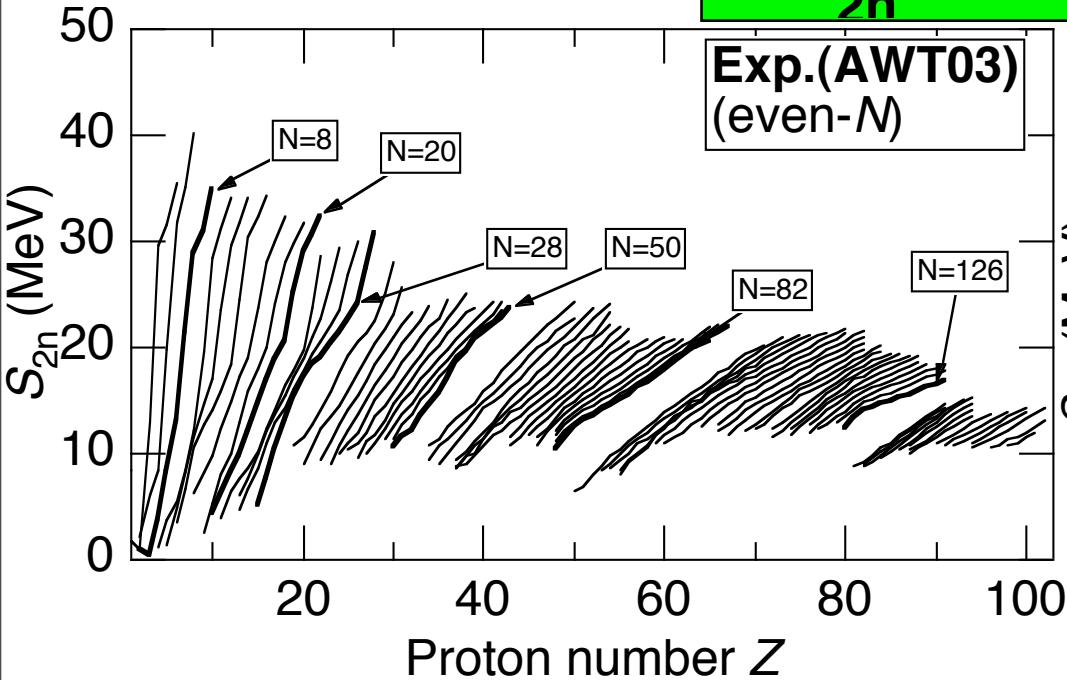
Obtained by **an appropriate mixture** of the above spherical shell energies + liquid-drop deform. energies

# RMS dev. of masses and separation energies from Exp.

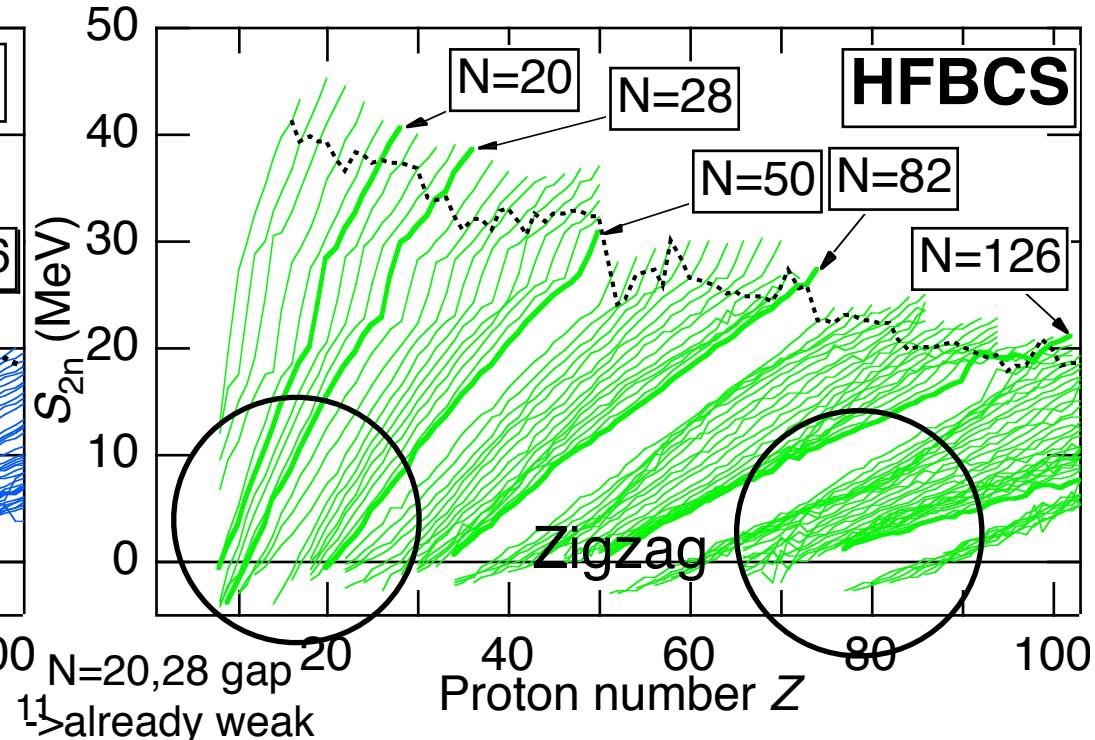
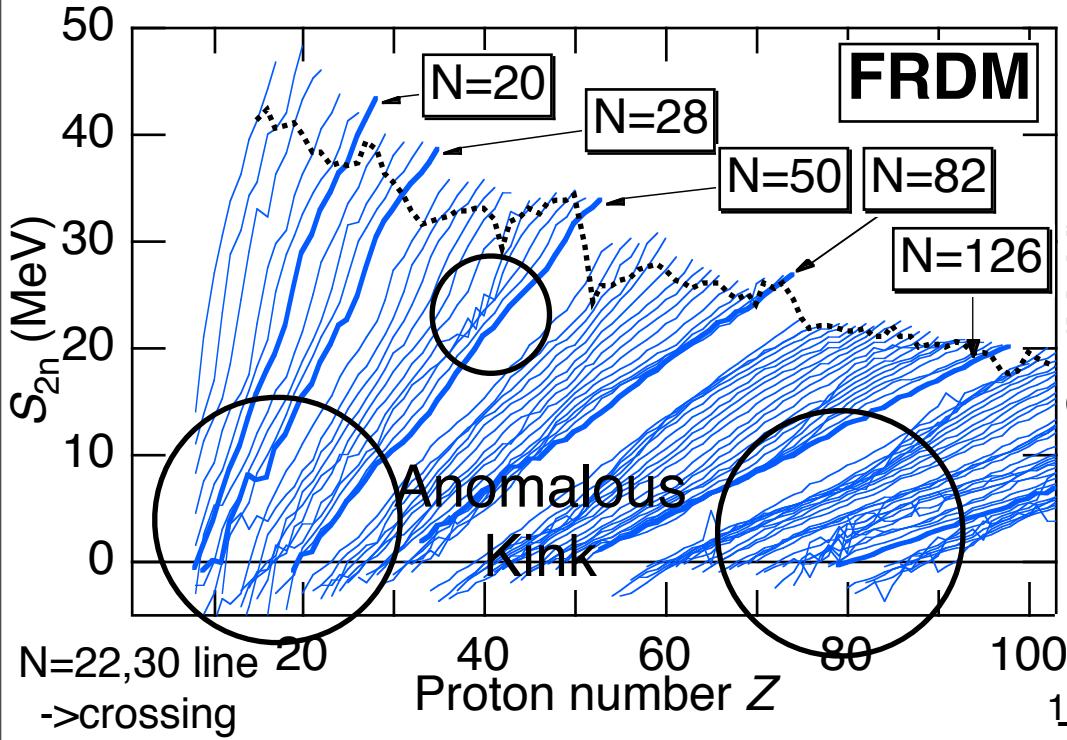
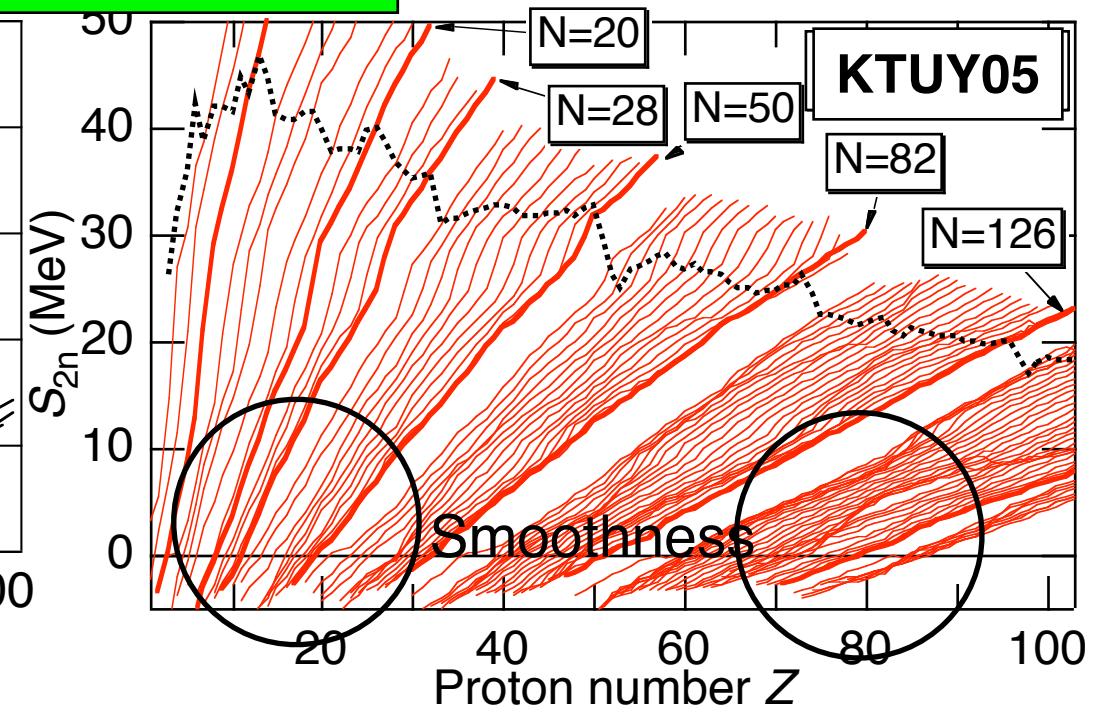
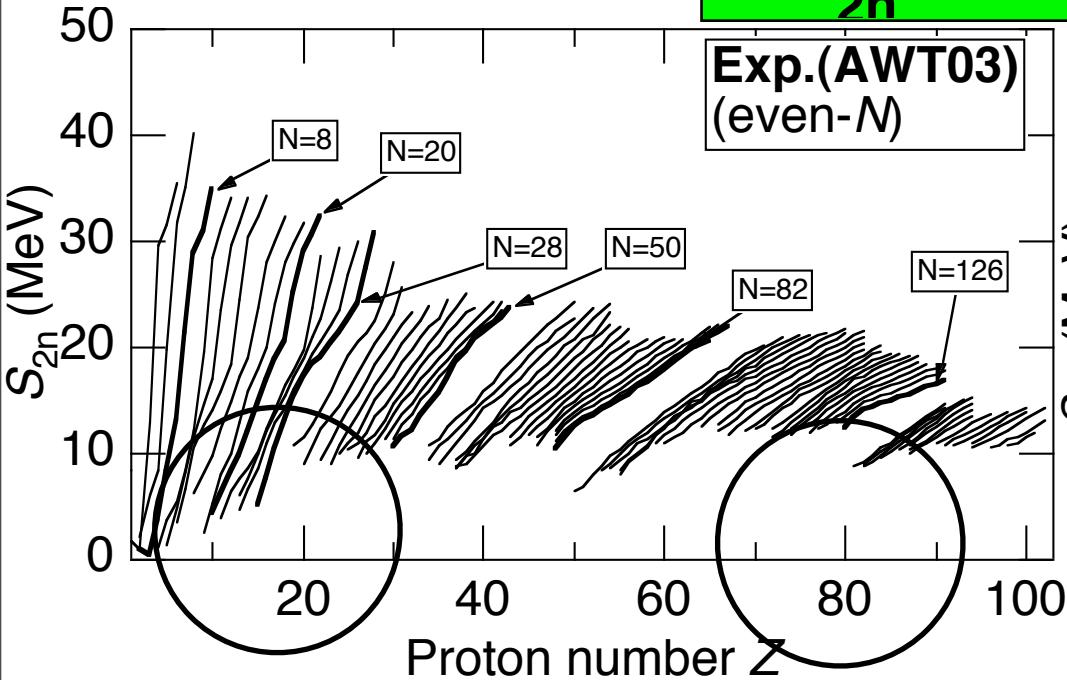
Mass formula	Masses	Neutron sep.		Proton sep.	
		$S_n$	$S_{2n}$	$S_p$	$S_{2p}$
$Z, N \geq 2$	(2219 nuclei)	(2054 nuclei)	(1997 nuclei)	(2016 nuclei)	(1897 nuclei)
<b>KTUY03(05)</b>	<b>666.7 keV</b>	<b>352.9 keV</b>	<b>442.0 keV</b>	<b>389.9 keV</b>	<b>532.2 keV</b>
<b>KUTY(00)</b>	<b>689.8 keV</b>	<b>389.1 keV</b>	<b>462.4 keV</b>	<b>473.6 keV</b>	<b>558.2 keV</b>
$Z, N \geq 8$	(2149 nuclei)	(1988 nuclei)	(1937 nuclei)	(1948 nuclei)	(1835 nuclei)
<b>KTUY03(05)</b>	<b>652.8 keV</b>	<b>316.2 keV</b>	<b>379.1 keV</b>	<b>353.0 keV</b>	<b>490.1 keV</b>
<b>KUTY(00)</b>	<b>670.7 keV</b>	<b>339.5 keV</b>	<b>386.5 keV</b>	<b>379.2 keV</b>	<b>499.7 keV</b>
FRDM(95)	655.5 keV	399.3 keV	511.7 keV	395.2 keV	493.6 keV
HFBCS-1(01)	770.7 keV	451.8 keV	477.3 keV	496.5 keV	603.8 keV



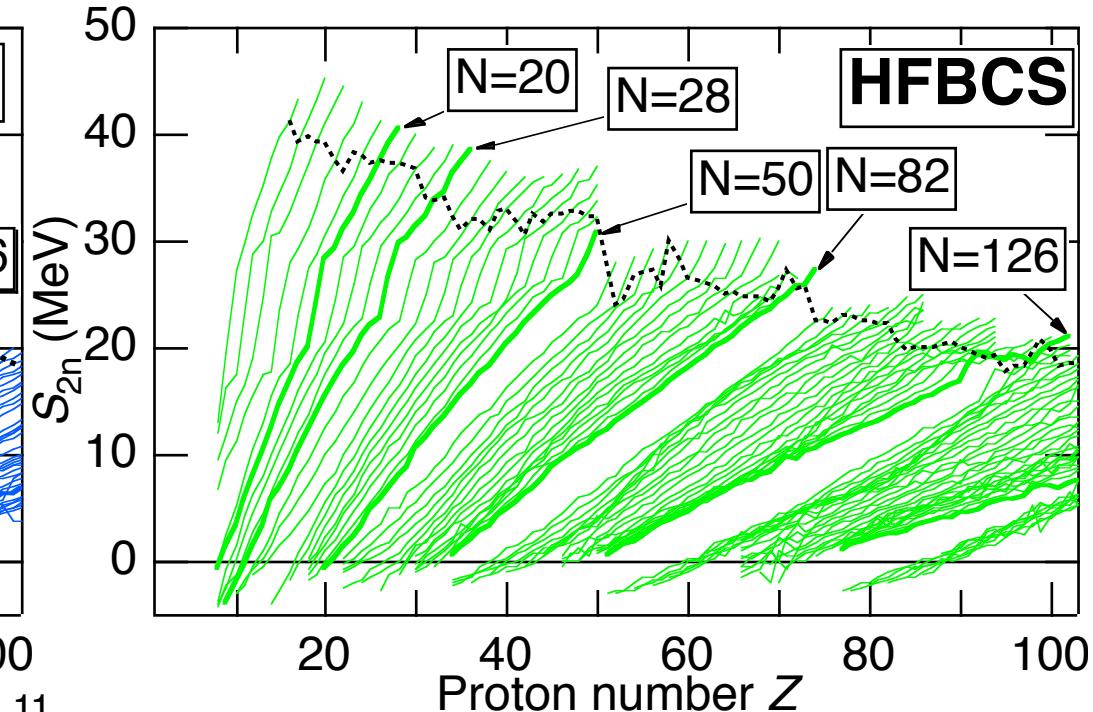
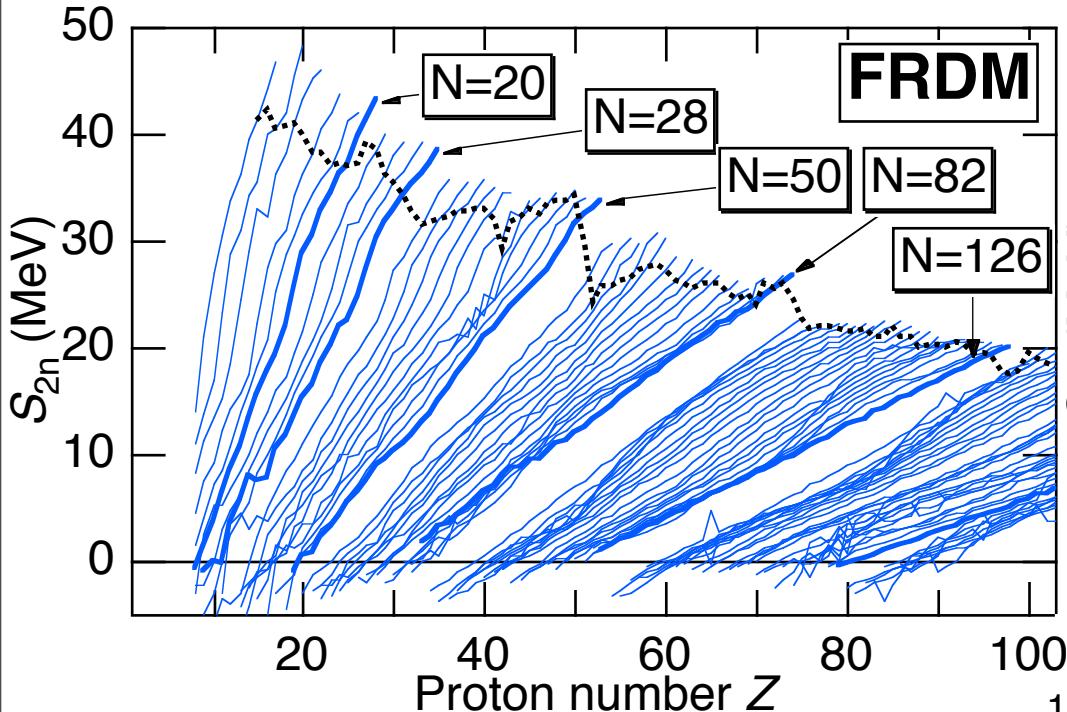
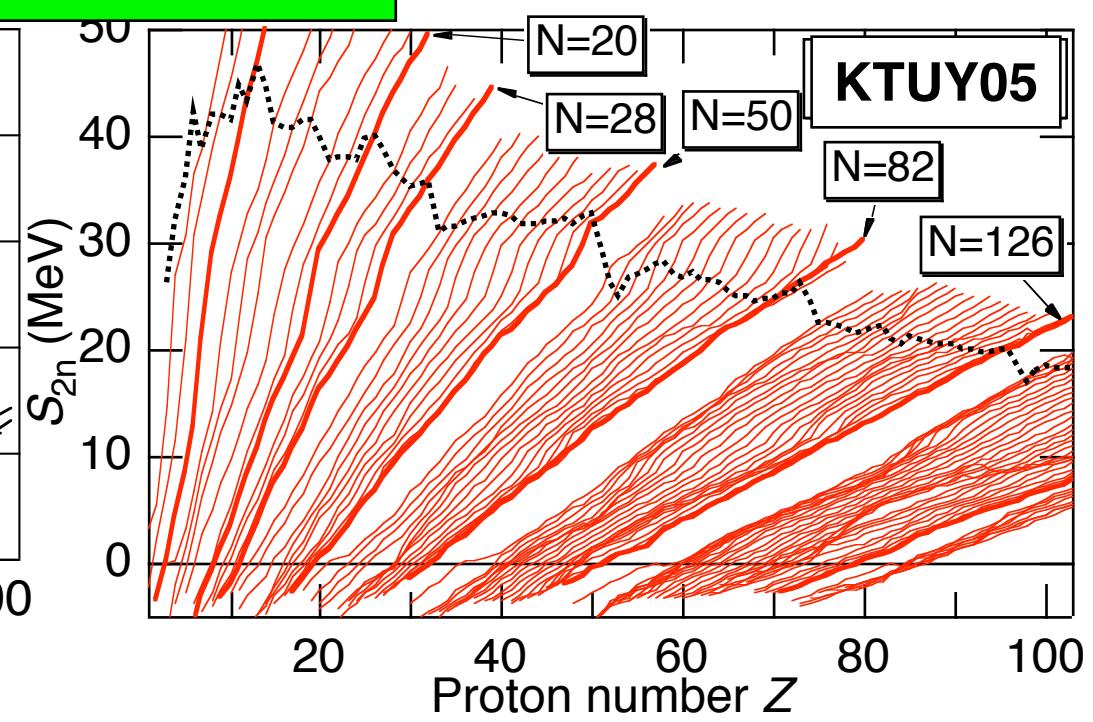
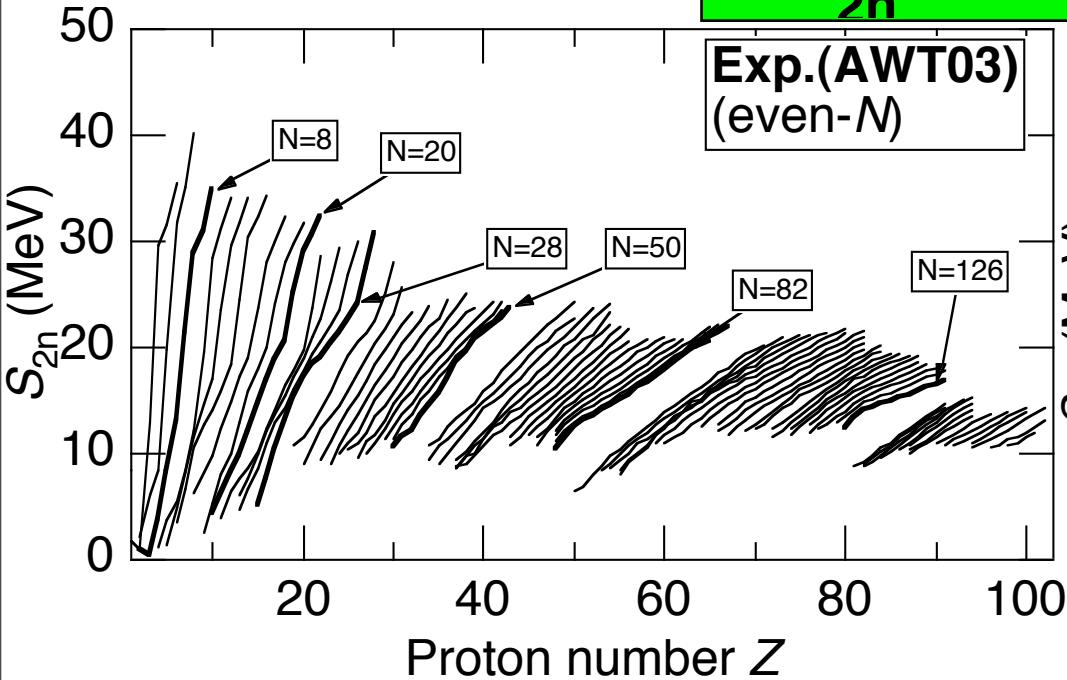
# $S_{2n}$ systematics



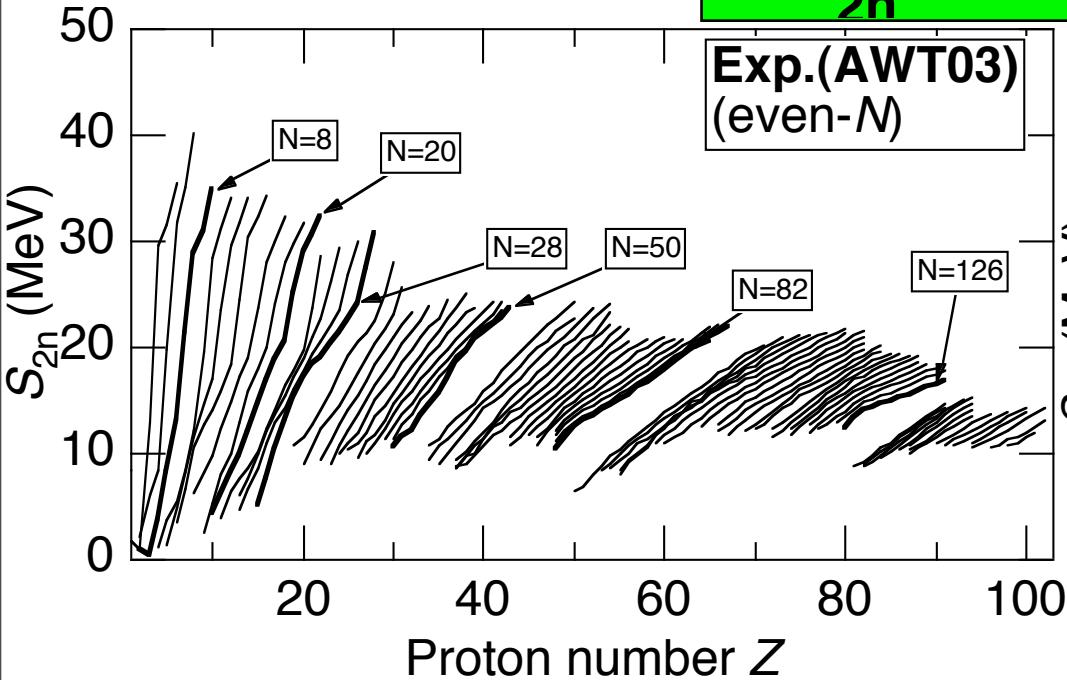
# $S_{2n}$ systematics



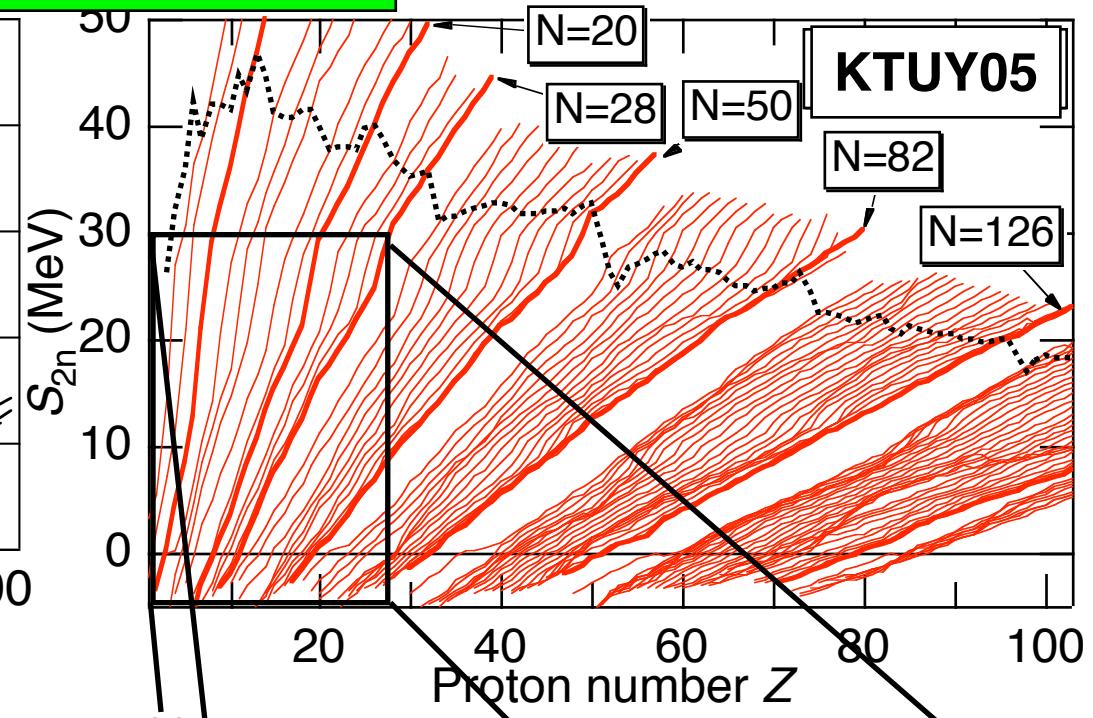
# $S_{2n}$ systematics



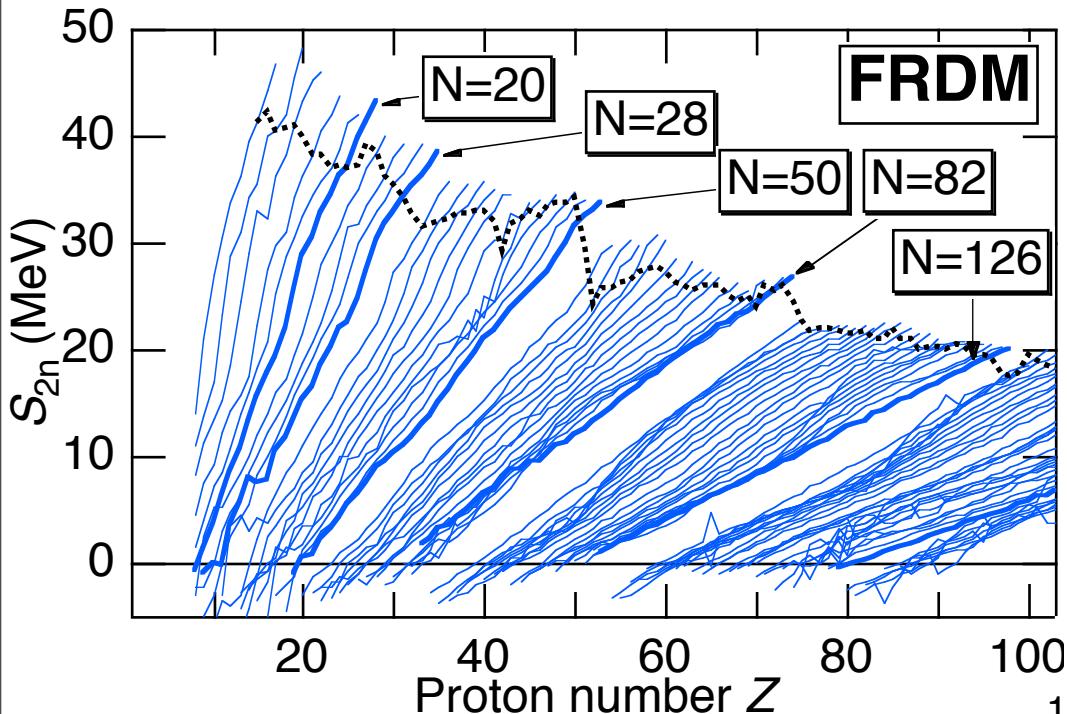
# $S_{2n}$ systematics



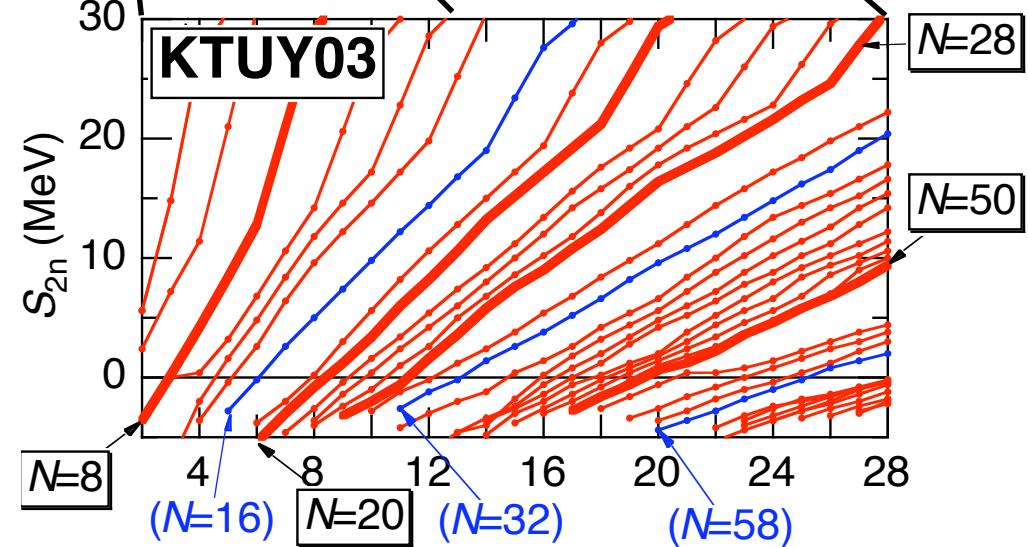
Exp.(AWT03)  
(even- $N$ )



KTUY05

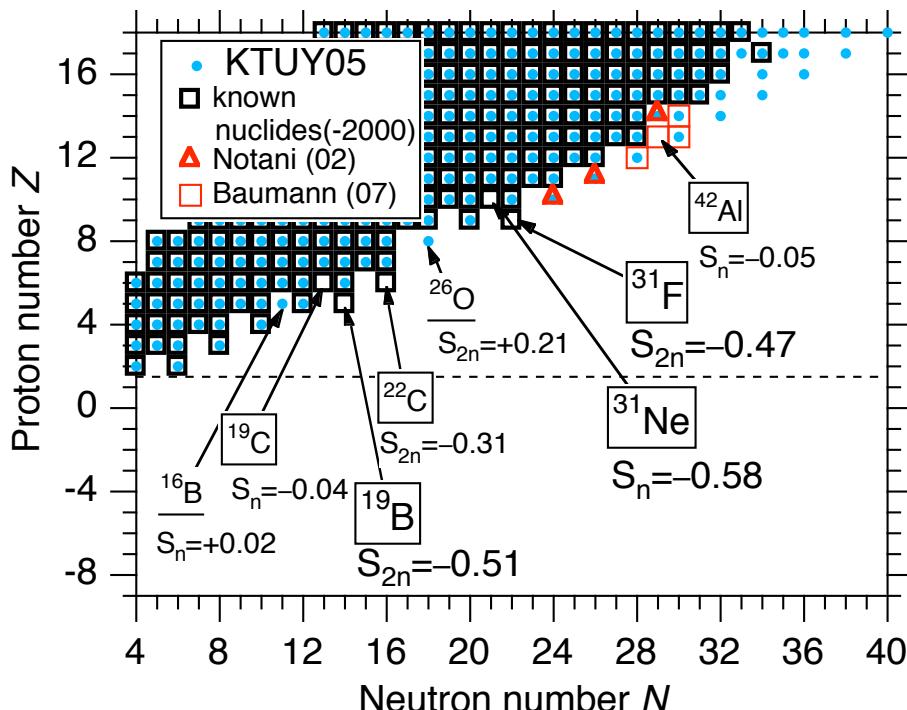


FRDM



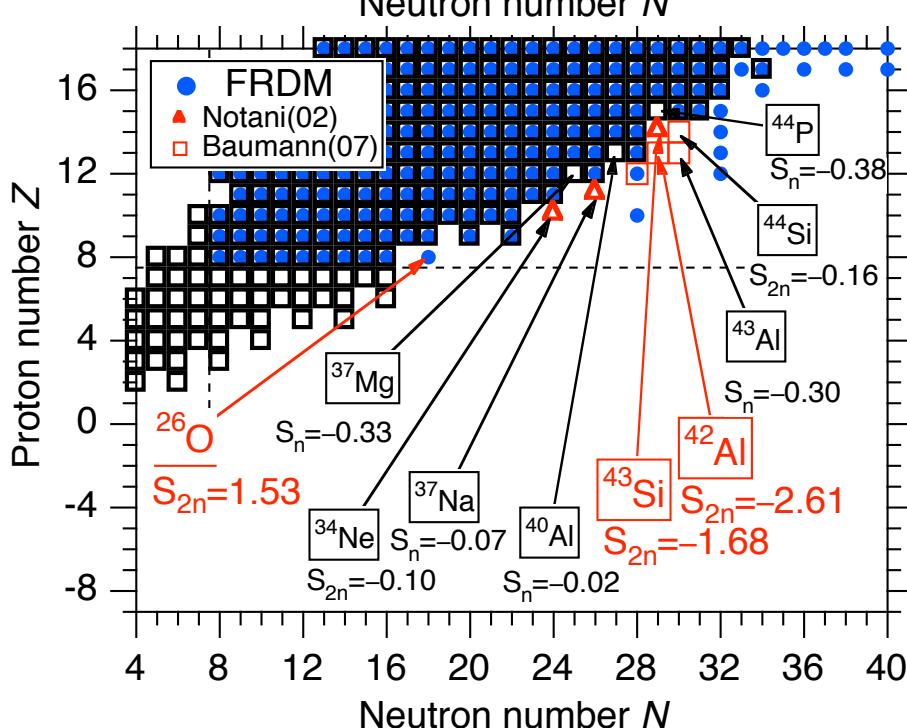
$N=14, 20, 28, 50$  gap  
->decreasing

# Light neutron-drip line



RMS dev. : 0.35MeV for  $S_n$   
0.44MeV for  $S_{2n}$

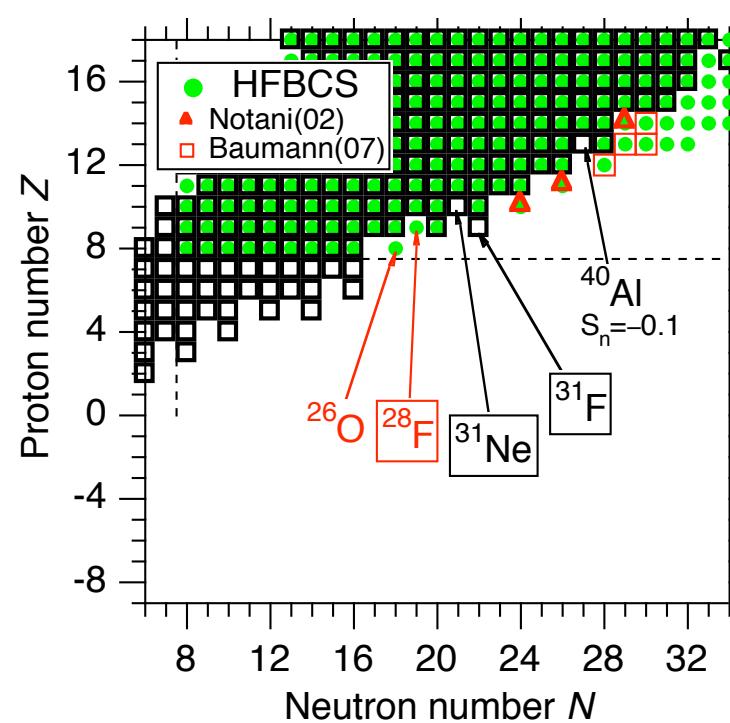
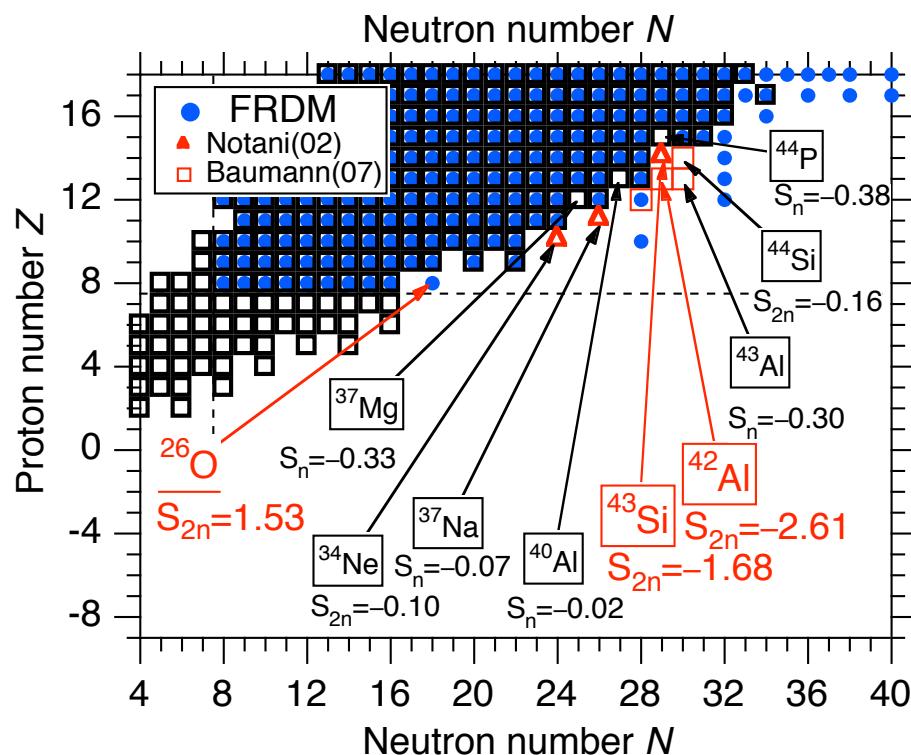
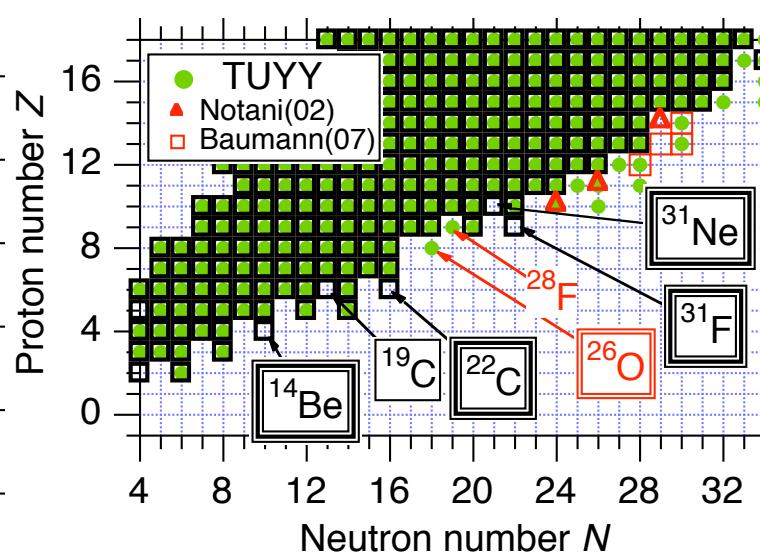
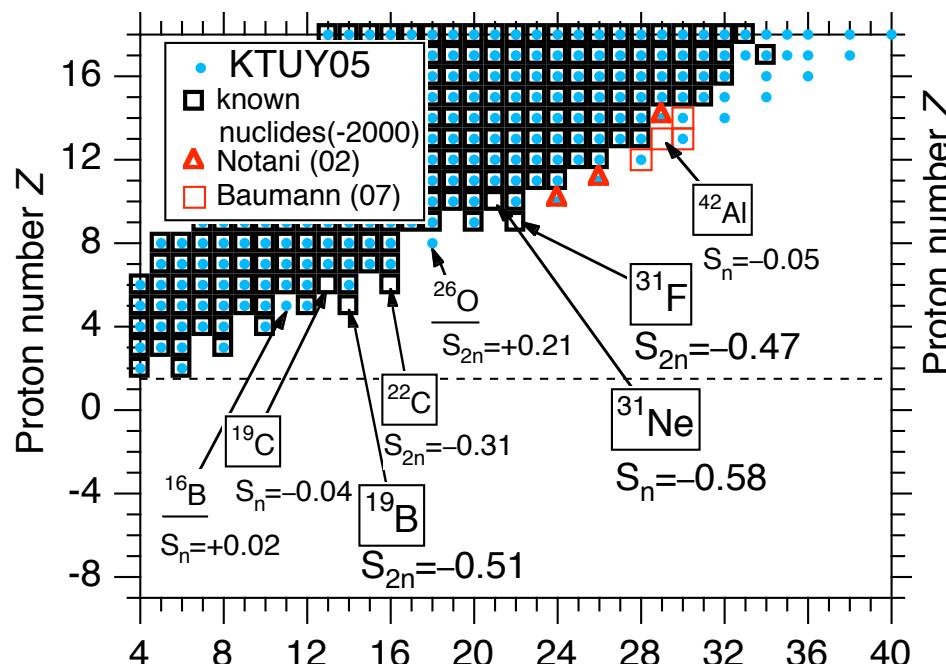
Fail to predict 8 nuclei whether bound/unbound  
All the n-sep. energy of these nuclei are within 1.5 times of RMS dev.



RMS dev. : 0.40MeV for  $S_n$   
0.51MeV for  $S_{2n}$

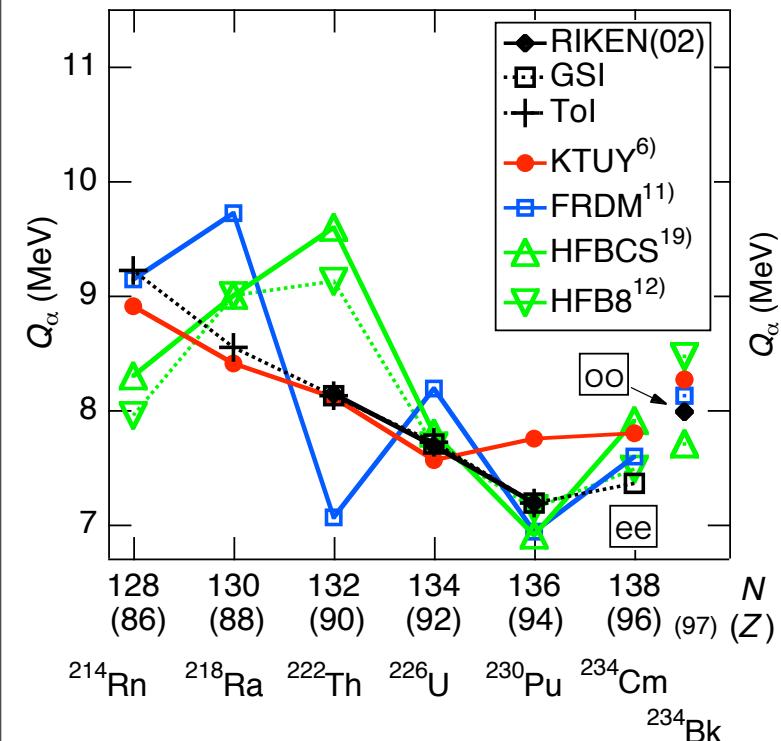
Fail to predict 10 nuclei whether bound/unbound  
The n-sep. energy of the most nuclei considered  
are within 1.5 times of RMS dev, while  
those of three nuclei,  $^{26}\text{O}$ ,  $^{43}\text{Si}$ ,  $^{42}\text{Al}$ , exceed 3.0 times of its RMS dev.

# Light neutron-drip line



# $\alpha$ -decay Q-values of heavy and superheavy nuclei

related to  $^{234}\text{Bk}$

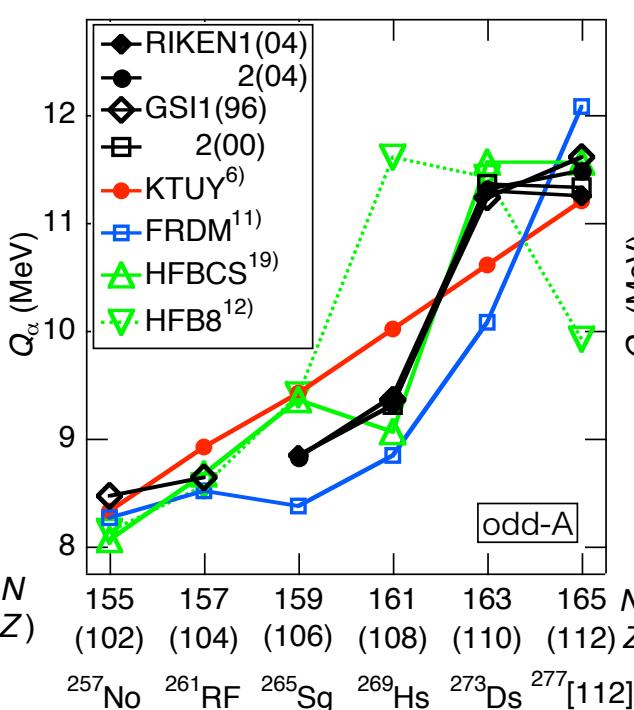


Exp.: gradually decreasing to  $N=136$

KTUY	O or $\Delta$
FRDM	X
HFBCS	X
HFB8	X

Black mark: exp. data

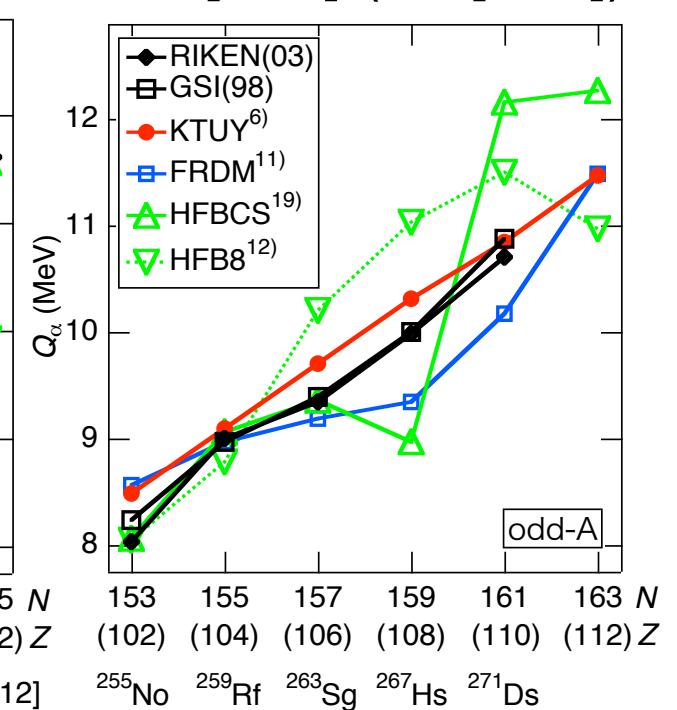
$^{277}[112]$



Exp.: steep increasing at  $N=162$   
suppressed at  $N=164$

KTUY	X
FRDM	$\Delta$
HFBCS	O
HFB8	X

$^{271}[110]$  ( $^{275}[112]$ )



Exp.: gradually increasing

KTUY	O
FRDM	$\Delta$
HFBCS	X
HFB8	X or $\Delta$

\*Measured  $Q_\alpha$  of odd- $A$  nuclei is not surely represented the g.s.-to g.s. decay.

# R-process nucleosynthesis

-Check the mass formulas as astrophysical data-

- Canonical model

Steady flow + Waiting point Approximation

Neutron-number density ( $N_n$ ) and temperature ( $T_9$ ) are constants  
( $n,\gamma$ )-( $\gamma,n$ ) equilibrium is established over an irradiation time  $\tau$

- Saha equation *(gives the r-process path)*

$$\log \frac{Y(Z, A+1)}{Y(Z, A)} = \log \frac{G(Z, A+1)}{G(Z, A)} - 34.075 + \log N_n + 1.5 \log \left( \frac{A}{A+1} T_9 \right) + \frac{5.04}{T_9} S_n(Z, A+1)$$



$$S_{2n}(Z, A+2)/2 \leq S_a^0 \equiv (34.075 - \log N_n + 1.5 \log T_9) T_9 / 5.04 \leq S_{2n}(Z, A)/2$$

$S_{2n}$ : 2-neutron separation energy

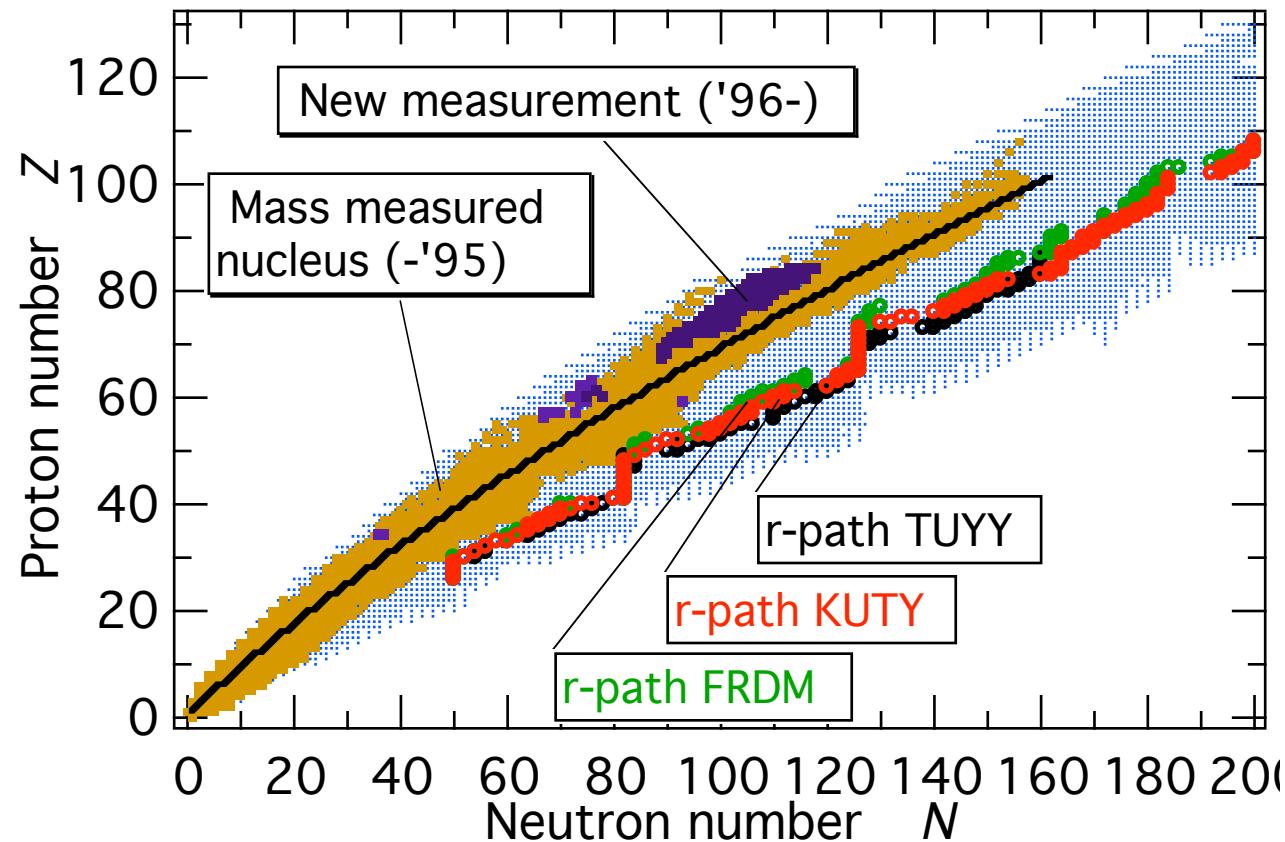
- Time evolution

$$dY/dt = -\lambda_Z Y_Z(t) + \lambda_{Z-1} Y_{Z-1}(t)$$

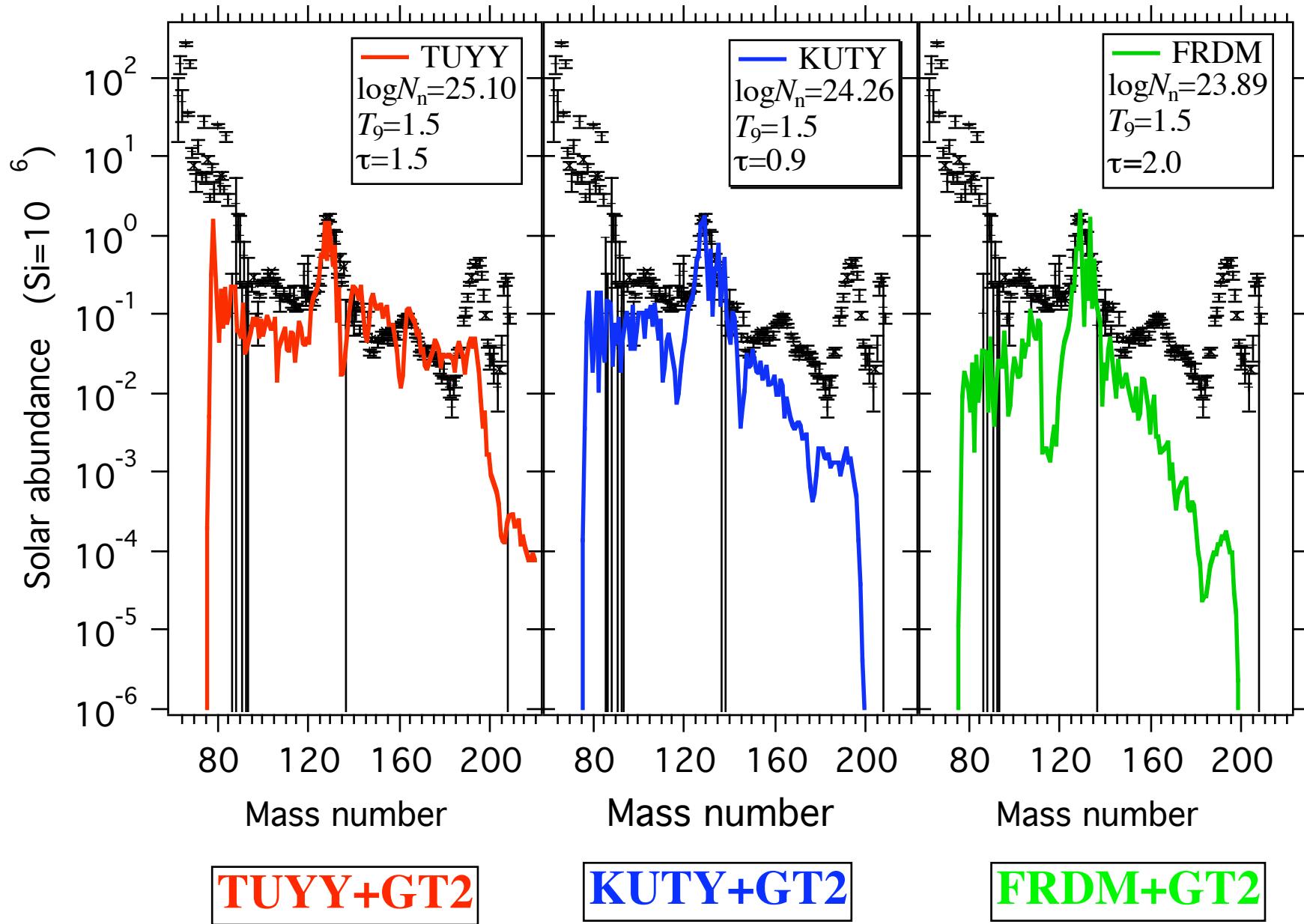
$Y_Z$ : abundance,  $\lambda_Z$ :  $\beta$ -decay constant (gross theory 2nd)

$N_n, T_9, \tau$ : chosen to reproduce the abundance peak at  $A=130$  (obs.)

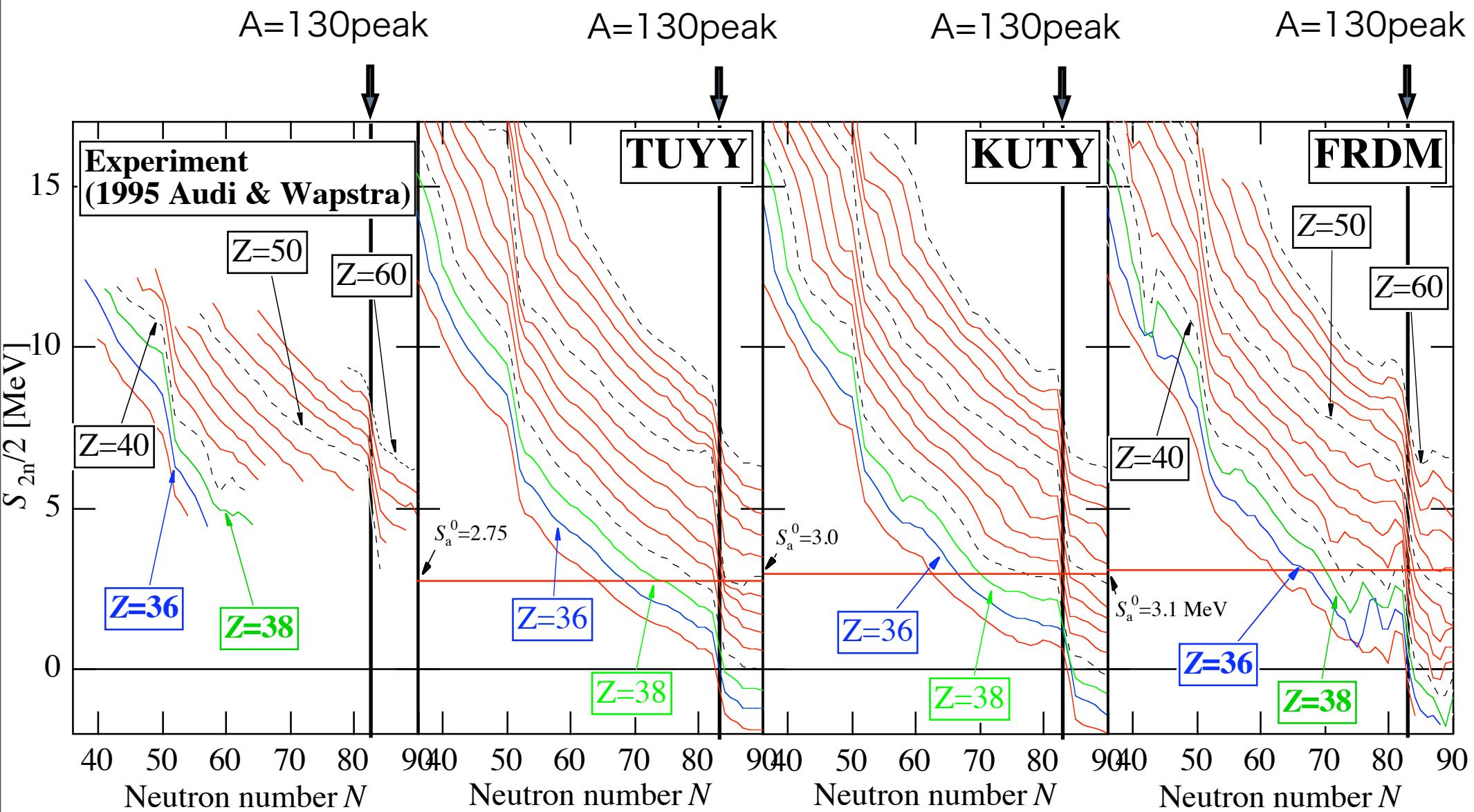
$S_{2n}, Q_\beta$ : estimated from mass formulas (TUYY, KUTY, FRDM)



$+$   $N_r = N(\text{Solar abund.}) - N_s$   
 $\times$   $N_r$  r-only nuclei



# $S_{2n}$ systematics



Experiment

TUYY

KUTY

FRDM

# $S_{2n}$ systematics

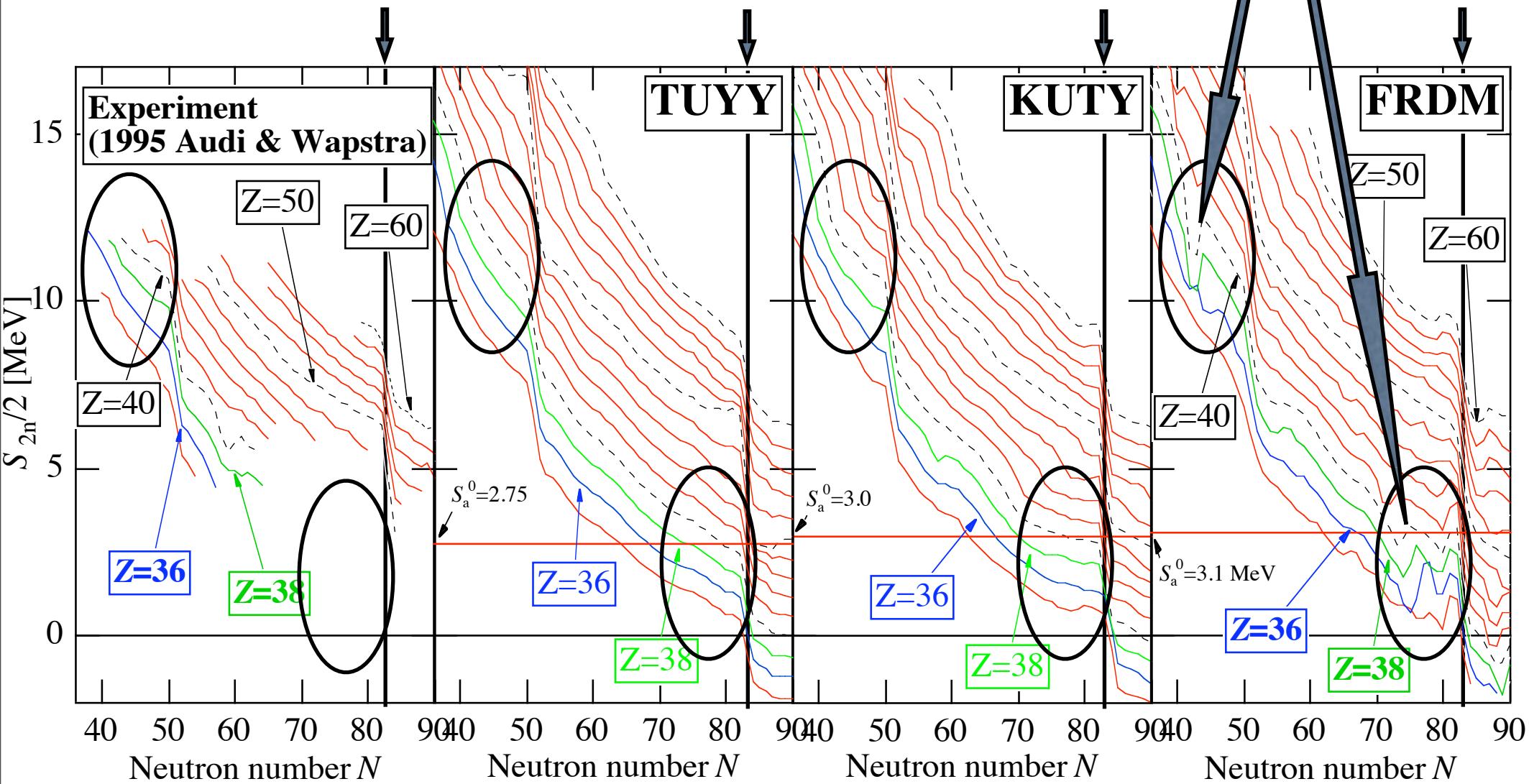
Kink

A=130peak

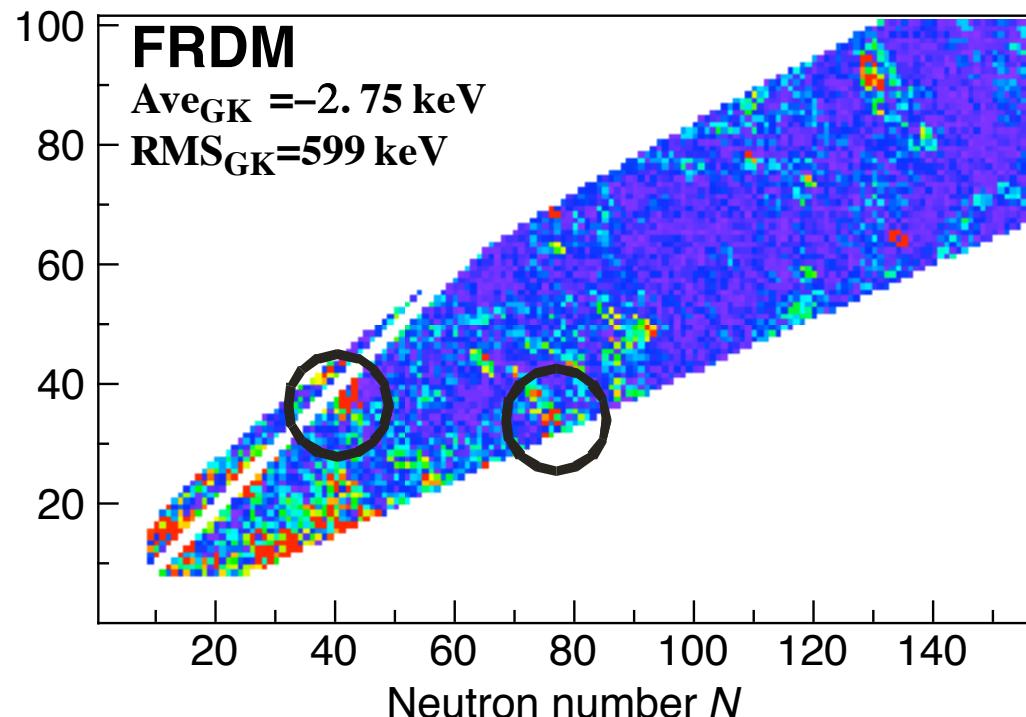
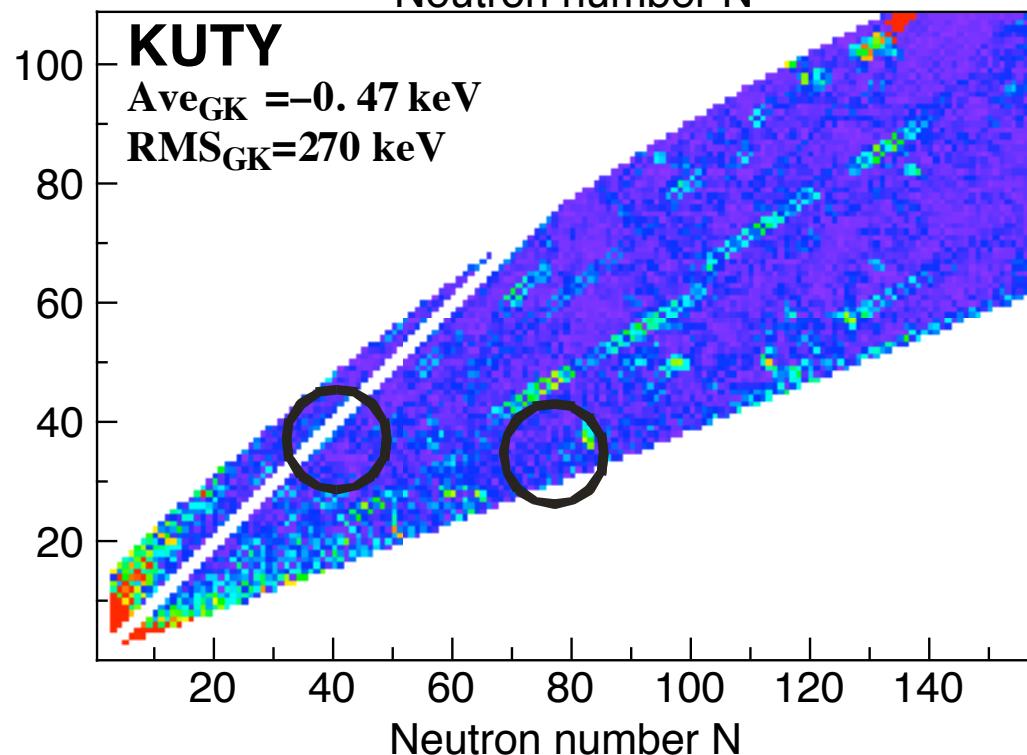
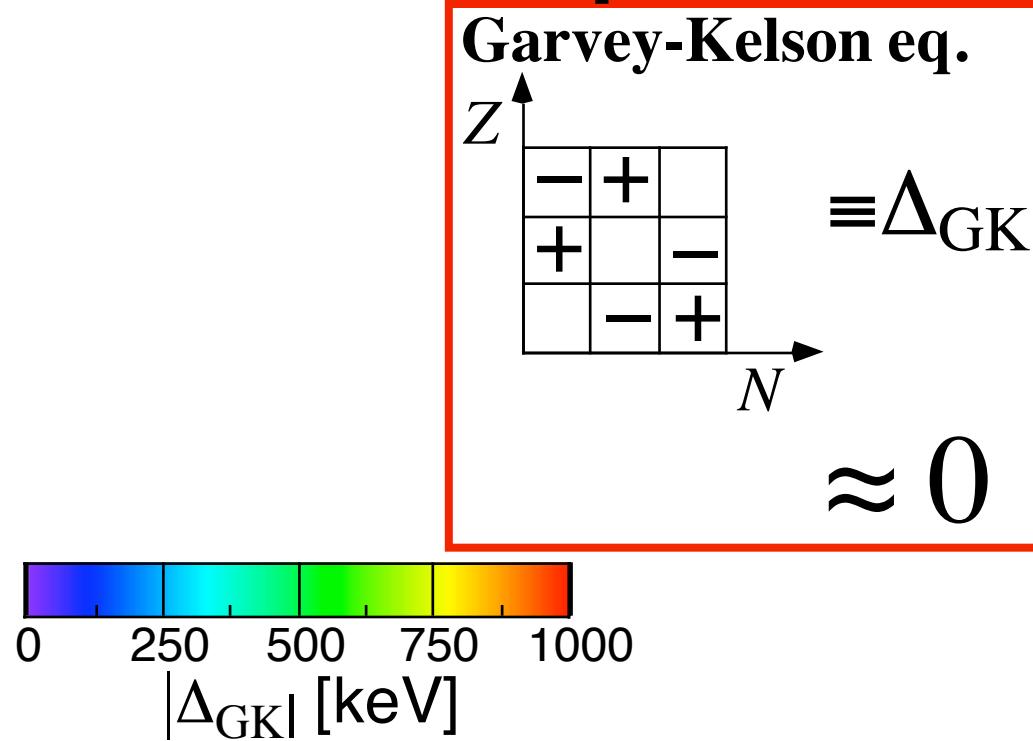
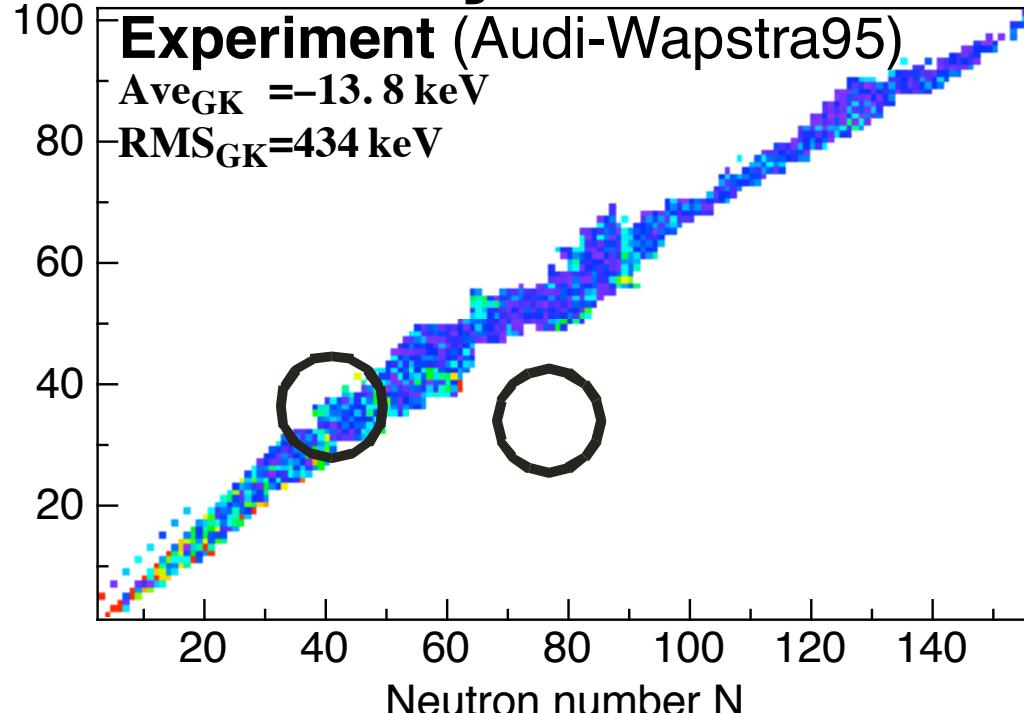
A=130peak

A=130peak

A=130peak

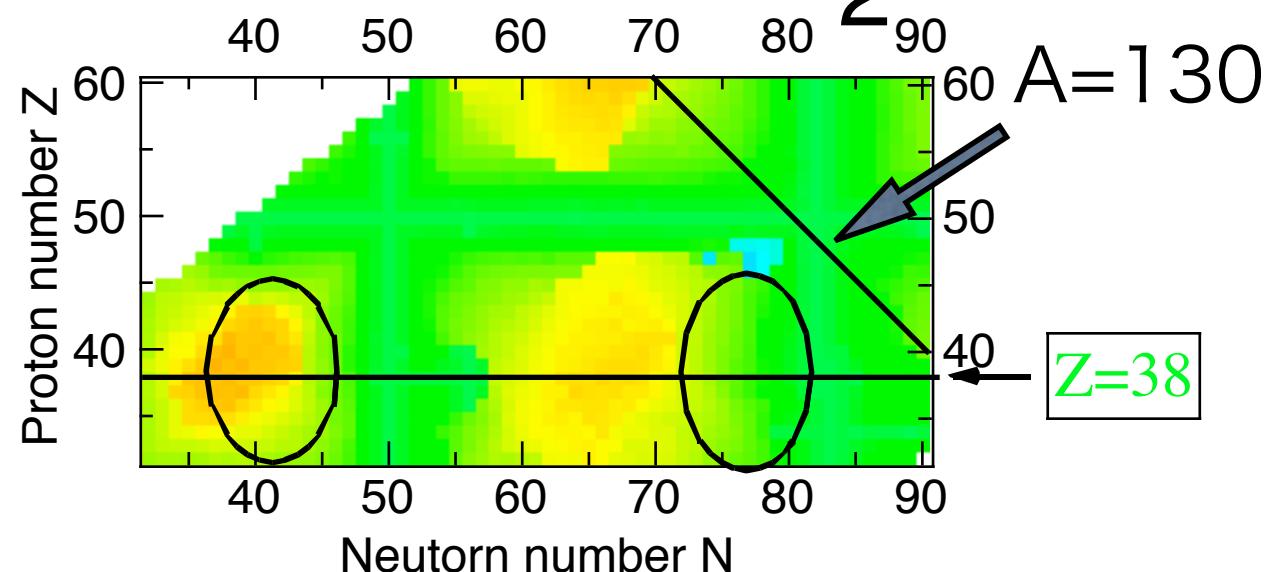


# Garvey-Kelson mass relationship

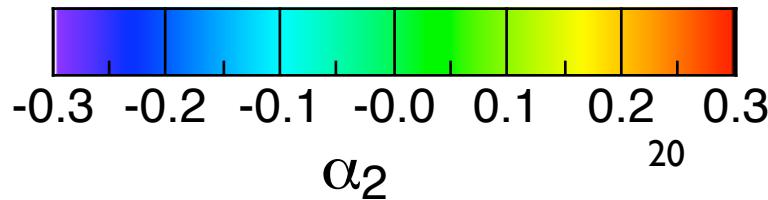
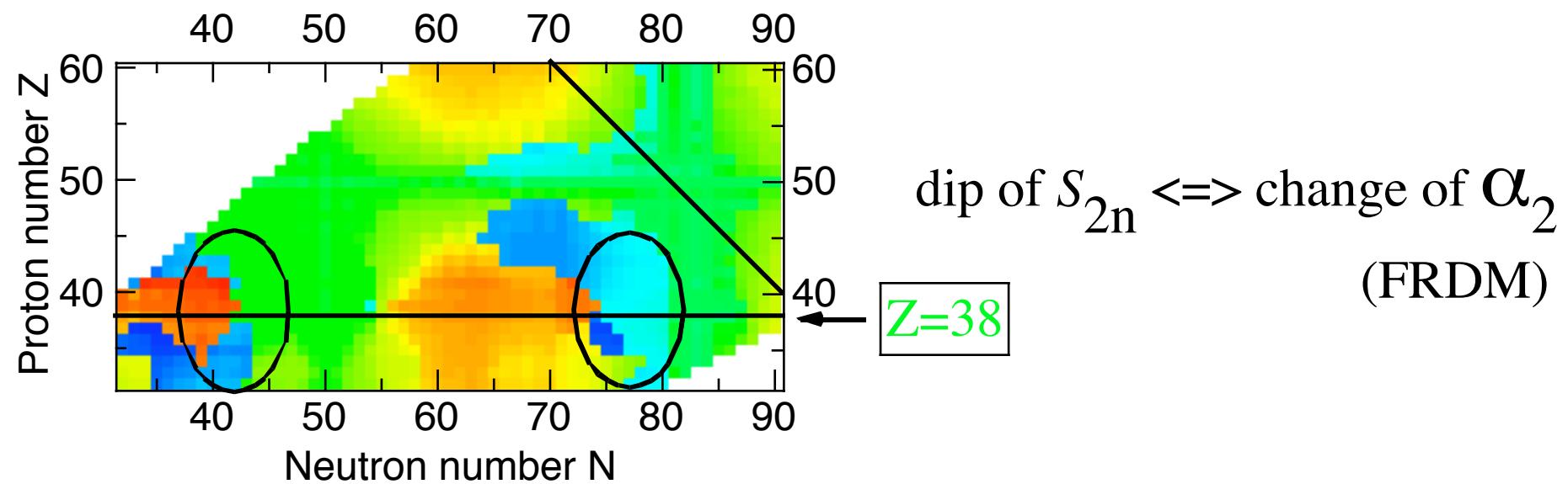


# Deformation parameter $\alpha_2$

KUTY



FRDM



# Influence of shell-quenching far from stability

B. Chen et al. / Physics Letters B 355 (1995) 37–44

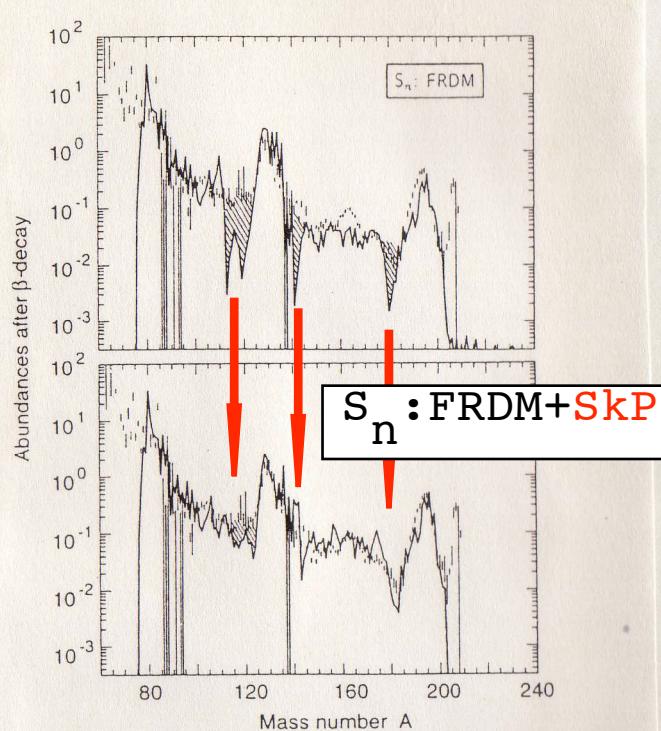


Fig. 2. r-process abundance fits obtained with ten equidistant neutron-density components from  $10^{20} \text{ cm}^{-3}$  to  $3 \times 10^{24} \text{ cm}^{-3}$  according to Fig. 1. In the upper part, the result is presented for FRDM [10] masses with the  $T_{1/2}$  and  $P_n$  values from the QRPA calculations according to Ref. [11]. In the lower part, masses of spherical nuclei around  $N = 82$  have been replaced by masses from HFB calculations with the Skyrme force SkP. The quenching of the  $N = 82$  shell gap (see Fig. 4) leads to a filling of the abundance troughs around  $A \approx 120$  and  $140$ , and to a better overall reproduction of the heavy-mass region.

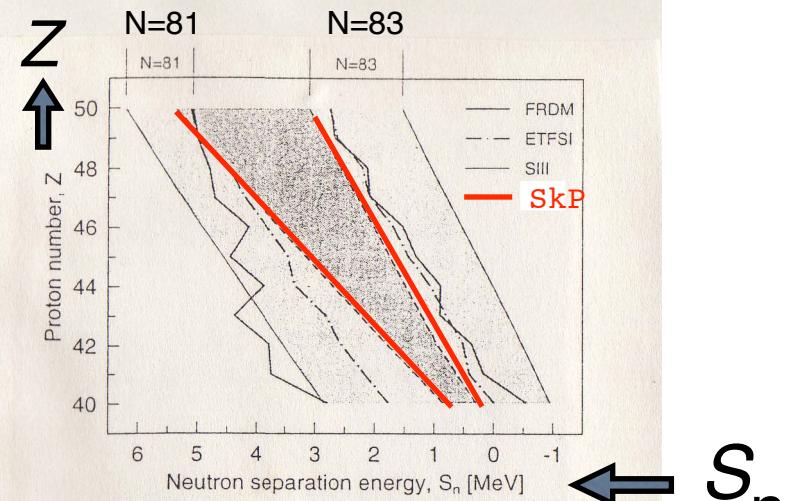


Fig. 4. Comparison of  $S_n$  values for the isotones  $N = 81$  and  $83$  as predicted by different mass models. The difference  $\delta S_n = [S_n(N = 81) - S_n(N = 83)]$  is a measure of the  $N = 82$  shell strength and is shaded for SIII (light) and SkP (dark). The shell quenching with distance from stability for SkP, in contrast to SIII, can be recognized. Masses of odd-odd nuclei have not been calculated in our SIII study.

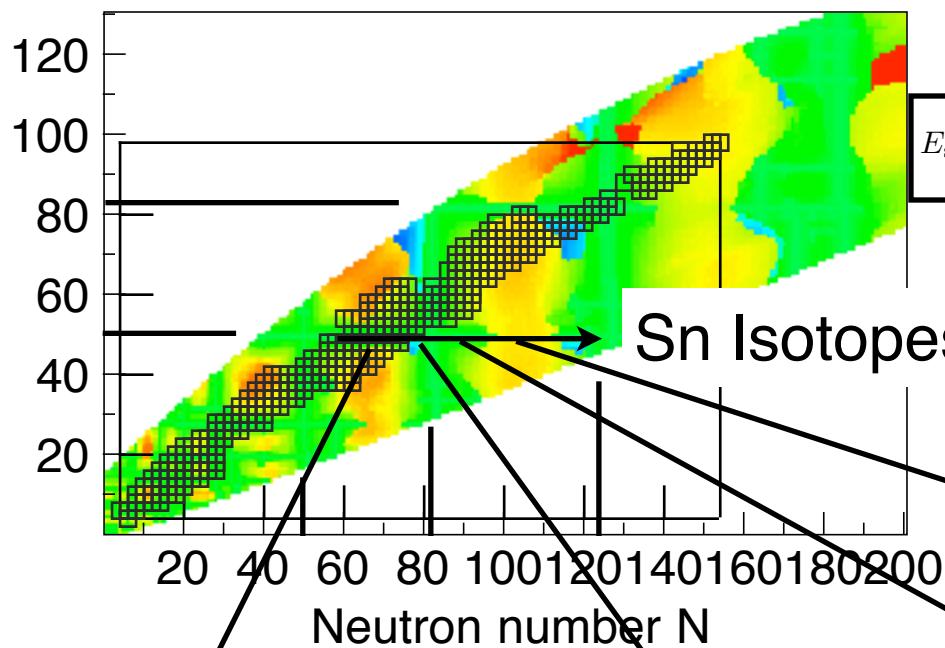
shell-quenching  
 => decreasing of dips  
 around the peaks  
 (Chen et al. 1995)

## Kink of $S_{2n}$ , or shell quenching?

# Deformation parameter alpha2 of KUTY

# Potential energy surface

Proton number  $Z$



Sn Isotopes

$$E_{sh}(Z, N) = \sum_{def.} (\langle E_{sh}^{sph}(Z, N) \rangle_{def.} + \Delta E_S(Z, N) - \Delta E_C(Z, N) - \Delta E_{pro}(Z, N))$$

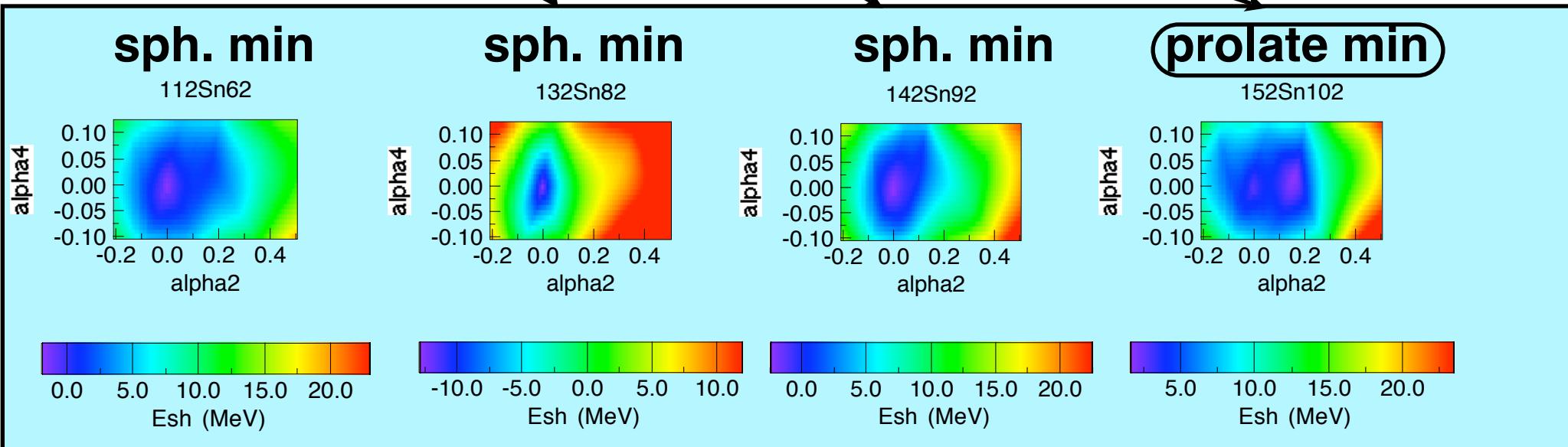
Possibility of shape isomer

sph. min

sph. min

sph. min

prolate min



$^{112}\text{Sn}_{62}$

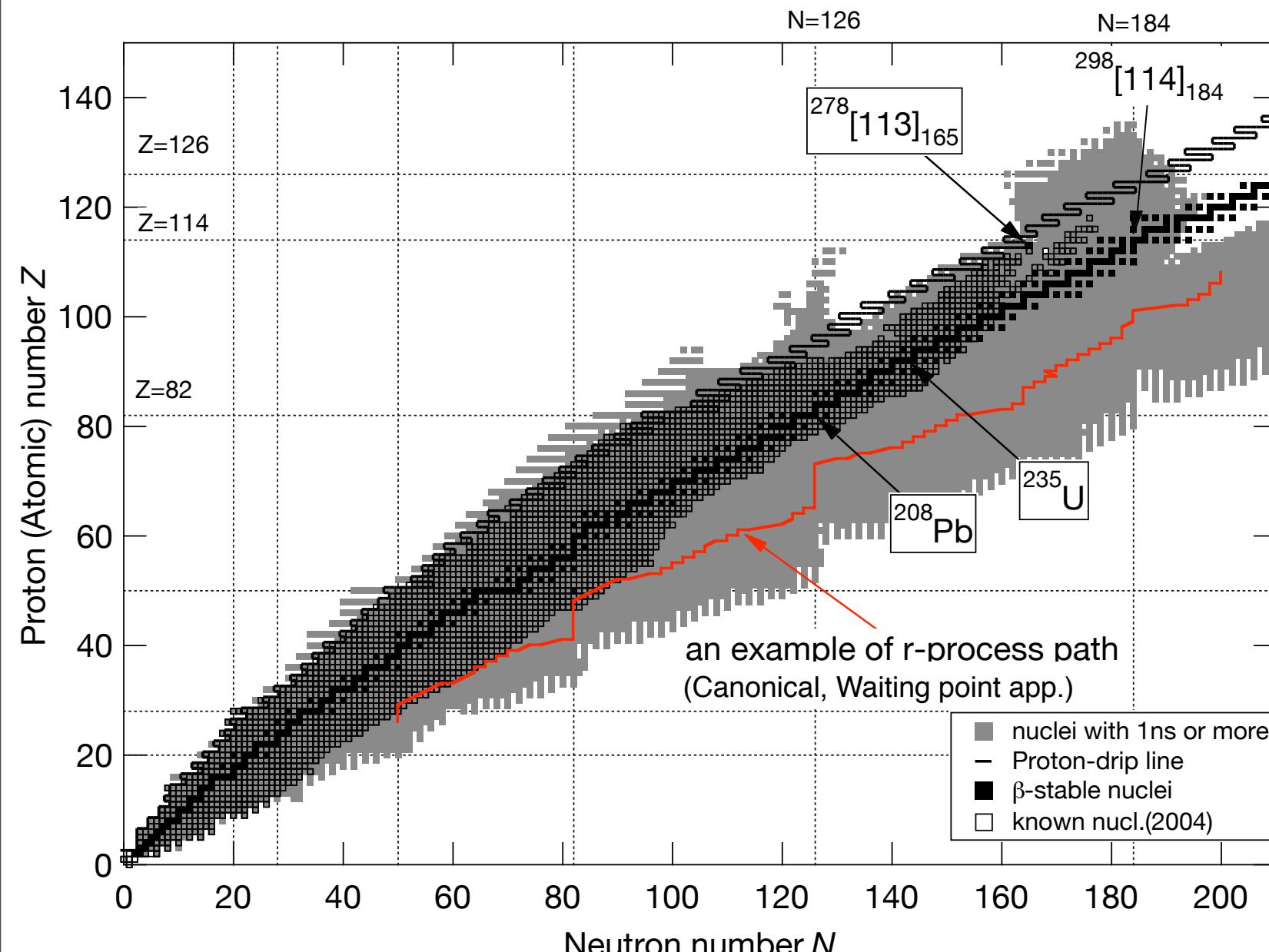
$^{132}\text{Sn}_{82}$

$^{142}\text{Sn}_{92}$

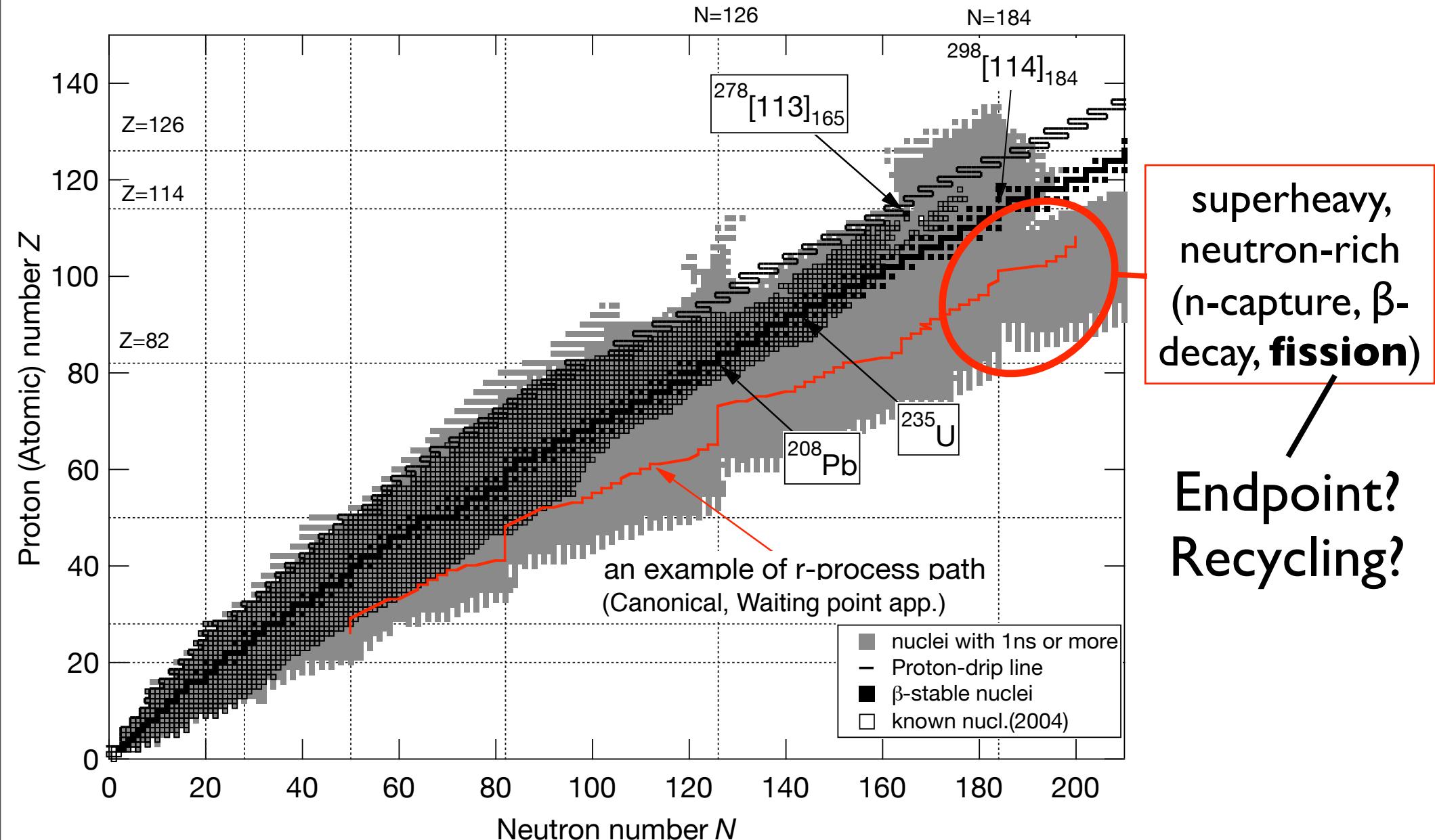
$^{152}\text{Sn}_{102}$

Systematical Study of Tin deformation (Shape coexistence)

# r-process mass region



# r-process mass region



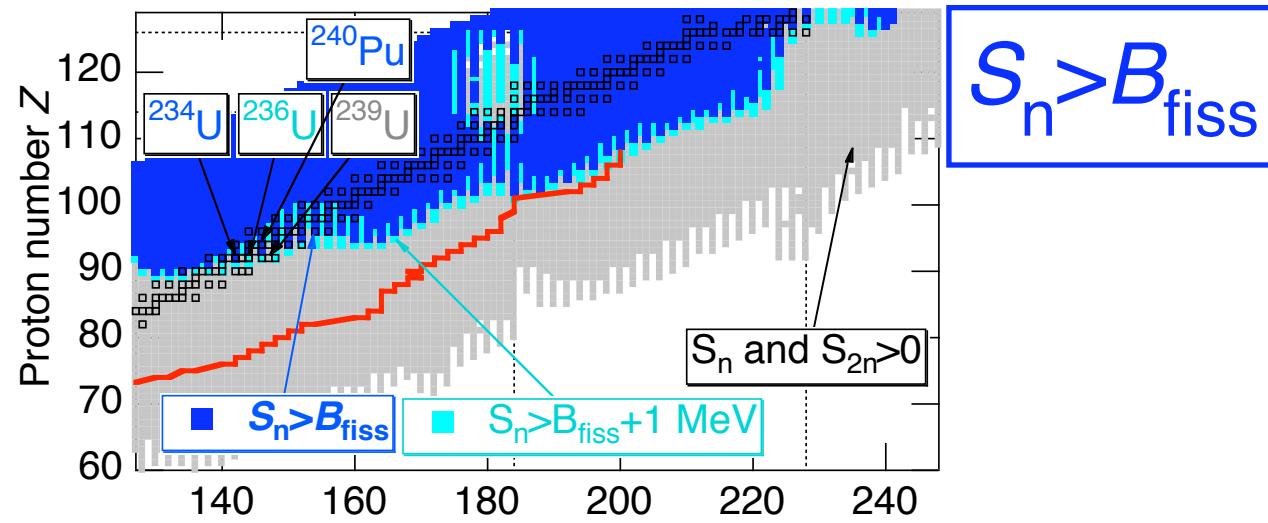
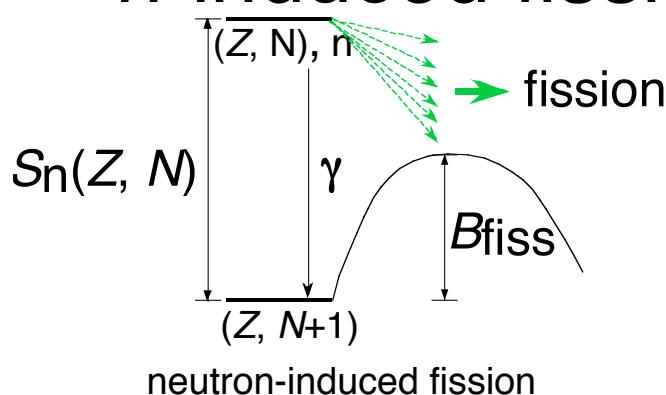
### 3. $\beta$ -delayed fission ( $\beta$ -df) probability

## Region of $\beta$ -delayed and n-induced fission

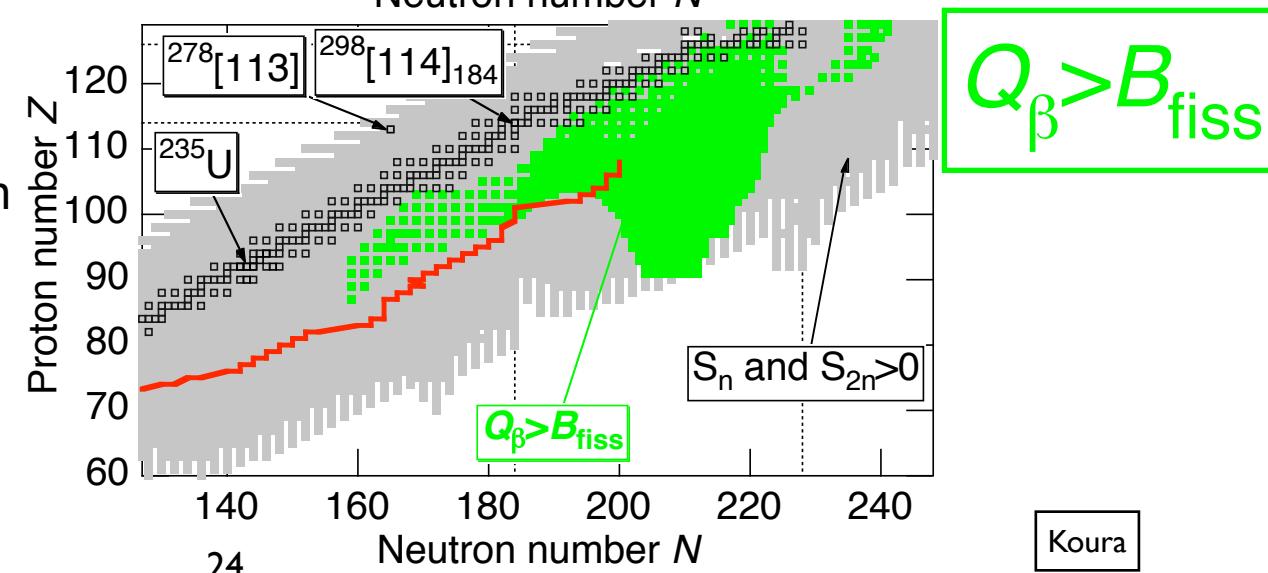
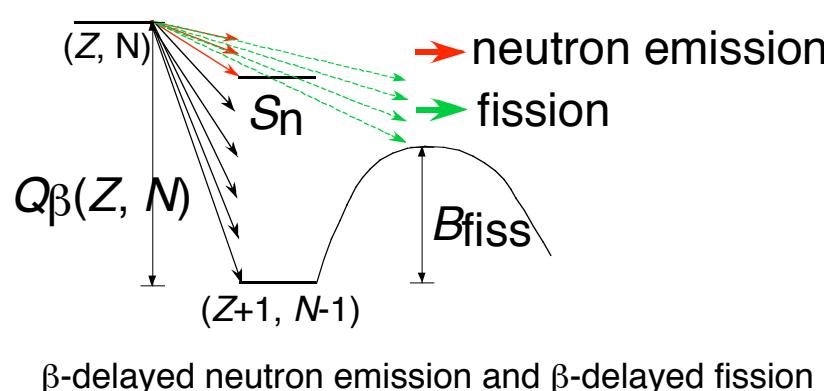
Nuclear masses and fission barrier:

KTUY (Koura-Tachibana-Uno-Yamada) mass formula

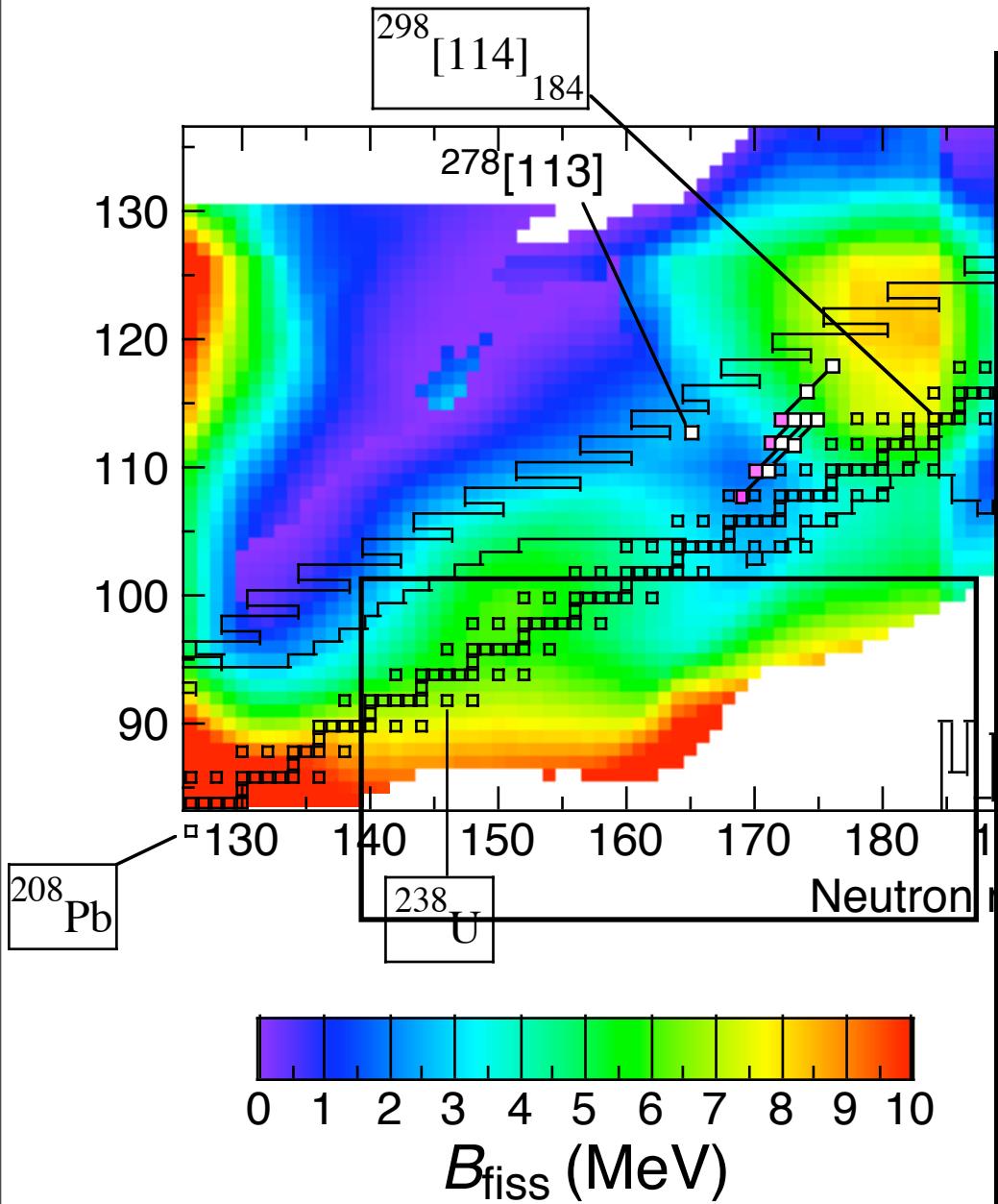
- n-induced fission



- $\beta$ -delayed fission

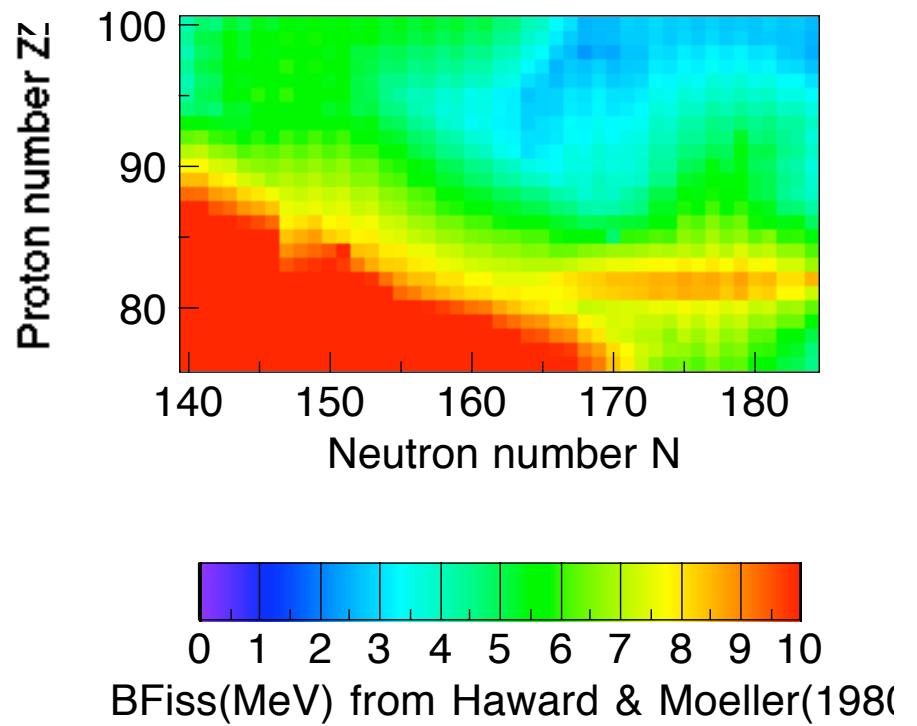


# Fission barrier height



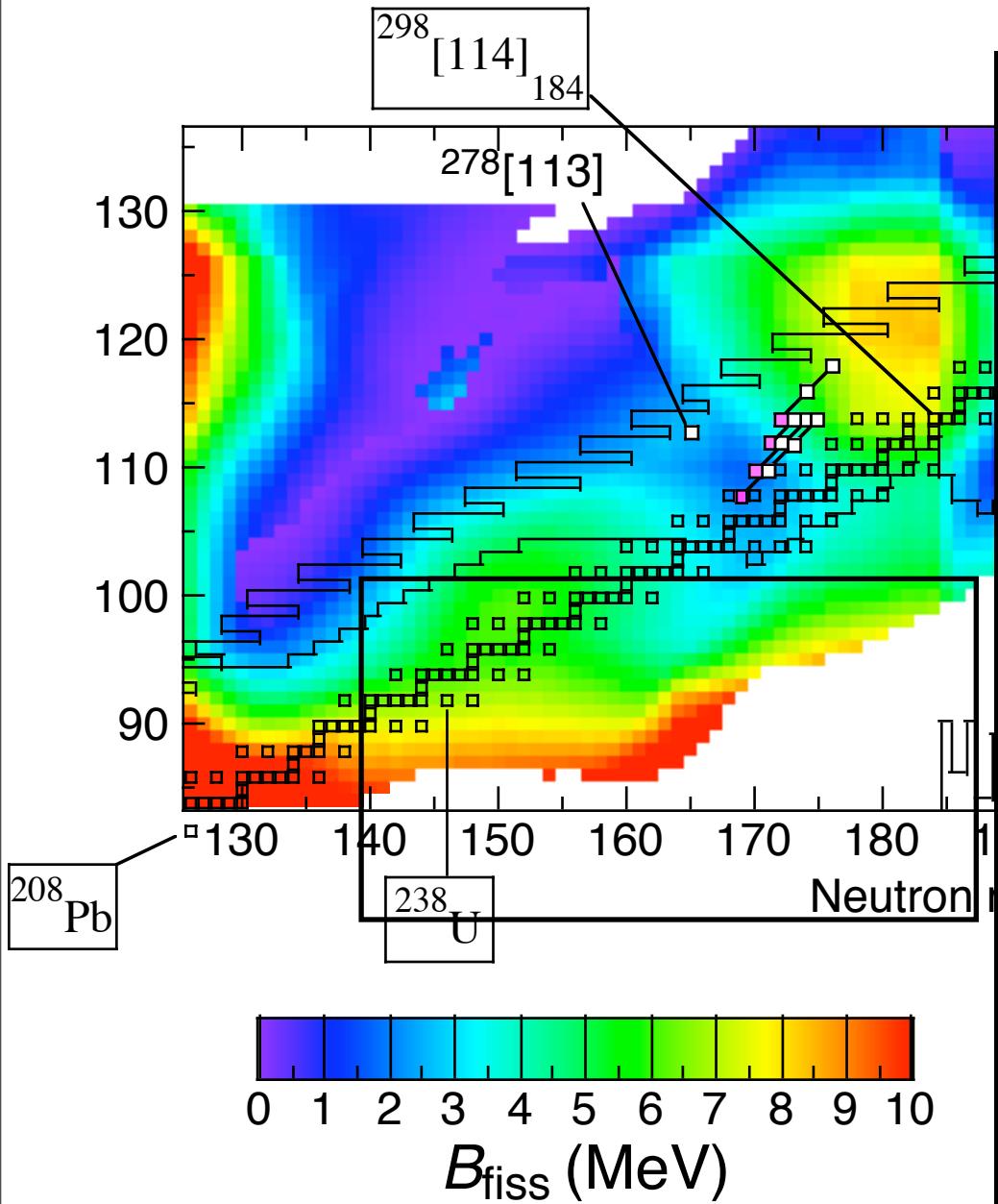
Fission Barrier height of Howard & Möller (1980):

Used for calc. of  $\beta$ -delayed fission prob. from QRPA (Klapdor, 88)

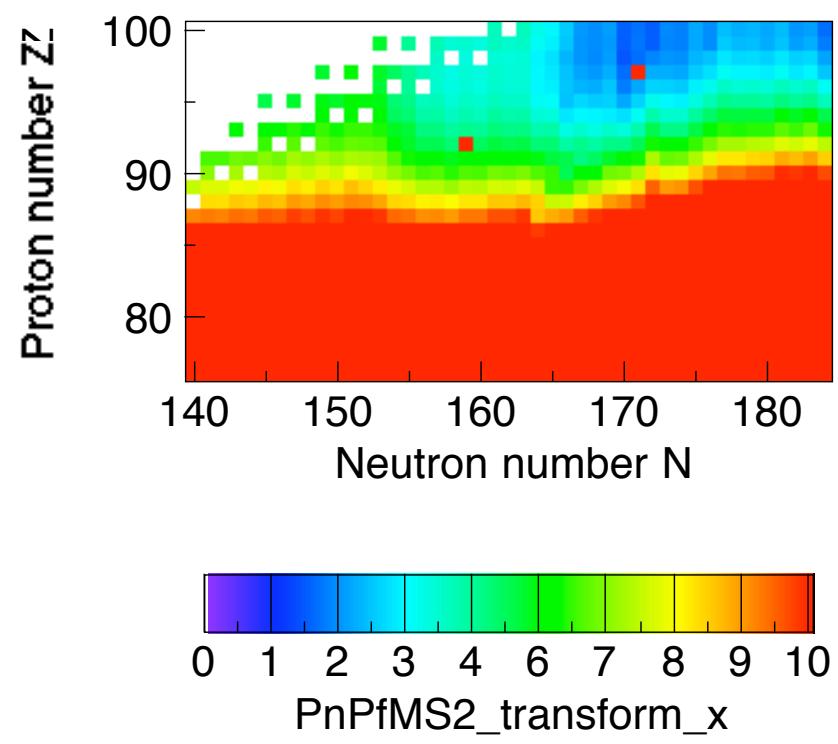


RMS dev. from exp.:  $\sim 1 \text{ MeV}$

# Fission barrier height

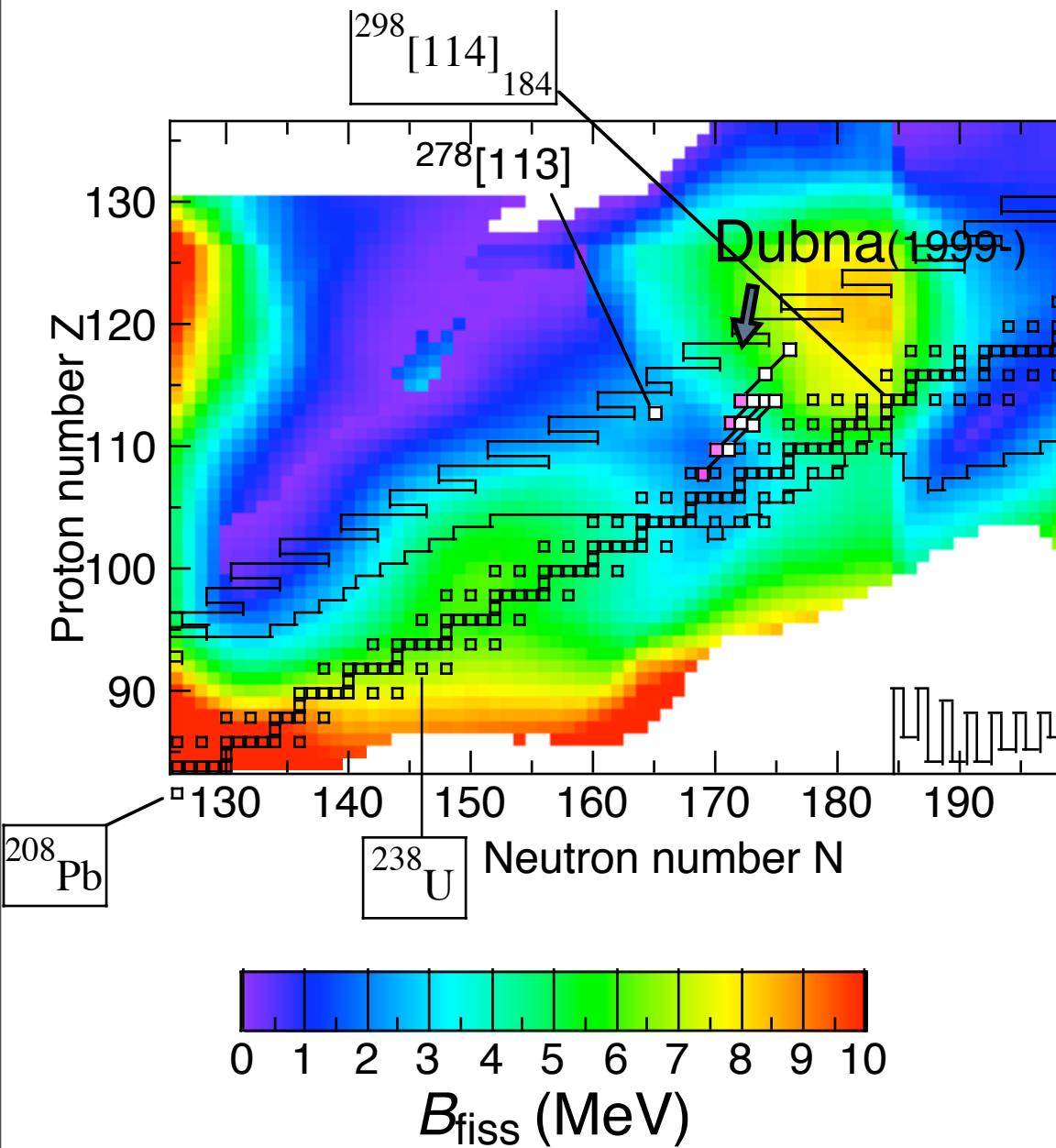


Fission Barrier height of  
Myers & Swiatecki (1996):

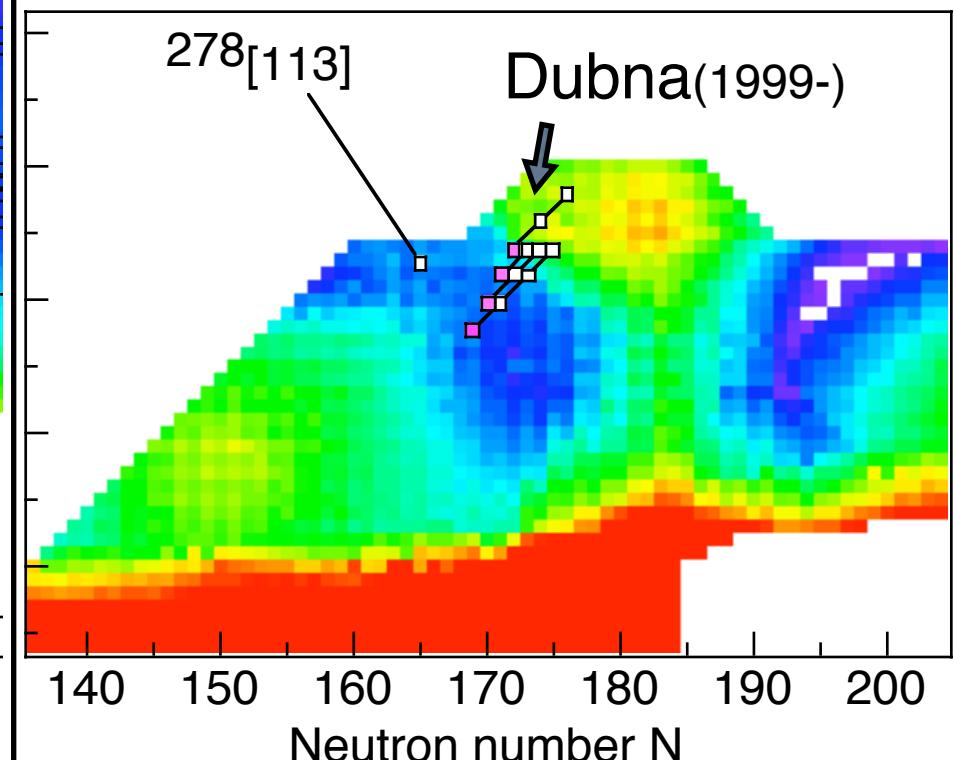


RMS dev. from exp.:  $\sim 1 \text{ MeV}$

# Fission barrier height of KUTY



ETFSI<sup>\*)</sup> ( $\beta_2, \beta_4, \beta_6$  deformation)



\*) Mamdouh, et al NPA679 (2001)

# Summary

Bulk properties of nuclear masses:

- **Notable differences in the n-rich region among mass formulae**

- Kink of the S2n systematics , Garvey-Kelson discrepancy, etc.

Relation between the r-process nucleosynthesis cal. and mass formulae:

- **R-process nucleosynthesis calculation with a canonical model**

- Abundance deficient both sides of  $A=130 \leq kink$  of S2n sys.