Seminar at G.S.I.

The mass evaluation:

adjustment procedure and some comments on statistics

Georges Audi Csnsm December 14, 2005

- the Atomic Mass Evaluation (AME)
  - the experimental data
  - data evaluation
  - data treatment
  - some special treatments
  - adjusted masses
- extrapolation - estimated unknown masses
- conclusion: best possible experimental masses
  & best possible evaluation of data

Ame2003 and Nubase2003

Aaldert H. Wapstra	Amsterdam
Olivier Bersillon	Bruyères-le-Châtel
Catherine Thibault	Orsay
Jean Blachot	Grenoble

Ame2008 and Nubase2008

Aaldert H. Wapstra	Amsterdam
....	....

Csnsm *Georges Audi*

"The 2003 Atomic Mass Evaluation"

Nuclear Physics A729 (2003) 129

"The Nubase Evaluation of Nuclear and Decay Properties"

Nuclear Physics A729 (2003) 3

- -

1993	1995	1997	2003	2008	2013
Ame'93	Ame'95	Nubase'97	Ame2003	Ame2008	Ame2013
full	update		Nubase2003	Nubase2008	Nubase2013

texts, tables, figs and bonus on the Web of Amdc

http://amdc.in2p3.fr/

http://www.nndc.bnl.gov/amdc/

The Ame ("Atomic Mass Evaluation")

- Experimental Data
  - Energy relation: reactions - decays $\longrightarrow$ relative meas.
  - Inertial mass in EM field $\longrightarrow$ relative measurement
- Data Evaluation
- Treatment of Data
  - Least Squares Method
  - Flow of Information
  - Consistency of Data
- Estimates for Unknown Masses
  - From S_{2n} - S_{2p} - Q_{α} - . . .
  - From difference with a smooth function

Experimental Data

- **Energy Relation**

  expressed in eV or keV

  keV*: *standard* volt

  adopt a value for $2e/h$ in Josephson

  keV: *international* volt

  from evaluation of fundamental constants

- **Inertial mass in EM field**

  expressed in u or μu, the

  "unified mass unit"

  $1\text{u} = \mathcal{M}(^{12}\text{C})/12$ since 1960

Conversion factor:

$1\text{u} = 931\,494.009\,0 \pm 0.007\,1$ keV*

$1\text{u} = 931\,494.013 \pm 0.037$ keV

Experimental Data II

- **Reaction Energies** eV

  A(a,b)B $Q_r = \mathcal{M}_\mathrm{A} + \mathcal{M}_\mathrm{a} - \mathcal{M}_\mathrm{b} - \mathcal{M}_\mathrm{B}$

  - close to stability
  - (n,γ) and (p,γ) $\Rightarrow$ backbone
  - self-calibrated A(a,b)B v/s C(a,b)D

- **Desintegration Energies** eV

  A(β^-)B $Q_{\beta^-} = \mathcal{M}_\mathrm{A} - \mathcal{M}_\mathrm{B}$ (“Atomic”)

  A(α)B $Q_\alpha = \mathcal{M}_\mathrm{A} - \mathcal{M}_\mathrm{B} - \mathcal{M}_\alpha$

  A(p)B $Q_p = \mathcal{M}_\mathrm{A} - \mathcal{M}_\mathrm{B} - \mathcal{M}_\mathrm{p}$

  - far from stability

- **Mass Spectrometry** u (often called “Direct”)

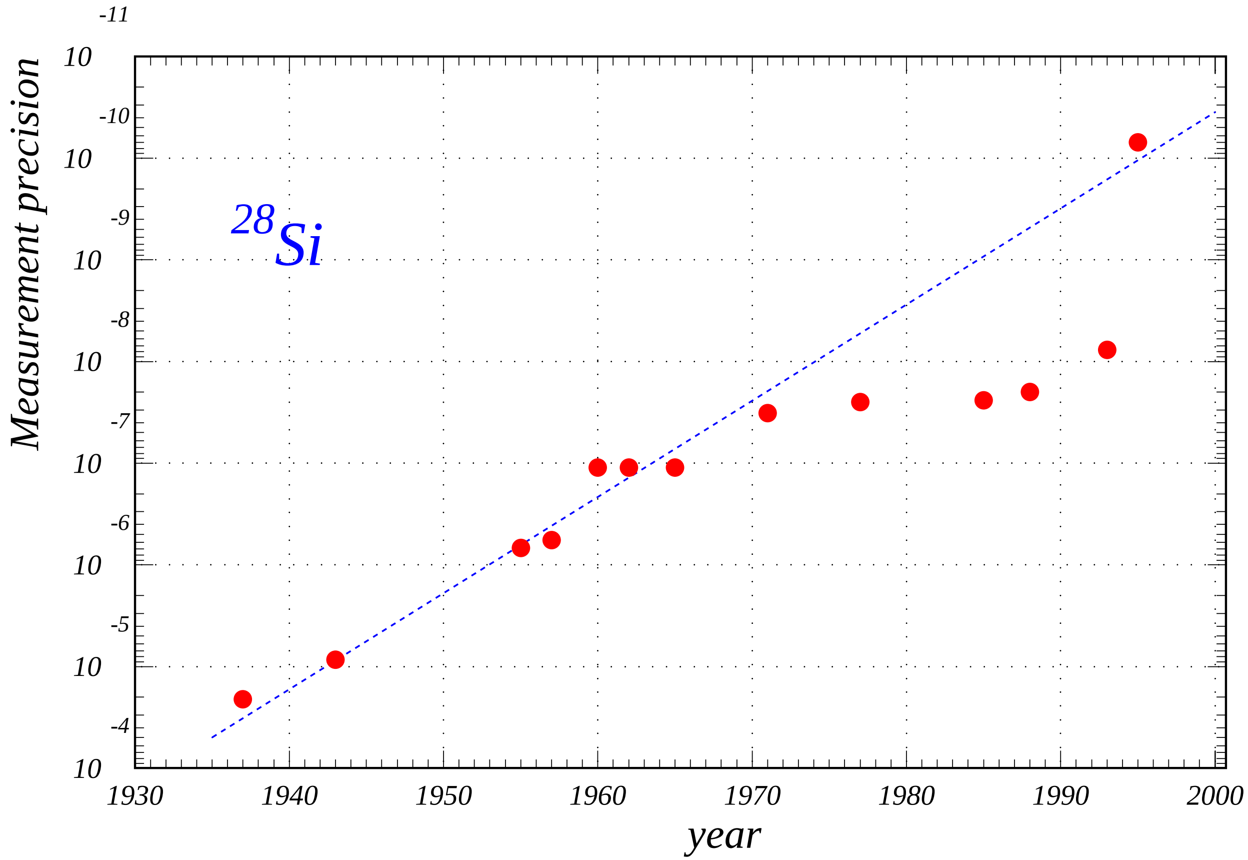
  1. Classical Spectrometers
  2. Time-of-Flight Spectrometers ($\mathcal{M}^t$ $(B\rho)$ and velocity)
  3. Cyclotron Spectrometers

     a. Radio-Frequency Spectrometer

     b. Penning Trap Spectrometer

     c. Storage Ring Spectrometer

Precision for ^{28}Si



One order of magnitude every 10 years

- 1937: 600 keV
- 1970-1990's "plateau" at 0.7 keV
- 1993: Stockholm-trap + (p,γ) + Manitoba-Spectr + (p,α)
- 1995: pure MIT-trap 2 eV
- 2005: expected 0.2 eV who & where

DATA EVALUATION

1 - Data Collection

* hidden data
* all available experimental data
  even poor ones (flagged accordingly)

2 - Careful Reading

* evaluate or re-evaluate
  calibration procedures & calibrants
  accuracies of the measurements
* examine spectra
* select PRIMARY information

3 - Comparaison

* to previous results
  ⟶ direct results
  ⟶ combination of other results
* to estimates from extrapolations
  (regularity of the Mass-Surface)
* to estimates from models

4 - Dialogue

* asking complementary information
* suggesting different analyses
* suggesting new measurements

evaluator = referee $\oplus$ anonymous collaborator $\oplus$ ……

csnsm *G. Audi*

DATA-file

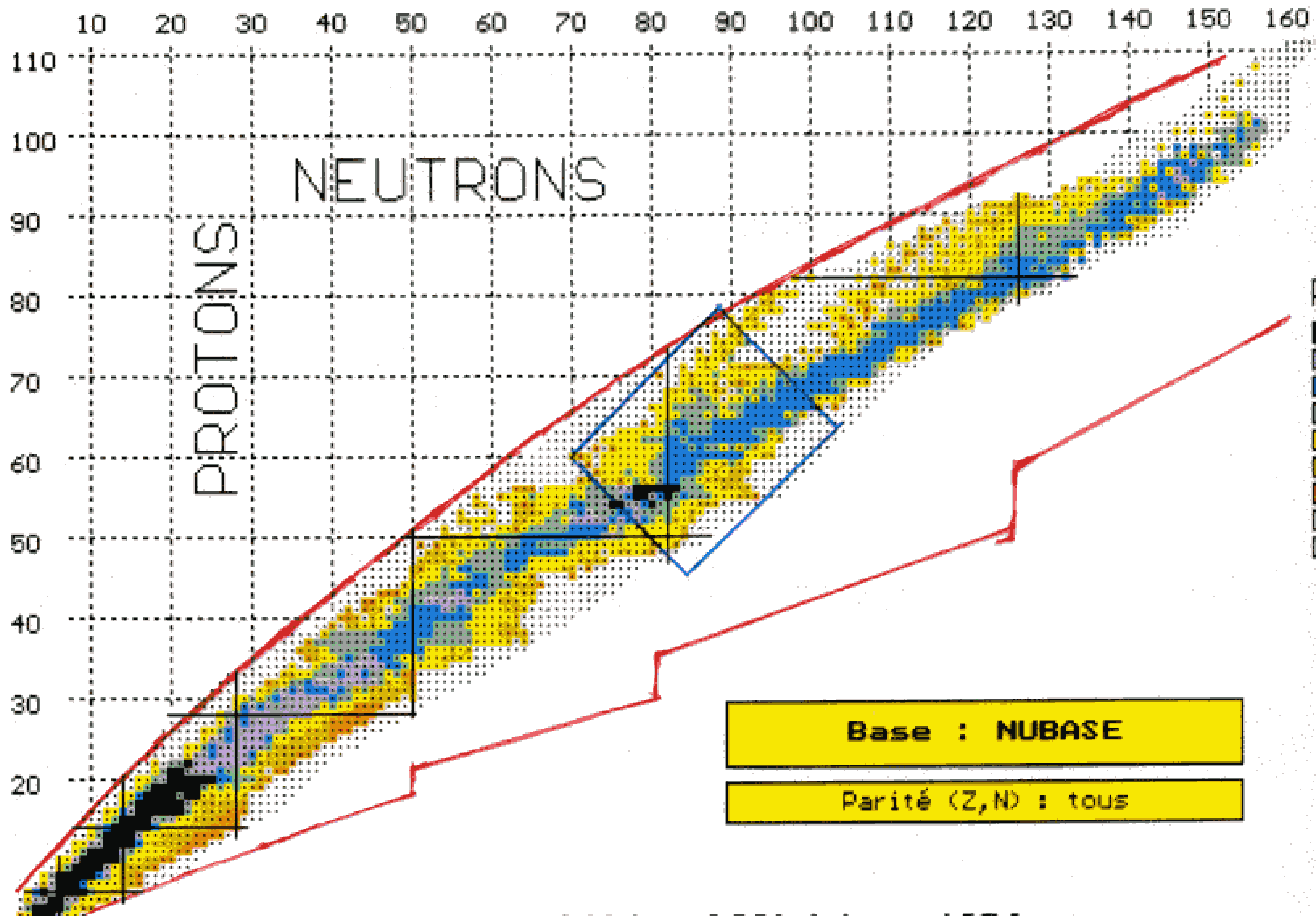
205 890806000a1 W	40Kr08	1620	200	205Hg(B-)205Tl				
205 890806000a2 W	51Ly10	1750	200	205Hg(B-)205Tl				
205 890816000c1 B	78Pe08	41.4	1.1	205Pb(e)205Tl		.525	.008	LM
205 890826000b1 P	62Bo25,W	2701.4	10.	205Bi(B+)205Pb		976	10	E+
205 890826000b2 P	62Pe08,W	2715.4	10.	205Bi(B+)205Pb		990	10	E+
205 890826000b3 W	AHW	*W E+ to 703.44 level						
205 890836000b1 W	69Ho37,W	3390	150	205Po(B+)205Bi		3E-3	1	p+
205 890836000b2 W	AHW	*W Positrons to 849.83 and 1001.22 levels						

REFERENCE-file

78Pa11	PRVCA	18,1249	Pardo,R.C., E.Kashy, W.Benenson, L.W.Robinson
78Pa12	.PRVCA	18,1277	Paschopoulos,I., E.Muller, H.J.Korner, I.C.Oelrich, K.E.Rehm, H.J.Scheerer
78Pe08	NUPAB 302,	1	Pengra,J.G., H.Genz, R.W.Fink
78Pf01	PRLTA	41, 63	Pfeiffer,L.P., A.P.Mills,Jr., R.S.Raghavan, F.Achandros
78Ra15	PRVCA	18,1085	Rao,G.R., G.Azuelos, J.C.Kim, J.P.Martin, P.Taras

MASS-file

204 0880	5990#	270#	204Ra			
205 0800	-22311	6	205Hg	5.2	m	1/2-
205 0810	-23845	4	205Tl	stbl		1/2+
205 0820	-23791	4	205Pb	15.2	My	5/2-
205 0830	-21083	8	205Bi	15.3	d	9/2-



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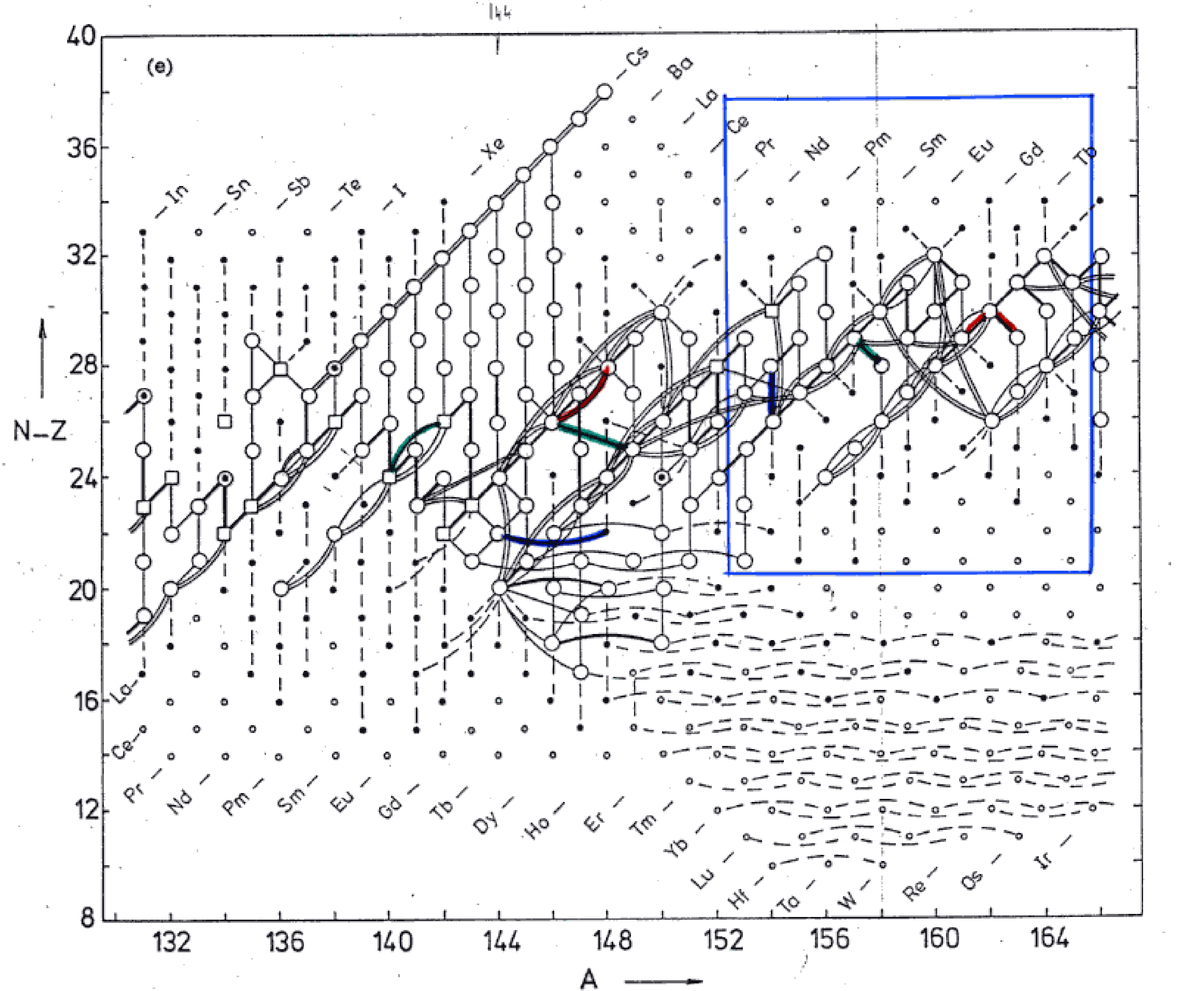
NEUTRONS
PROTONS
Base : NUBASE
Parité (Z,N) : tous



144
(e)
N–Z
A
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36
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In
Sn
Sb
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I
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Ce
Pr
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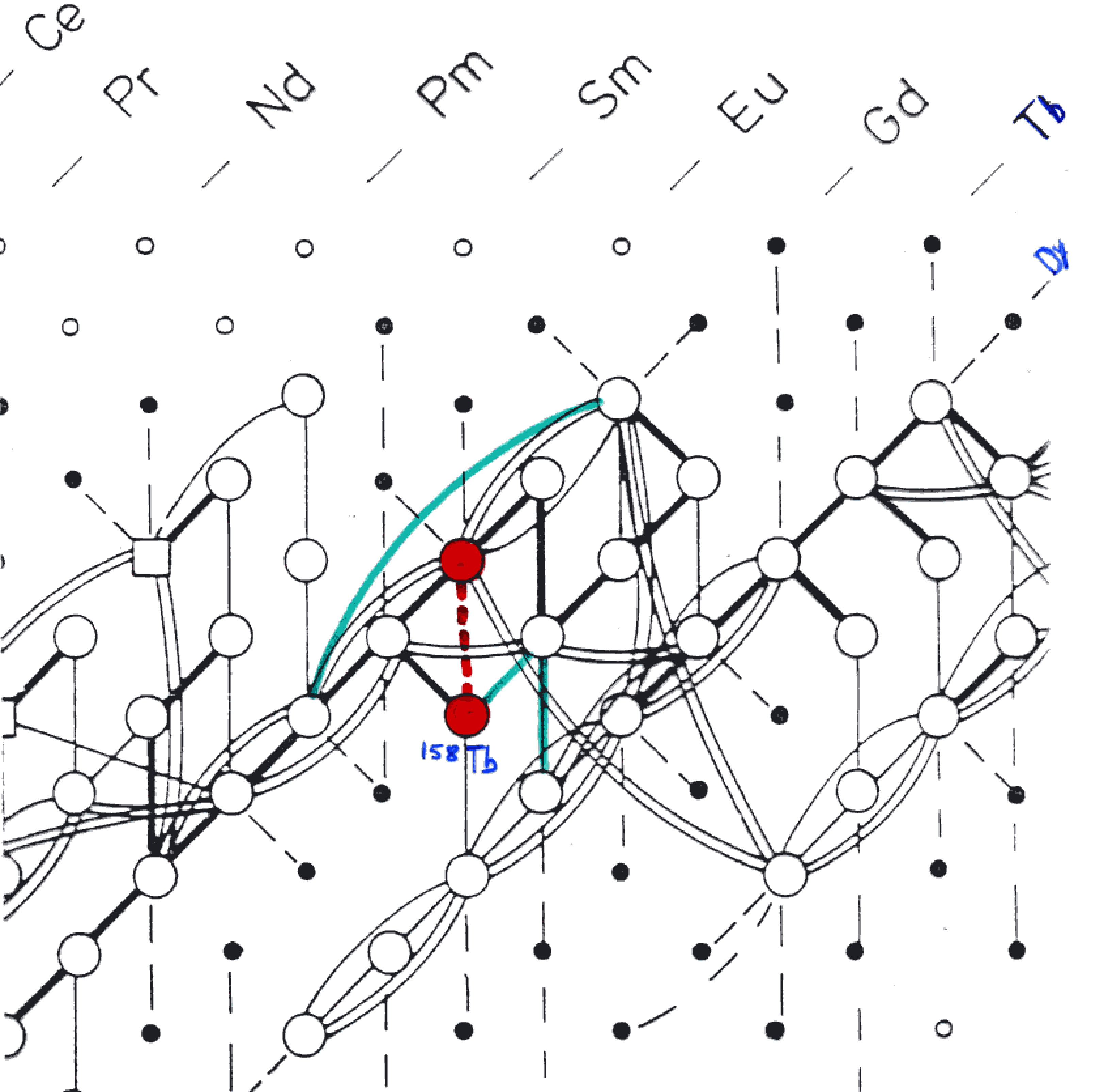

Ce
Pr
Nd
Pm
Sm
Eu
Gd
Tb
Dy
158 Tb

The Ame ("Atomic Mass Evaluation")

- ## Treatment of Data

  ### Least Squares Method

  answer vector

  adjusted values for the data

  ### Flow of Information

  influence of each datum on each mass

  ### Consistency of Data

  with other combination(s)

  with expectation from extrapolations

  with expectation from models

Treatment of Data - LSM - 1

Q data $q_i \pm dq_i$

M unknown quantities m_μ with $Q > M$

Q equations to M parameters overdetermined

$$\sum_{\mu=1}^{M} k_i^\mu m_\mu = q_i \pm dq_i \quad \Rightarrow \quad \boxed{\mathbf{K}|m\rangle = |q\rangle}$$

and the diagonal weight matrix $\mathbf{W}$: $w_i^i = 1/(dq_i dq_i)$

Very simple construction

$$^{t}\mathbf{KWK}|m\rangle = {}^{t}\mathbf{KW}|q\rangle$$

$$\mathbf{A}|m\rangle = {}^{t}\mathbf{KW}|q\rangle$$

$\mathbf{A}$ normal matrix square, positive, symmetric and regular

$\Rightarrow$ invertible : $\mathbf{A}^{-1}$

$$|\overline{m}\rangle = \mathbf{A}^{-1}\ {}^{t}\mathbf{KW}|q\rangle \quad \Rightarrow \quad \boxed{|\overline{m}\rangle = \mathbf{R}|q\rangle}$$

"Flow-of-information" matrix : $\Rightarrow$ $\boxed{\mathbf{F} = {}^{t}\mathbf{R} \otimes \mathbf{K}}$

NIM 249 (1986) 443

Treatment of Data -

adj. value of exp. data $\Rightarrow$ $|\overline{q}\rangle = \mathbf{KR}|q\rangle$

Consistency of data

$v_i = (\overline{q}_i - q_i)/dq_i \quad \Rightarrow \quad \chi^2 = \sum_{i=1}^{Q} v_i^2$

expected $\quad \chi_{expect} = Q - M \pm \sqrt{2(Q-M)}$

normalized χ_n = consistency factor = Birge ratio

$\chi_n = \sqrt{\chi^2/(Q-M)} \quad \chi_{n-expected} = 1 \pm 1/\sqrt{2(Q-M)}$

Partial consistency factor, χ_n^p, for a group of p data:

$$\chi_n^p = \sqrt{\frac{Q}{Q-M}\ \frac{1}{p}\ \sum_{i=1}^{p} v_i^2}.$$

Treatment of Data -

Least Squares Method - 2

Typical Sizes (Ame'2003 numbers)

6848 experimental data

(but U=1230 B=207 C=58 D=37 F=72)

5244 valid input exp. data + 887 estim. $\Rightarrow$ $Q = 6131$

3504 masses (including 1073 systematics) $\Rightarrow$ $M = 3504$

Reducing the System

Pre-averaging $\Rightarrow$ $Q = 4038$ $M = 3504$

Separating "Secondaries" (2657) $\Rightarrow$ $Q = 1381$ $M = 847$

Least Squares Adjustment

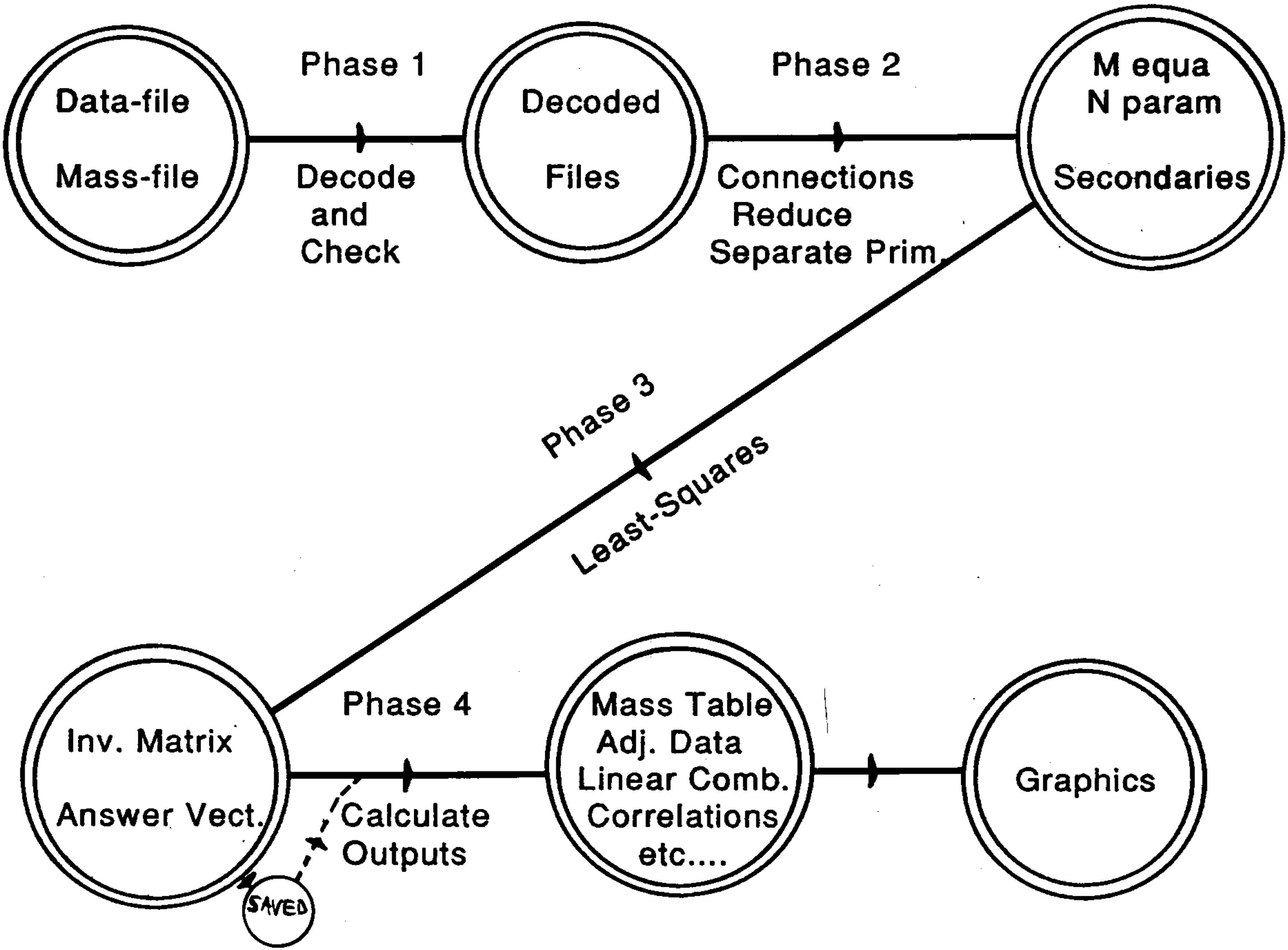
Total $\chi^2 = 814$ (expected 534 ± 33)

$\Rightarrow$ on the average σ's underestimated by 27% for energy data
and 16% for mass spectrometry

Distribution of the deviations (v/s)

$\sigma > 1$	$\sigma > 2$	$\sigma > 3$
15%	3.2%	0.007%

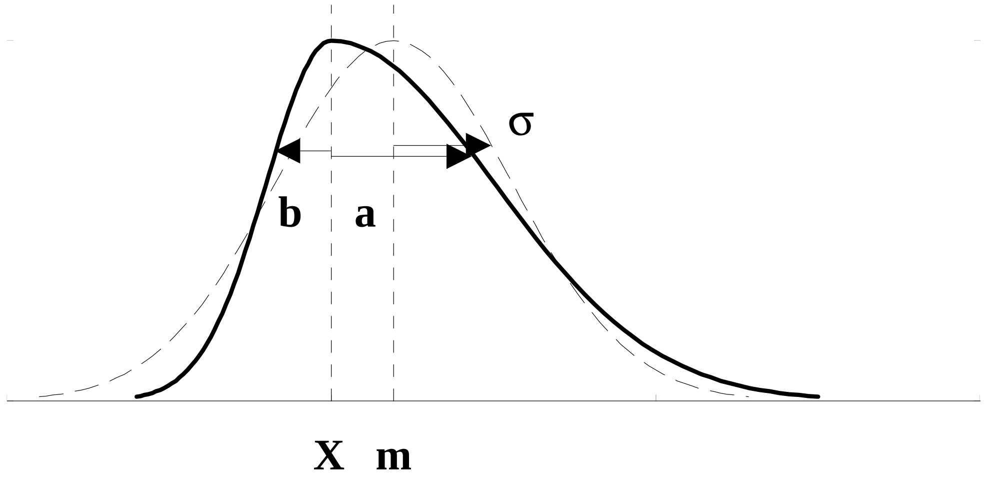
TREATMENT OF DATA - Least Squares Method - 3



Special Treatments I

- Asymmetric Errors X^{+a}_{-b}

Symmetrize the probab. distribution:



- Rough symmetrization

$$X + \tfrac{1}{2}(a-b) \qquad \pm \qquad \tfrac{1}{2}(a+b)$$

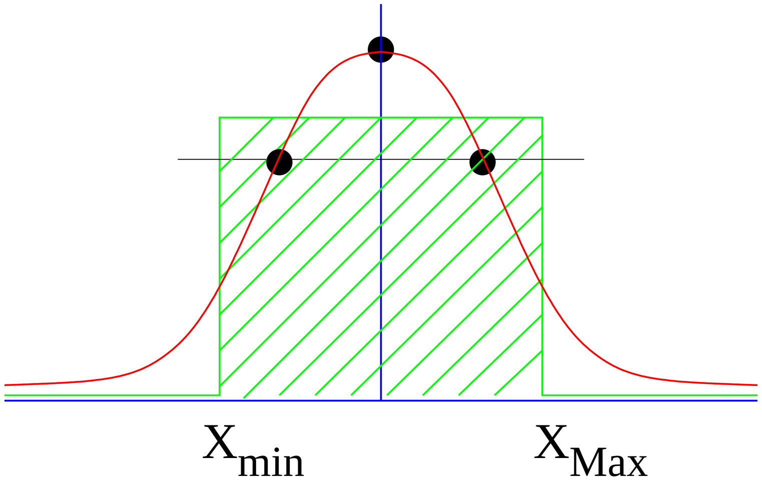
- Rigourous symmetrization (cf. Nubase2003)

$$X + 0.64(a-b) \quad \pm \quad \sqrt{\left(1-\tfrac{2}{\pi}\right)(a-b)^2 + ab}$$

Special Treatments II

- Range of Values X_{min}-X_{Max}

Moments of the probab. distribution:



$$\frac{1}{2}(X_{min} + X_{Max}) \quad \pm \quad 0.29(X_{Max} - X_{min})$$

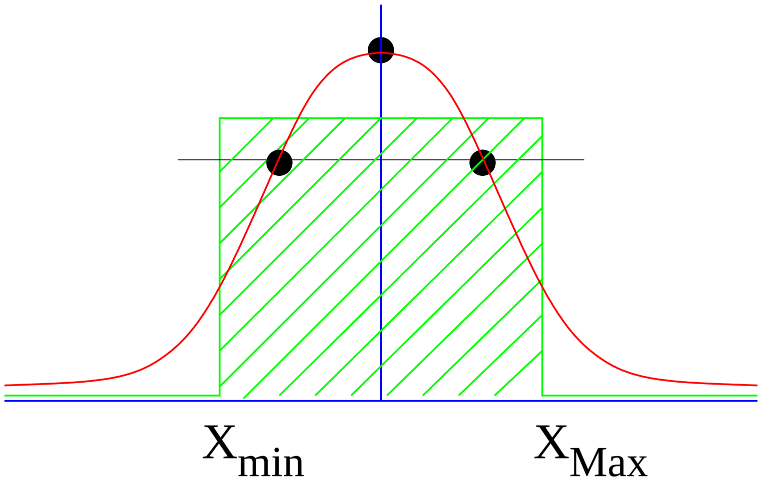
Special Treatments III-a

- Mixture of two lines

Two lines are known to exist at: M_{gs} M_m
but relative population NOT known

Assume equal probablitiy for all population ratio

The mixture will appear at any value between M_{gs} and M_m



same as preceding view: $M_{exp} = \frac{1}{2}(M_{gs} + M_m) \quad \pm \quad 0.29(M_m - M_{gs})$

the ground-state mass ($E_1 = M_m - M_{gs}$) :

$$M_{gs} = M_{exp} - 0.5E_1 \quad \pm \quad \sqrt{(\sigma_{exp}^2 + (\frac{1}{2}\sigma_1)^2 + (0.29E_1)^2}$$

Special Treatments III-b

- Mixture of three lines

Three lines are known to exist at: M_{gs} M_{m1} M_{m2}

(see demonstration in Ame2003, p. 176):

the ground-state mass:

$$M_{gs} = M_{exp} - \frac{1}{3}(E_1 + E_2)$$

and its error:

$$\sigma_{gs}^2 = \sigma_{exp}^2 + (\frac{1}{3}\sigma_1)^2 + (\frac{1}{3}\sigma_2)^2 + \frac{1}{18}(E_1^2 + E_2^2 - E_1 E_2)$$

The Ame ("Atomic Mass Evaluation")

- Regularity of the mass-surface

  Smoothness and structures

  Surface in 3D space

  Structures on the Surface: Shells - Deformations - Wigner

  Regularity is a basic property of the surface of masses

  Consequences :

  New Physics

  Outliers

  Conflict among Data

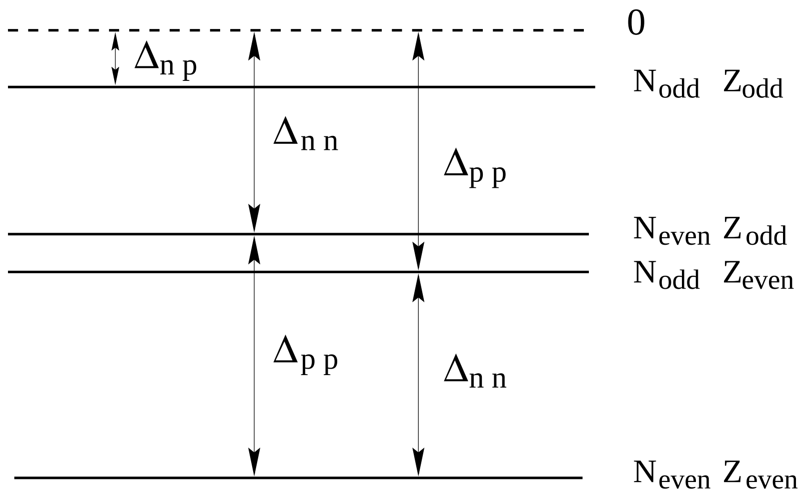
  Estimate unknown masses

Regularity of the Mass Surface I

- Surface in 3D space
- Pairing Energy $\Rightarrow$ 4-sheets
  - nearly parallel in all directions
  - smooth variations in N and Z

  Caveat: smooth = continuous
  non-staggering

  smooth $\neq$ slow



- Structures on the Surface:
  Shells - Deformations - Wigner
- Conclusion: **Regularity** is a **Basic Property**

Regularity of the Mass Surface II

- New Physics
  - Coherent deviations in (N, Z)

    $\Rightarrow$ new physical property (e.g. $^{23}N_{15}$ $N = 108 - 115$ Cs_{63-112})

- Outliers
  - One single 'Irregularity'

    $\Rightarrow$ question correctness of datum

    re-measure same and/or measure neighbors

    strongly deviating 1-experiment (chaotic surf.):

    $\Rightarrow$ replace by 'recommended' value

- Conflict among Data

  $\Rightarrow$ which one agrees with estimate?

- Unknown Masses

  $\Rightarrow$ Estimates : Interpolate - Extrapolate

Regularity of the Mass Surface III

- Extrapolations (short extrapolations)

  from regularity of the surface of masses

  for medium and heavy nuclides

  knowledge of n-stable or n-unstable

  for light n-rich nuclides

  similar for p-rich ← but Coulomb !!

  mirror and IMME

  for light p-rich nuclides

Scrutinizing the surface of masses

Derivatives of the Mass Surface

Separation energies : S_n S_{2n} S_p S_{2p}
Decay energies: Q_α Q_β $Q_{\beta\beta}$
Pairing energies : Δ_{nn} Δ_{np} Δ_{pp}

function of Z N A $N{-}Z$ $2Z-N$

1-2 isolines Z N A $N{-}Z$ $2Z-N$

(pb: same sheet - extrap. - double movement - ....)

Subtracting a simple function

subtracting results from a model

spherical Groote-Hilf-Takahashi

spherical Duflo-Zuker

(pb: shell migrations ...)

subtracting a Bethe and Weizsäcker formula

$$\mathcal{M}(N,Z) = N\mathcal{M}_{\mathrm{n}} + Z\mathcal{M}_{\mathrm{H}} - \alpha A + \beta\frac{(N-Z)^2}{A} + \gamma A^{\frac{2}{3}} + \frac{3}{5}\frac{e^2Z^2}{r_0A^{\frac{1}{3}}}$$

plus a pairing term to lessen oscillations

Fig. 6. Mass Exp-Mass Duflo-Z 96 sph. N= 70 to 118

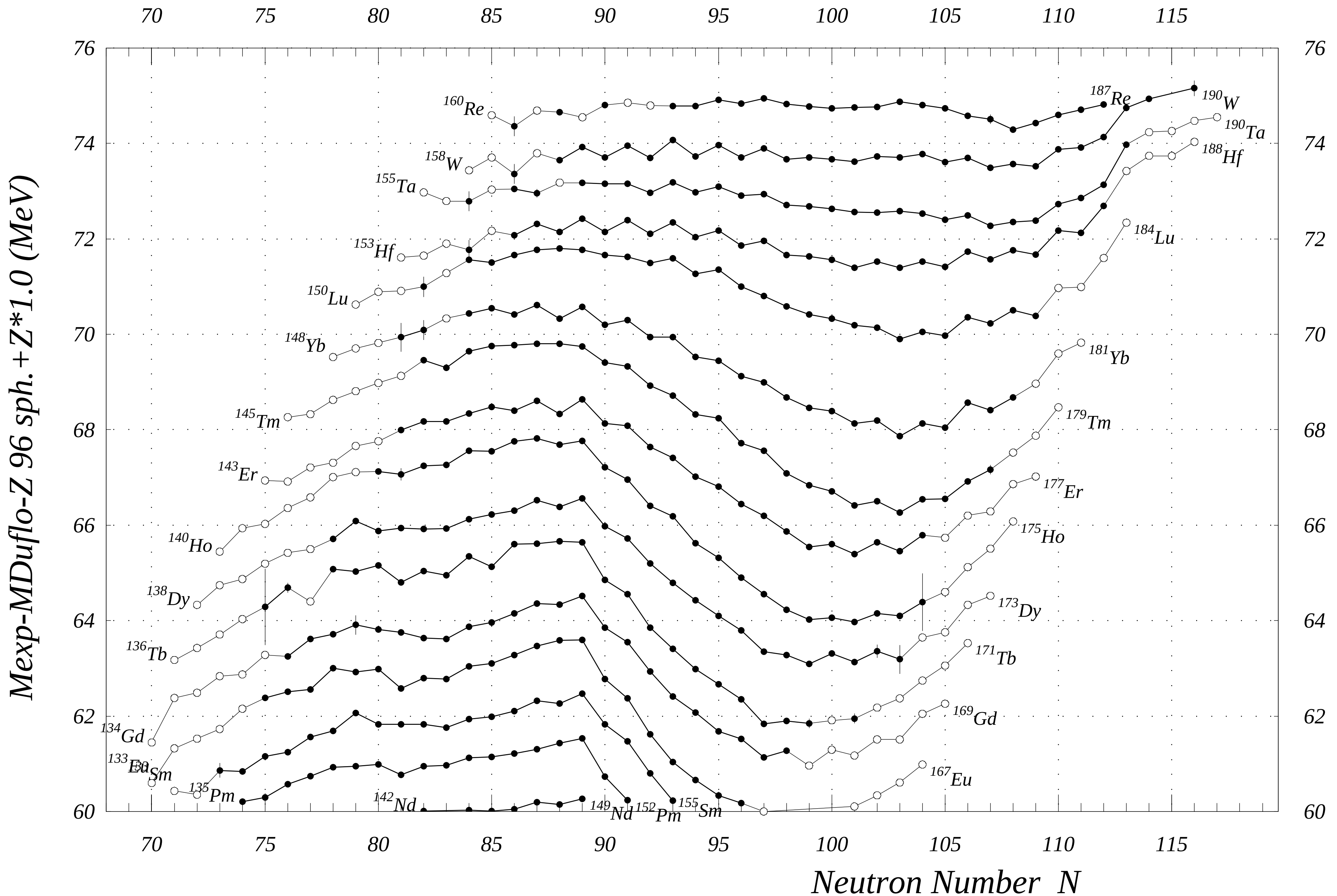
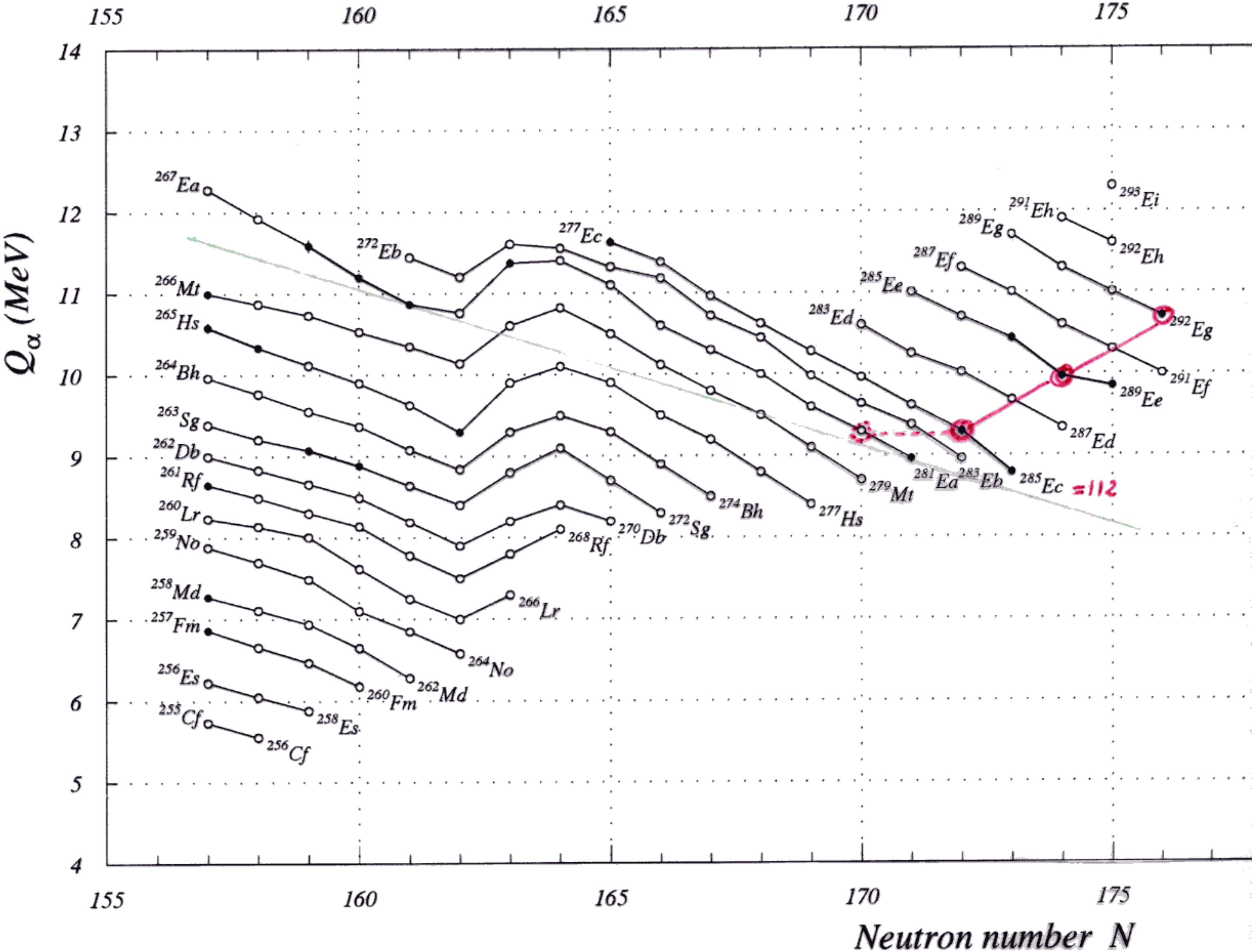
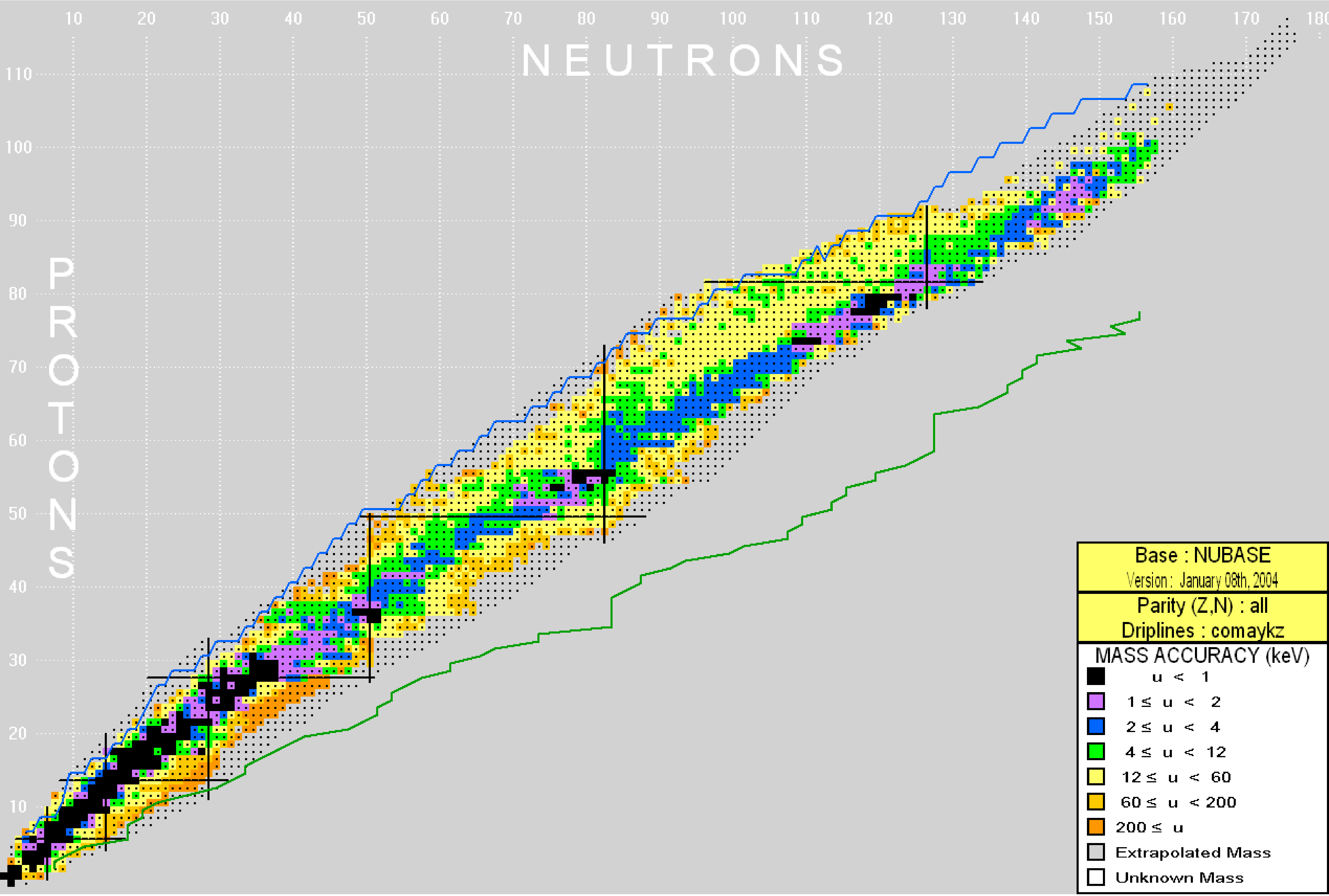


Fig. 9. α-decay energies N = 157 to 178




NEUTRONS
PROTONS
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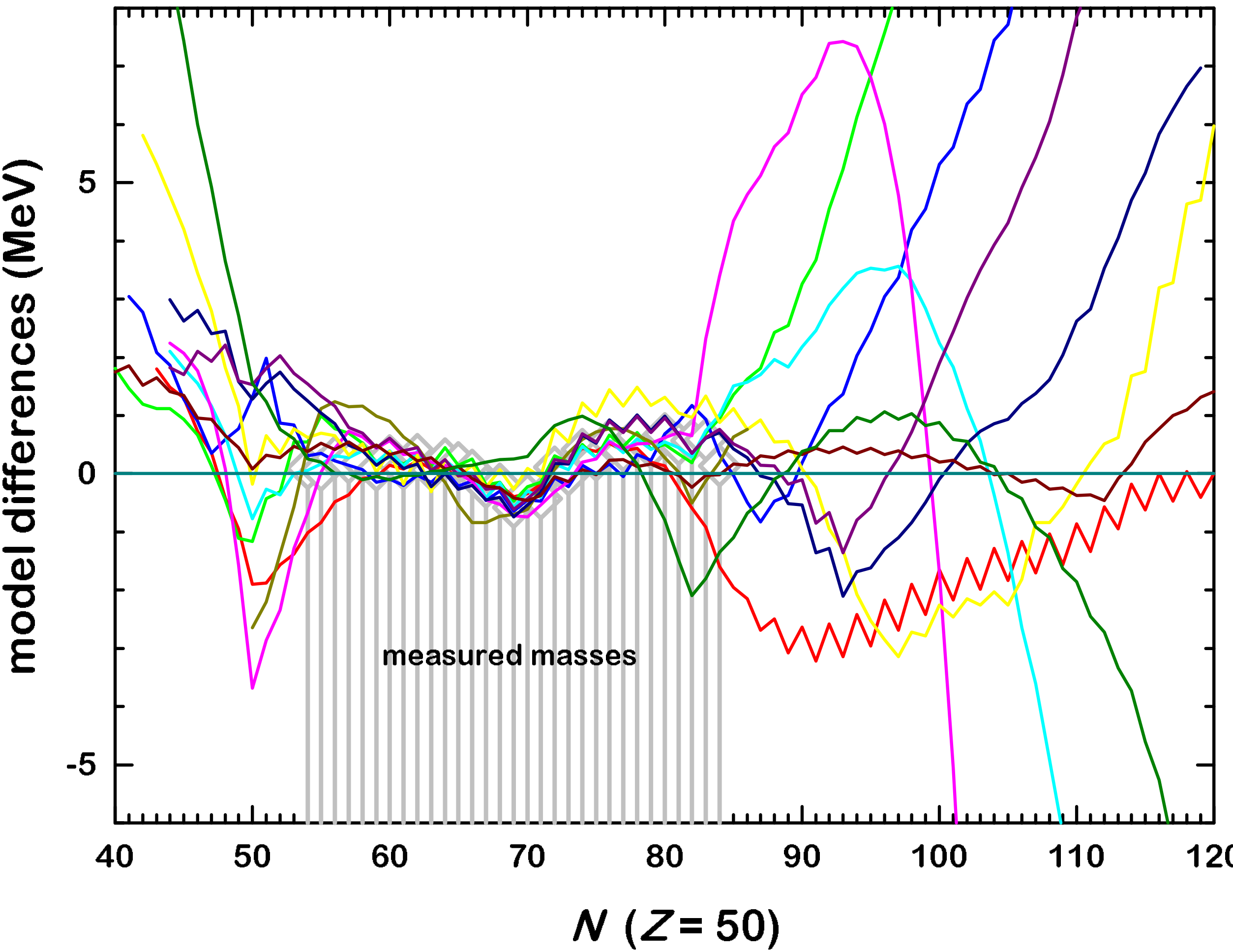
Base : NUBASE
Version : January 08th, 2004
Parity (Z,N) : all
Driplines : comaykz
MASS ACCURACY (keV)
u < 1
1 ≤ u < 2
2 ≤ u < 4
4 ≤ u < 12
12 ≤ u < 60
60 ≤ u < 200
200 ≤ u
Extrapolated Mass
Unknown Mass

comparison of mass model predictions



TO CONCLUDE

- Deriving a mass value from one or several experiments

  sometimes not easy

- Mathematical tools (LSM)

  + computer tools
  + evaluator's judgment

  are essential ingredients to reach the best possible mass-values

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- unknown masses

  - close to last ones : predicted from extension of mass surface
  - further out : derived from models.

  but models diverge!!! (10's of MeV in region of r-process)

- therefore (besides best possible experimental data):

  - best possible evaluation of masses $\longrightarrow$best set of mass values

    on which models may 1) adjust their parameters
    2) better predict masses further away