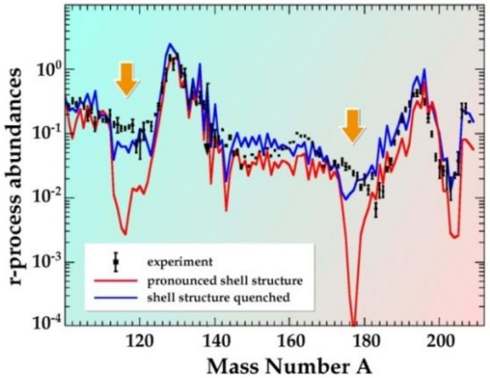
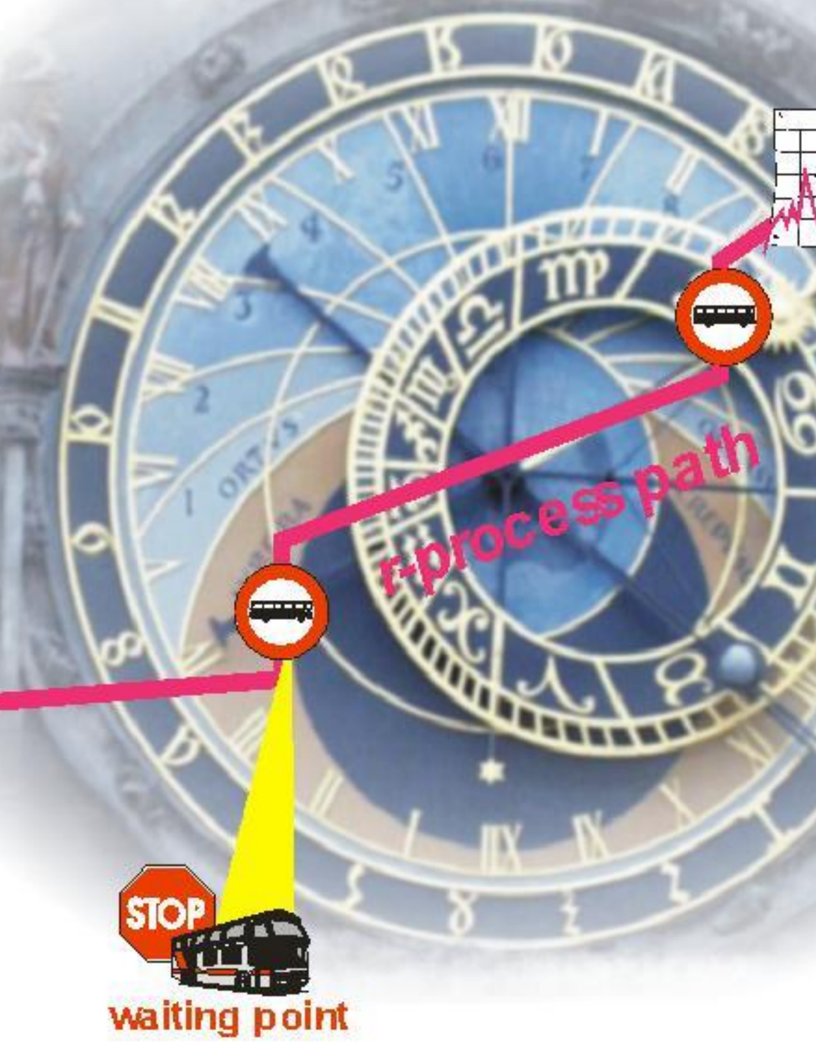
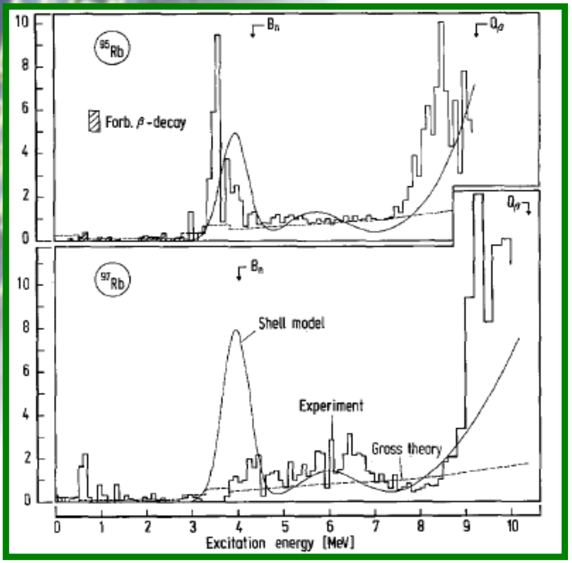
# Thirty years of collaboration with Peter Möller: From RPA (1984) to FRDM & QRPA (today)

JOHANNES GUTENBERG UNIVERSITÄT MAINZ

MAX-PLANCK-INSTITUT FÜR CHEMIE




**ASRC Workshop (JAEA)**
**Tokai, Dec. 2014**

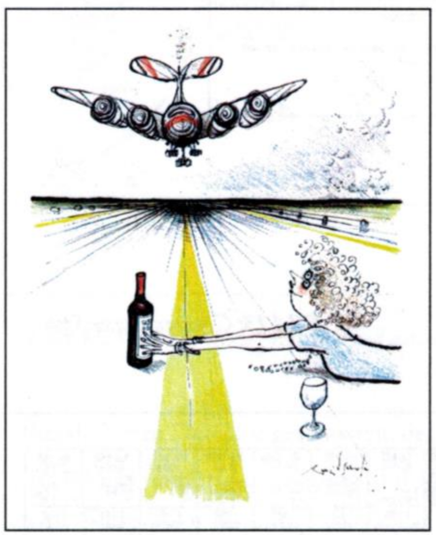
**Karl-Ludwig Kratz**

# The starting-point: my PhD-thesis

Because of the important contribution of **halogen** isotopes to the **ß-delayed neutron** groups occurring in fission, rapid separation procedures for **Br** and **I** were already developed in the 1950's by several groups.

In those days, chemical **ELEMENT** separation was (still) superior to physical **MASS** separation.

**"SRAFAP"**
(**S**tudents **R**unning **A**s **F**ast **A**s **P**ossible)



**"HITSEP"**
(**HI**gh-**T**ech **SE**paration **P**rocedure)

In my **PhD thesis,** I worked out an **ultra-fast separation procedure** based upon formation of methyl-halides in a hot-atom reaction between fission halogens recoiling from a solid U-235 target into gaseous methane:

$$Br^* / I^* + CH_4 \Longrightarrow CH_3Br^* / I^* + H^\circ$$

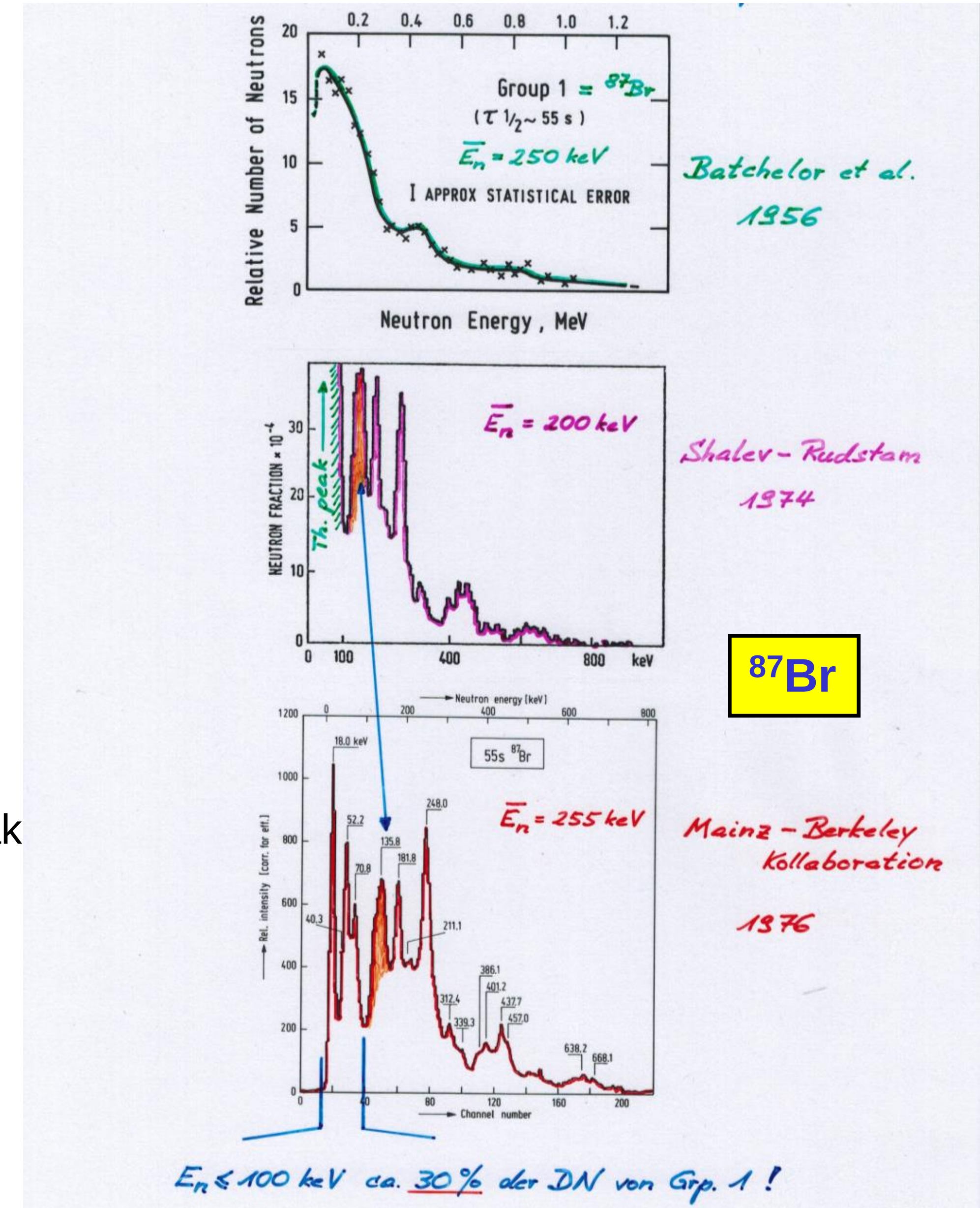
... shortest-lived isotopes detected :

**0.65 s $^{91}$Br, 0.25 s $^{92}$Br and 0.45 s $^{141}$I, 0.2 s $^{142}$I**

# Development of βdn-spectroscopy, as Mainz postdoc

## Neutron detector:

**He-3 ionisation chambers**




**Energy resolution:**

10 keV for $E_n$ = thermal peak

20 keV for $E_n$ = 2 MeV

**Efficiency:**

$10^{-4} – 10^{-5}$

**…new spectroscopic method ?**

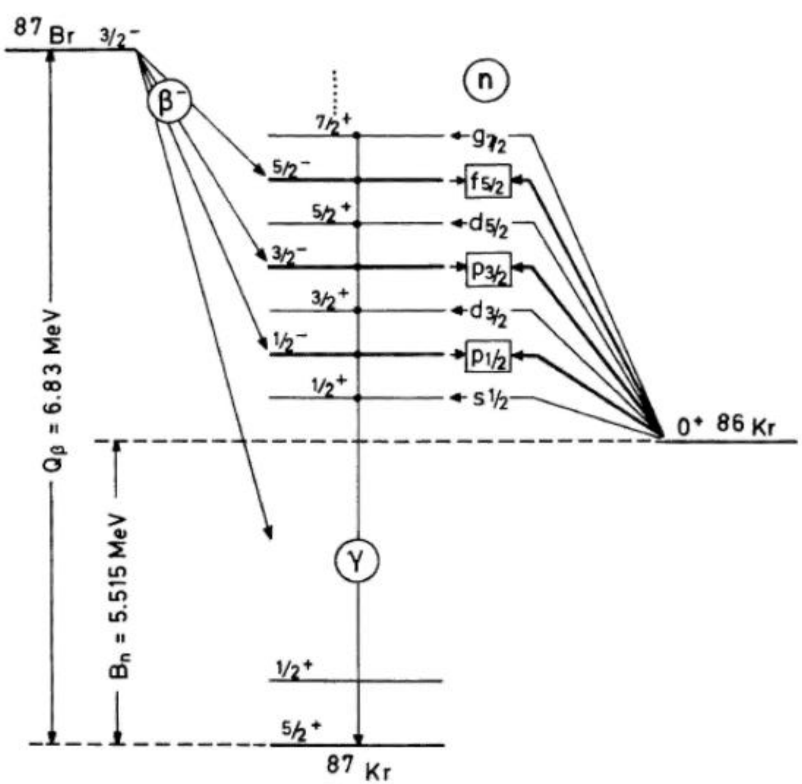
**Importance of low-energy βdn's for astrophysics**

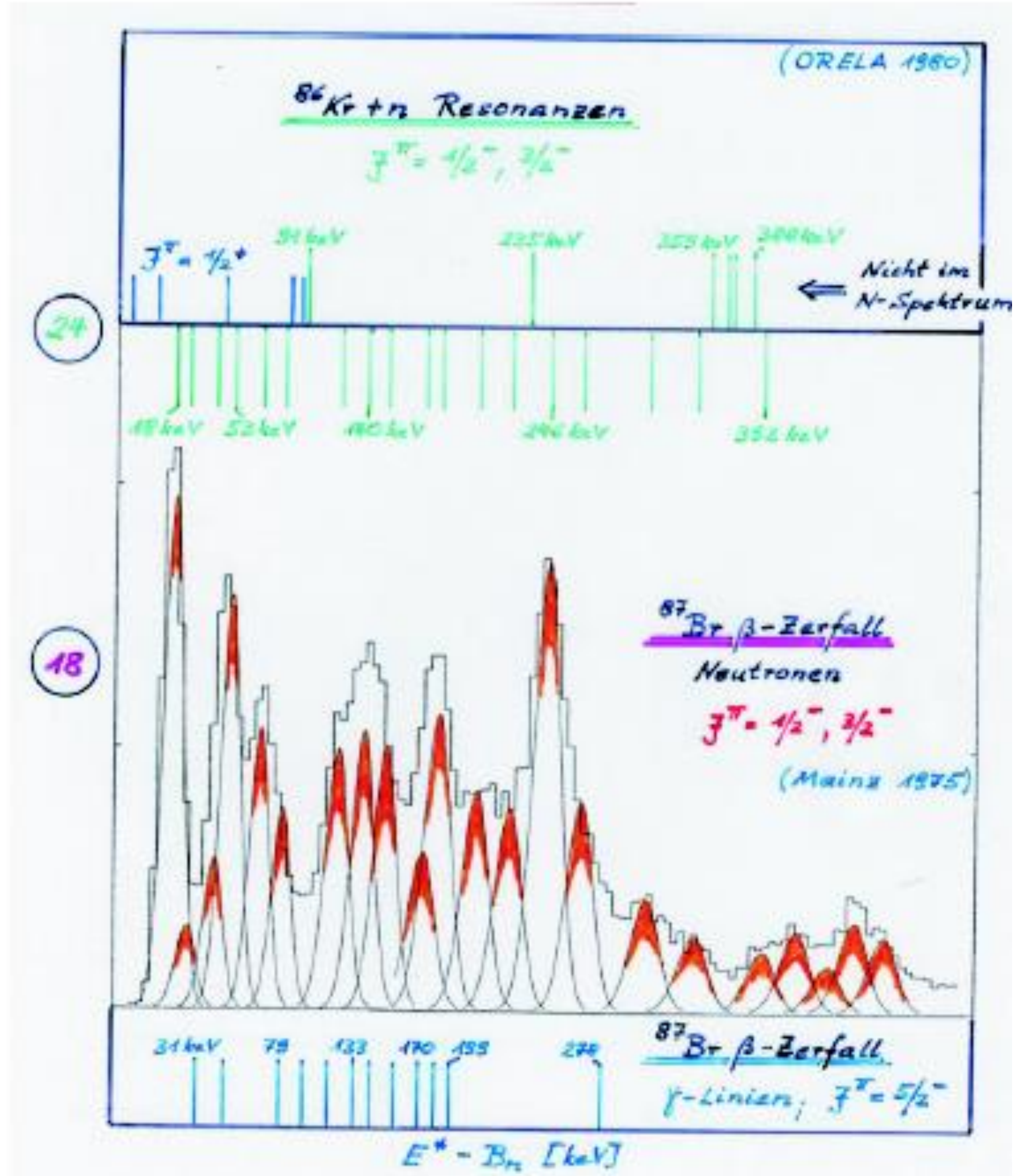
# βdn-emission as inverse process to n-capture

## Two experiments:

$^{86}Kr(n,\gamma)^{87}Kr$ at **ORELA** (Oak Ridge)

$^{87}Br(\beta^-)^{87}Kr(n)^{86}Kr$ at **TRIGA** Mainz



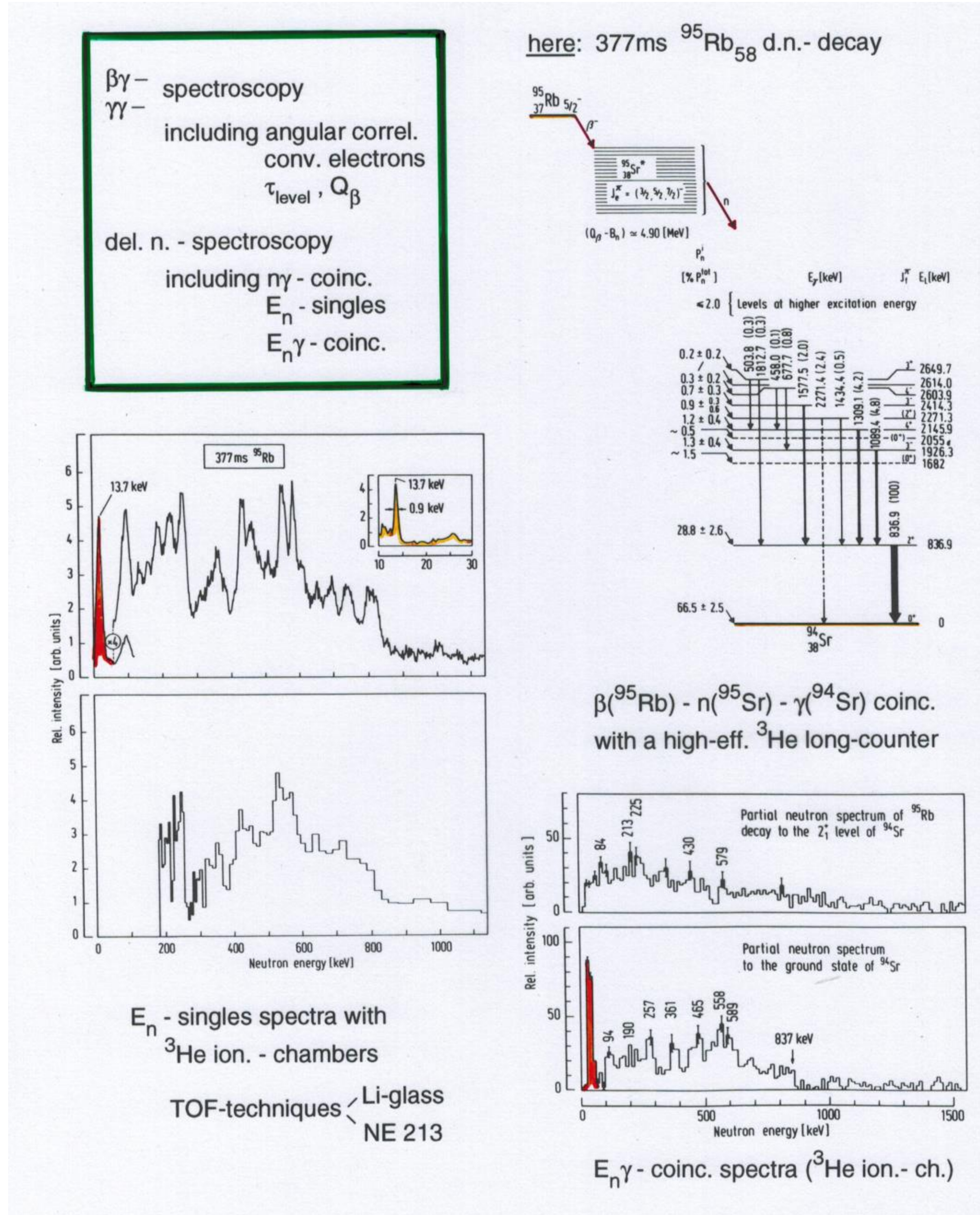



# The early 1980s: the “OSTIS Period” at ILL

## Detailed nuclear structure studies of neutron-rich Rb isotopes

$(Q_\beta - B_n)$ in $^{95}$Rb large enough to populate many excited states in the final nucleus $^{94}$Sr

**13.7 keV** peak in βdn ground-state spectrum
⇨ **p-wave neutron**



# βdn-Data ⇨ high-energy part of $S_\beta(E)$

Z. Phys. A312, 43 (1983)

## The Beta-Decay of $^{95}Rb$ and $^{97}Rb$

K.-L. Kratz, H. Ohm, A. Schröder et al.

The high-energy part of $S_\beta(E > B_n)$ is given by the βdn-energy spectra and $P_n(i)$-values

Combination of γ- and βdn-data ↷ exp. $S_\beta(E)$

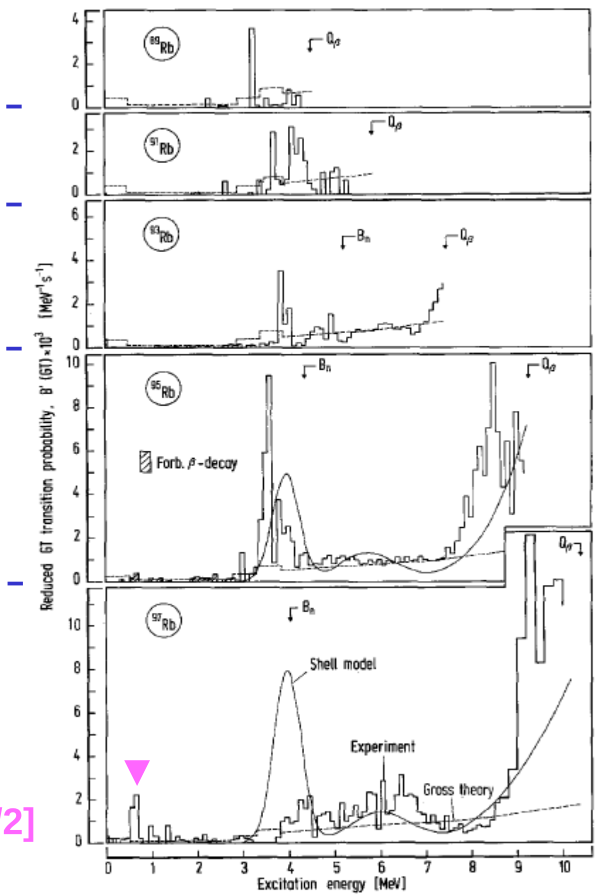
N=52
15.2 m

N=54
58 s

N=56
5.8 s

N=58
377 ms

N=60
170 ms




spherical

$\nu p_{1/2} \rightarrow \pi p_{3/2}$

$(\nu g_{7/2} \rightarrow \pi g_{9/2})$

$\nu g_{7/2} \rightarrow \pi g_{9/2}$

deformed

ν[420 1/2] ⇨ π[431 3/2]

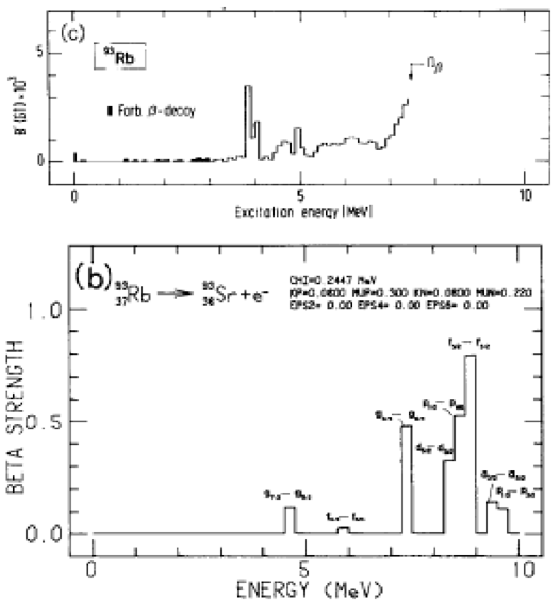
# $S_\beta(E)$ of Rb isotopes: the starting point of my collaboration with Peter

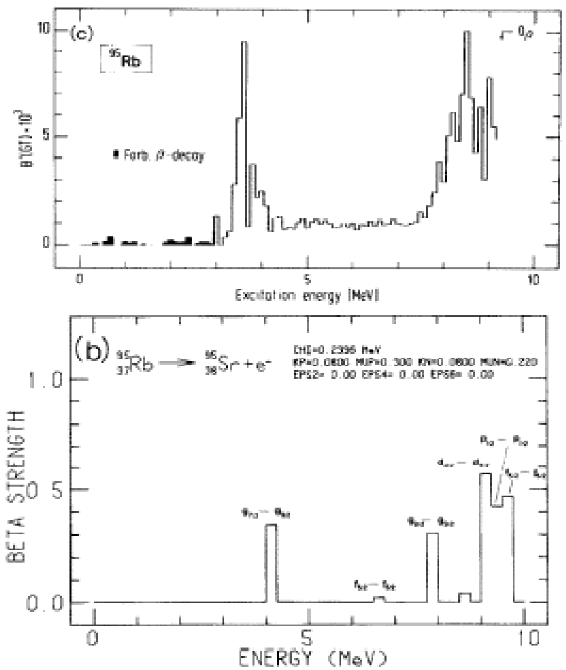
**Nucl. Phys. A417 (1984)**

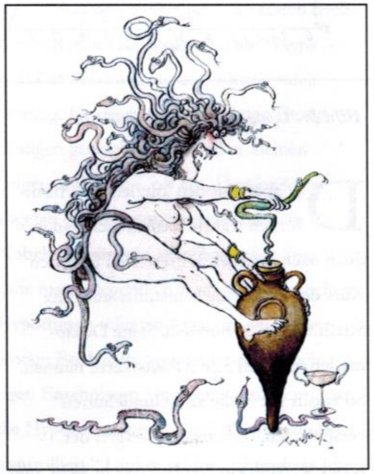
**CALCULATION OF GAMOW-TELLER β-STRENGTH FUNCTIONS IN THE RUBIDIUM REGION IN THE RPA APPROXIMATION WITH NILSSON-MODEL WAVE FUNCTIONS**

JOACHIM KRUMLINDE and PETER MÖLLER

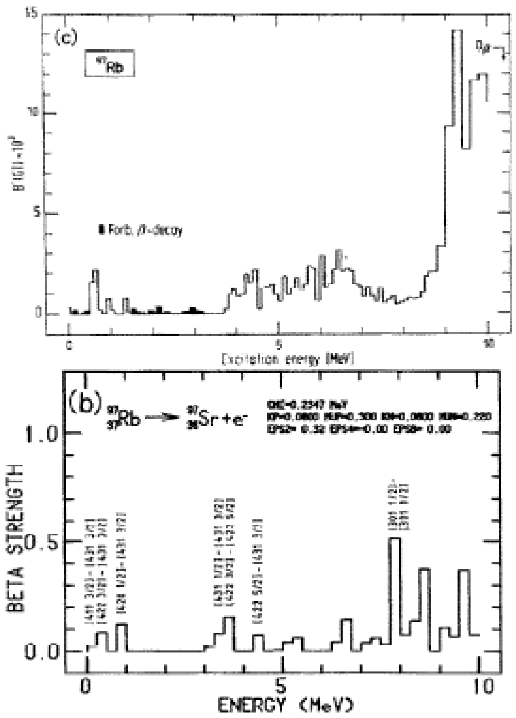
*Departments of Physics and Mathematical Physics, Lund University, Box 725, S22007 Lund, Sweden*



**The “antique” $S_\beta(E)$ paper**



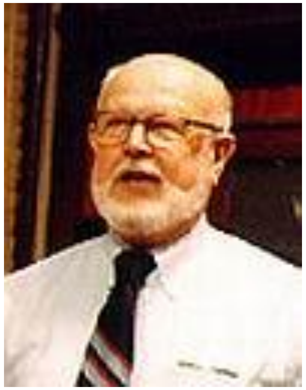

“We find good agreement between calculated and experimental spectra, provided an appropriate choice of single-particle parameters and deformation is made.”

## How we became interested in "astro" and "cosmo"

In 1981, I got an invitation to a USA – EU workshop on **"Nuclear Astrophysics",** to give a review talk about **"Beta-decay detection methods and limits"**

At this workshop, Willy Fowler gave a talk on isotopic **FUN** anomalies of Ca and Ti found in the EK-1-4-1 inclusion of the Allende meteorite

...in particular **$^{48}Ca/^{46}Ca = 250$ !**



"... Agreement for the **$^{46}Ca$** and **$^{49}Ti$** anomalies was obtained (within the assumed **"nβ"** nucleosynthesis process) by increasing the theoretical Hauser-Feshbach cross sections for $^{46}K(n,\gamma)$ and **$^{49}Ca(n,\gamma)$** by a factor 10 on the basis of probable thermal (30 keV, s-wave) resonances [....] in the compound nuclei **$^{47}K$** and **$^{50}Ca$**, respectively. ..."

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Already during this talk I wondered,

if we had already measured this resonance at **CERN / ISOLDE** via high-resolution β-delayed neutron spectroscopy of

**$^{50}K(\beta^-)^{50*}Ca(n)^{49}Ca$**

as "inverse process" to neutron capture of

8.7 min **$^{49}Ca(n,\gamma)^{50}Ca$** ....

# This led to the EK-1-4-1 story (I)

## Astron. Astrophys. 125 (1983)

**Determination of stellar neutron-capture rates for radioactive nuclei with the aid of $\beta$-delayed neutron emission**

**K.-L. Kratz, W. Ziegert, W. Hillebrandt & F.-K. Thielemann**

we discuss the reaction $^{49}Ca(n,\gamma)\ ^{50}Ca$ [$T_{1/2}(^{49}Ca) = 8.7$ min] with its inverse process [$^{50}K(\beta^-)$] $^{50}Ca^*(n)$ $^{49}Ca$ [$T_{1/2}(^{50}K) = 740$ ms]. The observed non-statistical behaviour of this reaction supports recent attempts to explain the isotopic anomalies in Ti observed in meteoritic inclusions.

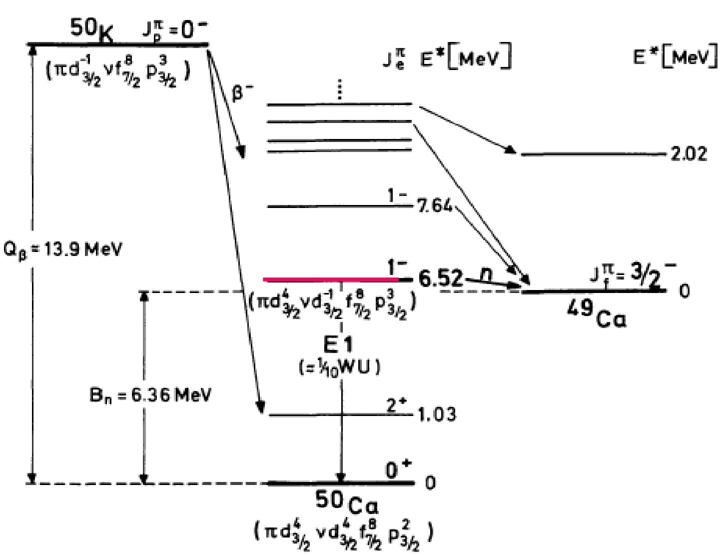
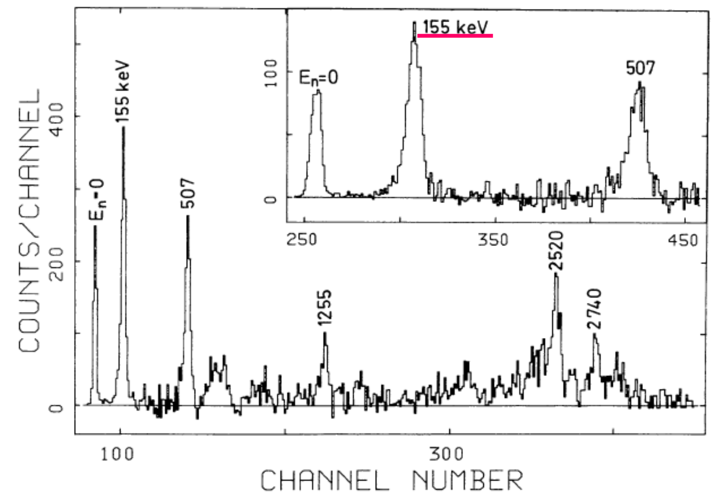



**Fig. 4.** Principal characteristics of $\beta$-delayed neutron decay of 740 ms $^{50}K$. The neutron-emitter state at 6.52 MeV ($J^\pi = 1^-$) in $^{50}Ca$ may have the properties of the $s$-wave neutron-capture state required by Sandler et al. (1982) (see text)




**Low-lying s-wave resonance in $^{50}Ca$ does exist; however, not at 30 keV, but at 155 keV.**

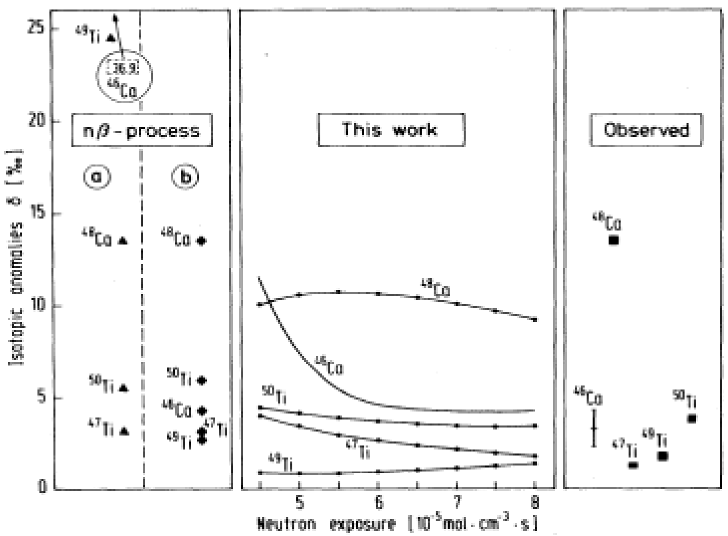
**nβ-process ⇨ r-process**

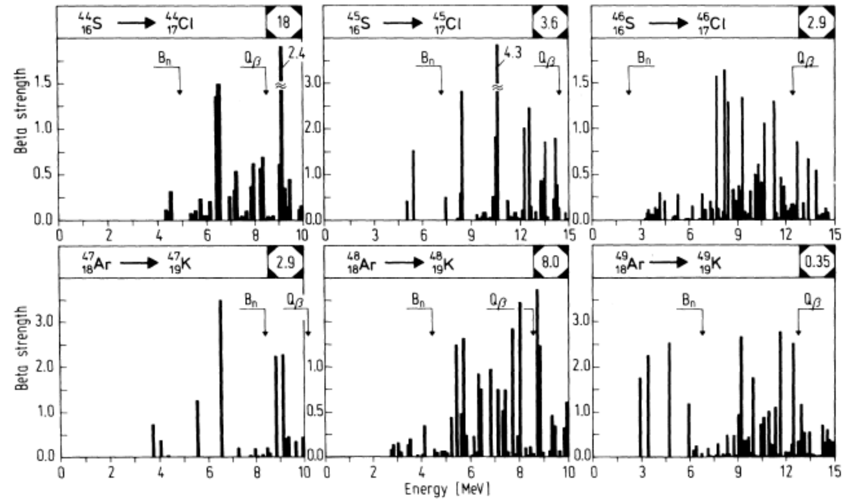
# The EK-1-4-1 story (II)

**Phys. Rev. Lett. 55 (1985)**

**Interpretation of the Solar $^{48}Ca/^{46}Ca$ Abundance Ratio and the Correlated Ca-Ti Isotopic Anomalies in the EK-1-4-1 Inclusion of the Allende Meteorite**

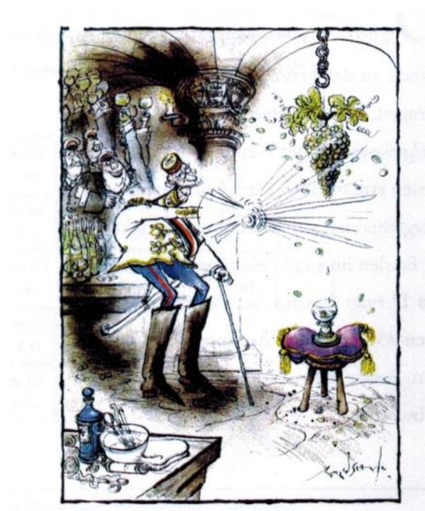

**W. Ziegert, M. Wiescher, K.-L. Kratz**
**P. Möller, J. Krumlinde**
**F.-K. Thielemann, W. Hillebrandt**


**GT strength functions from RPA**

**Left: Ca-Ti anomalies predicted by nβ-process;**
**(a) HF rates for all nuclei**
**(b) HF x 10 for $^{46}K$ and $^{49}Ca(n,\gamma)$.**
**Middle: Our astro-calculations.**
**Right: EK-1-4-1 observations.**



**Cleverness required**

# The EK-1-4-1 story (III) – 15 years later

MEMORIE DELLA
SOCIETÀ ASTRONOMICA ITALIANA
JOURNAL OF THE ITALIAN ASTRONOMICAL SOCIETY

ON THE ORIGIN OF THE CA-TI-CR ISOTOPIC ANOMALIES IN THE INCLUSION EK-1-4-1 OF THE ALLENDE-METEORITE

K.-L. KRATZ[1], W. BÖHMER[1], C. FREIBURGHAUS[2], P. MÖLLER[3], B. PFEIFFER[1], T. RAUSCHER[2], F.-K. THIELEMANN[2]

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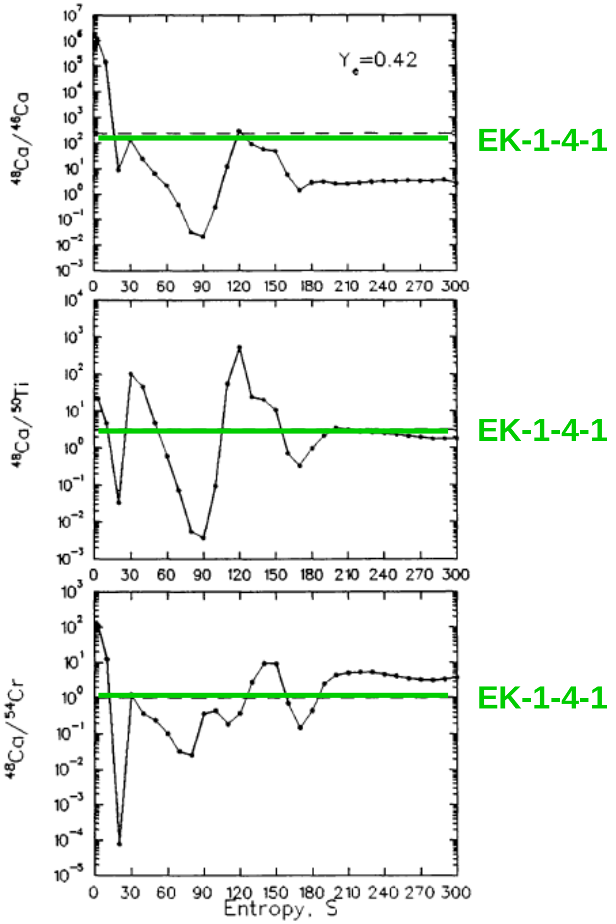
**Updates:**

Experiments at **CERN / ISOLDE** & **GANIL / LISE**
Theoretical n-capture rates (CN + DC)
Astrophysical network calculations



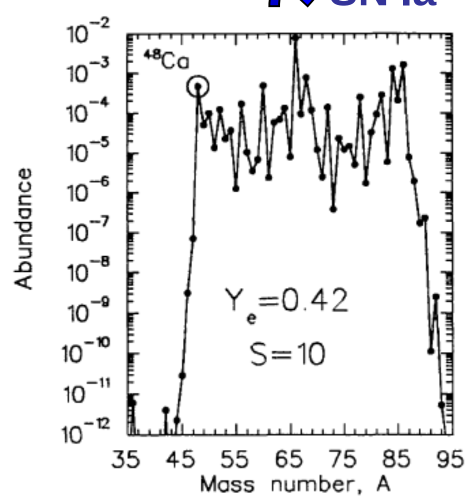

Two astrophysical scenarios:

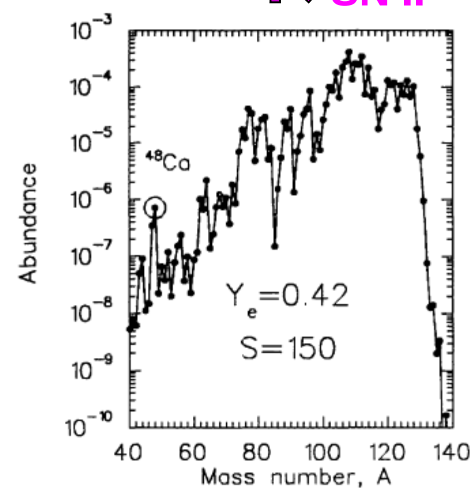
(i) **α-process** (ii) **weak r-process**

α-rich freezeout from

**Si-QSE** **Fe-QSE + n-capt.**

**SN Ia** **SN II**



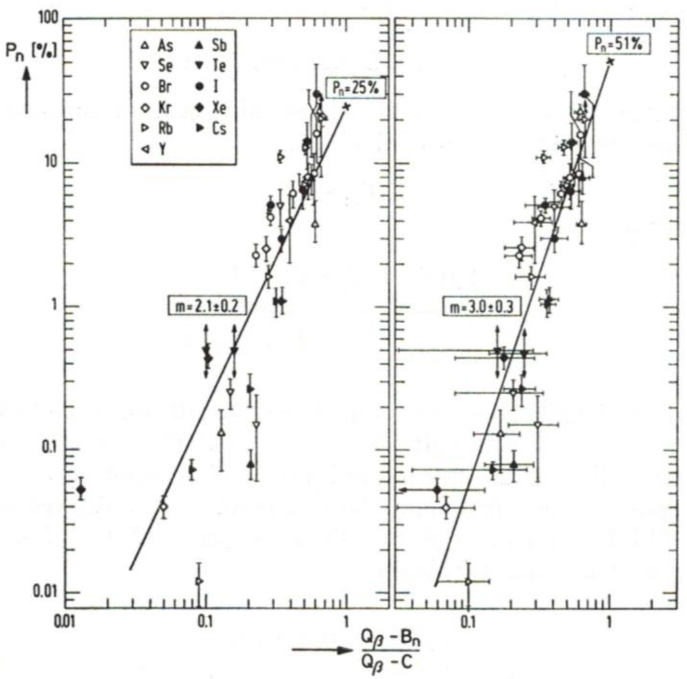
# Systematics of β-decay properties

**Z. Phys. 263, 435 (1973)**

## Systematics of Neutron Emission Probabilities from Delayed Neutron Precursors

K.-L. Kratz* and G. Herrmann

Institut für Kernchemie der Universität Mainz




Theoretically,

the two gross / integral β-decay quantities, $T_{1/2}$ and $P_n$, are interrelated via their traditional definition in terms of the so-called **β-strength function [$S_\beta(E)$]**

"Experimental" definition (Duke et al., 1970)

$$S_\beta(E) = \frac{b(E)}{f(Z, Q_\beta - E) \cdot T_{1/2}} \quad [s^{-1}MeV^{-1}]$$

| | |
|---|---|
| b(E) | absolute β-feeding per MeV, |
| $f(Z, Q_\beta-E)$ | Fermi function, |
| $T_{1/2}$ | β–decay half-life. |

$P_n$ as ratio of $S_\beta(E)$ x f above $B_n$ to total $S_\beta(E)$ x f within $Q_\beta$    $T_{1/2}$ as reciprocal $S_\beta(E)$ x f

assuming $S_\beta(E)$ = const.; $f \sim (Q_\beta - E)^5$ and cut-off energy C

**The "Kratz-Herrmann Formula"**

$$P_n = a[(Q_\beta - B_n)/(Q_\beta - C)]^b$$

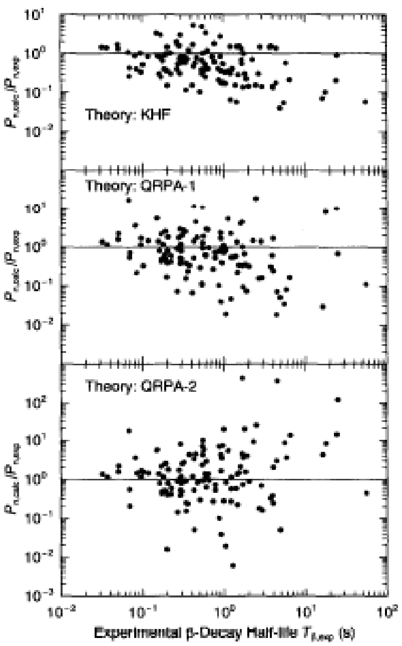
$$T_{1/2} = c[1/(Q_\beta - C)]^d$$

# From KHF to MPK (I)

**Progr. Nucl. Energy 41, 39 (2002)**

**STATUS OF DELAYED-NEUTRON PRECURSOR DATA: HALF-LIVES AND NEUTRON EMISSION PROBABILITIES**

Bernd Pfeiffer[1] and Karl-Ludwig Kratz
*Institut für Kernchemie, Universität Mainz, Germany*
Peter Möller
*Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545*

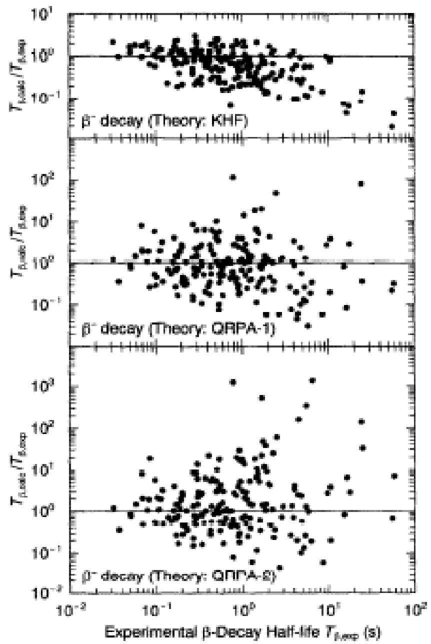



$\sigma_{rms}^2$

2.8

4.1

5.6

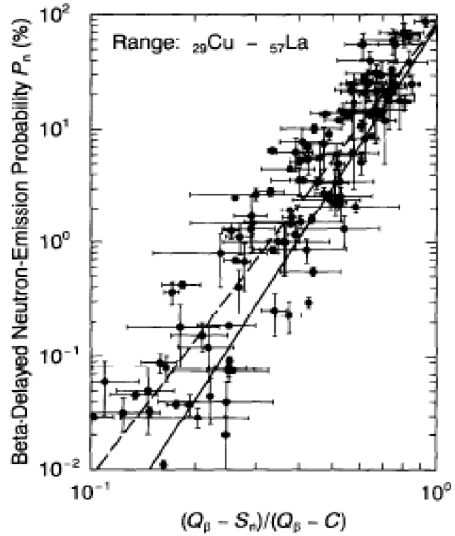



$\sigma_{rms}^2$

2.6

3.9

5.8




**Ratios of calculated to experimental $P_n$ (left) and $T_{1/2}$ (right):**

upper part: Kratz - Herrmann **Formula** (KHF)

lower parts: QRPA(GT); Pfeiffer – Kratz – Möller **Model** (MPK)

**…and Peter was not amused !**

# From KHF to MPK (II)

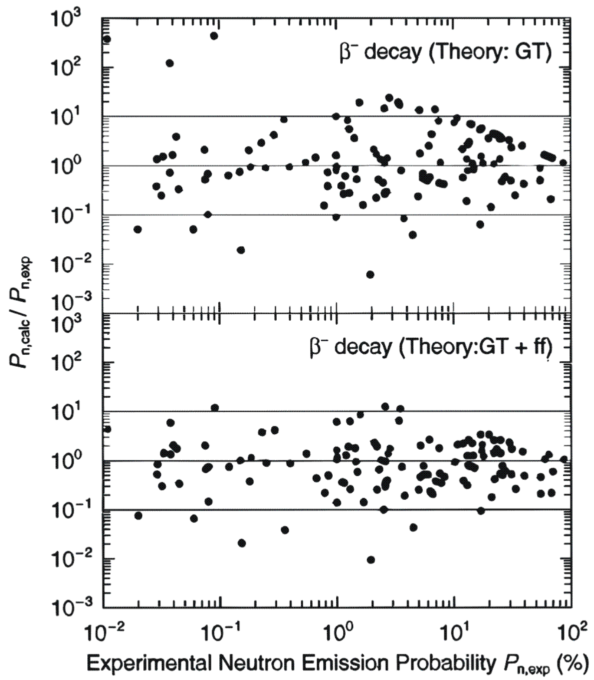
…a simple **formula** cannot be better than a microscopic **model** !

**Phys. Rev. C67 (2003)**

**New calculations of gross β-decay properties for astrophysical applications: Speeding-up the classical r-process**

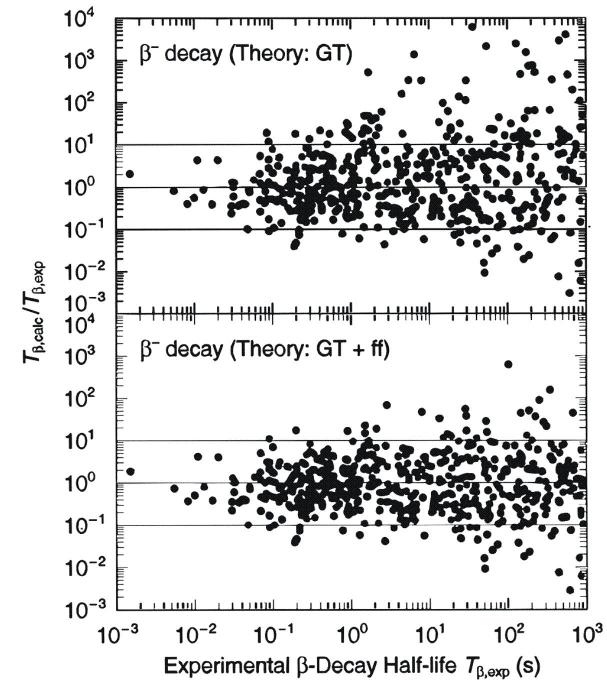
P. Möller, B. Pfeiffer, K.-L. Kratz

**Let's think about possible improvements…**




**Total error 3.5**

**$T_{1/2}$(GT+ff) become shorter**
**↷ faster r-process matter flow**




**Total error 3.1**

- **add ff-part of Gross Theory to GT-strength**
- **include empirical spreading of GT-strength**

# From KHF to MPK (III)

## $T_{1/2}$ and $P_n$ calculations in 3 steps:

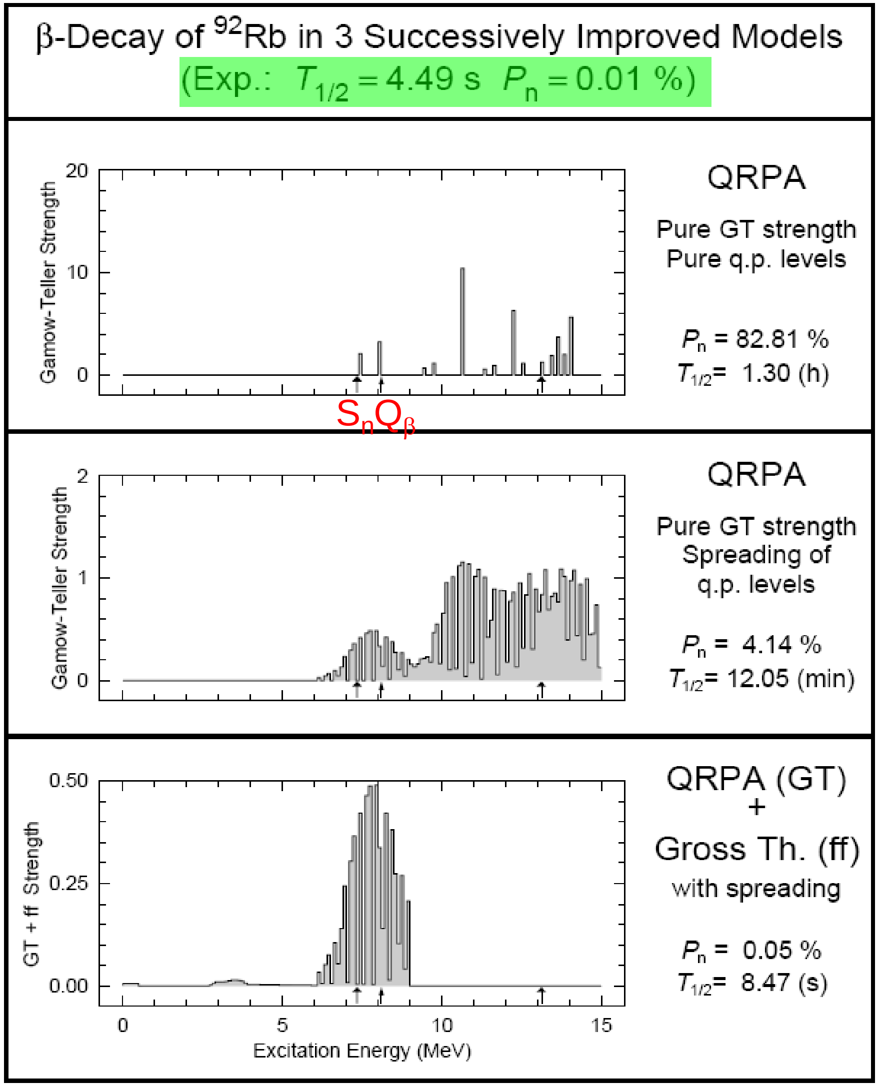
(1) **Mass model** FRDM
↷ $Q_\beta$, $S_n$, $\varepsilon_2$
Folded-Yukawa wave fcts.

**SP shell model** QRPA (pure GT)
with input from FRDM
potential: Folded Yukawa
pairing-model: Lipkin-Nogami

(2) as in (1) with empirical spreading of SP transition strength, as shown in experimental $S_\beta(E)$

(3) as in (2) with addition of first-forbidden strength from Gross Theory

**"Typical spherical example":**



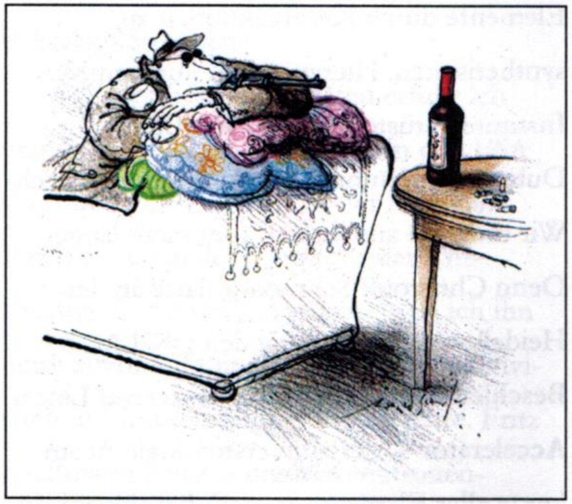

note: effects on $T_{1/2}$ and $P_n$ !

# From KHF to MPK (IV) -- TODAY

**The Astrophys. Journal 792 (2014)**

**A High-Entropy-Wind r-Process Study Based on Nuclear-Structure Quantities from the New Finite-Range Droplet Model FRDM(2012)**

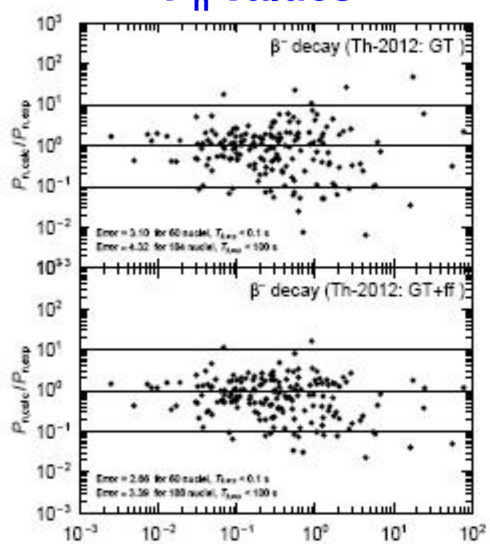
K.-L. Kratz, K. Farouqi, P. Möller



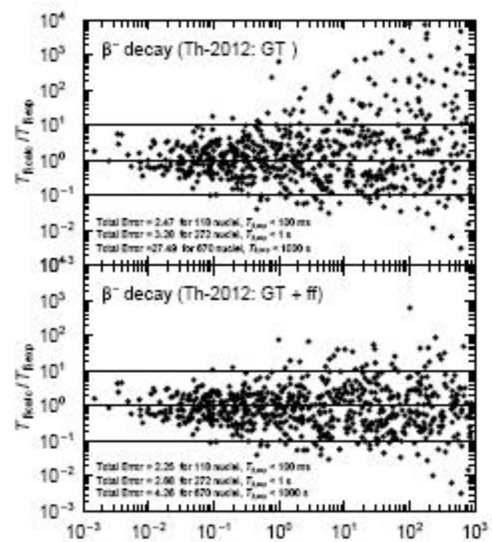
**Patience is required…**

**…consistent nuclear-data input for masses and β-decay properties from FRDM(2012) and QRPA(2012)**

**$P_n$ values**




**Half-lives**



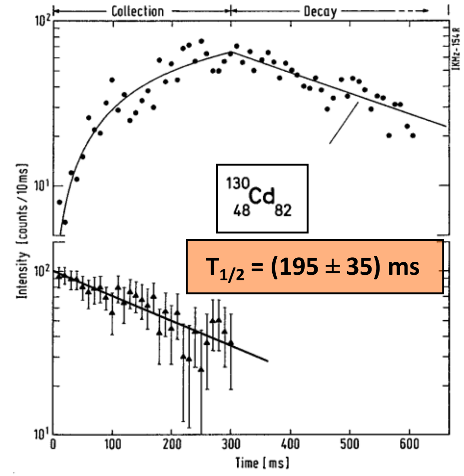

| $T_{1/2}(calc)/T_{1/2}(exp)$ | |
|---|---|
| 2002 | 3.9 |
| 2003 | 3.1 |
| 2012 | 2.7 |

# Solar system r-process abundances

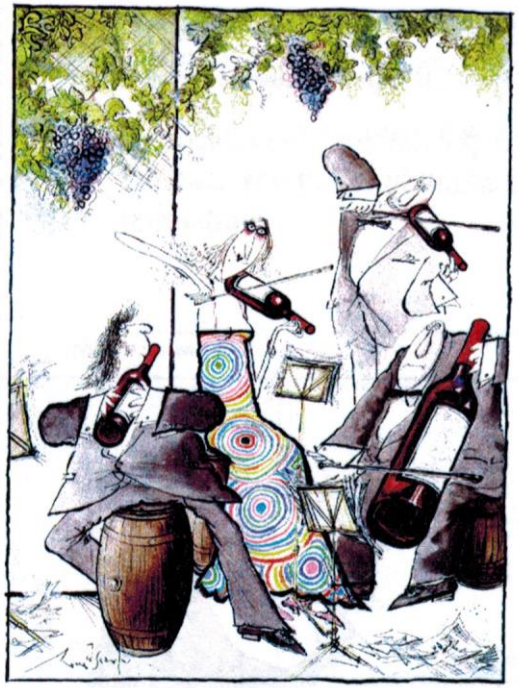
Inst. Phys. Conf. Ser. No. 88 / J. Phys. G: Nucl. Phys. 14 Suppl. (1988)

**Constraints on r-process conditions from beta-decay properties far off stability and r-abundances**

K-L Kratz, F-K Thielemann, W Hillebrandt, P Möller, V Harms, A Wöhr and J W Truran




**Model predictions at that time:**
**30 ms ≤ $T_{1/2}$ ≤ 1.2 s**



**Concerted action**

The Astrophys. J. 403 (1993)

ISOTOPIC *r*-PROCESS ABUNDANCES AND NUCLEAR STRUCTURE FAR FROM STABILITY: IMPLICATIONS FOR THE *r*-PROCESS MECHANISM

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Institut für Kernchemie, Universität Mainz, Fritz-Straβmann-Weg 2, D-W-6500 Mainz, Germany
JEAN-PHILIPPE BITOUZET[1] AND FRIEDRICH-KARL THIELEMANN
Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138
AND
PETER MÖLLER AND BERND PFEIFFER
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*Received 1991 August 13; accepted 1992 July 14*

# The FK$^2$L waiting-point approach (I)

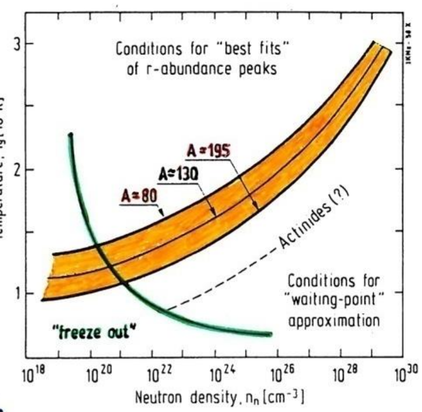
## With the nuclear physics knowledge at that time…

J. Phys. G 24 (1988)

With $T_{1/2}$(exp) and $N_{r,\odot}$ test of "waiting-point concept":

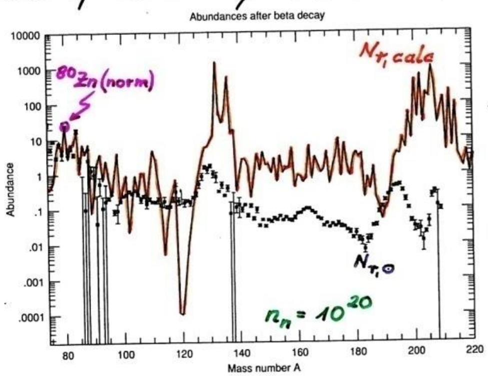
correlate $T_{1/2} \rightleftharpoons N_{r,\odot}$

→ deduce $T_9 - n_n$ band conditions to fit the $A \simeq 80$ and 130 $N_{r,\odot}$-peaks.




Ap. J. 403 (1993)

Static and time-dependent r-process calculations for "freeze-out" conditions.
Use of internally consistent nuclear-physics input (FRDM + QRPA).




Steady-flow NOT global

- wrong trend, increasing $N_r$ with A
- $A \simeq 130$ and 195 peaks shifted, too large; ⇒ indicates too low $n_n$

When we (Hillebrandt, Kratz, Möller, Thielemann) startet in 1986, already numerous attempts existed to search for the site(s) of the r-process…
but **none really successful**.

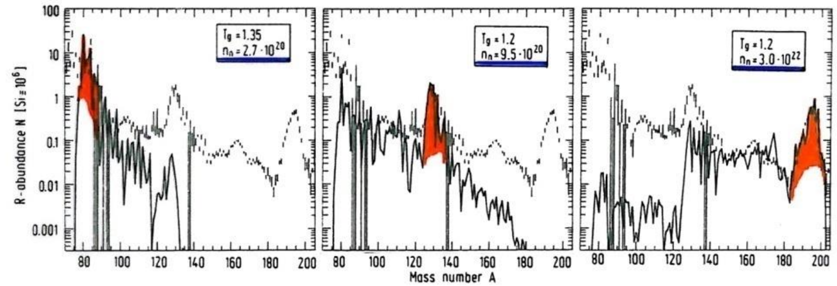
**Therefore, our approach:**

The **"site-independent"** waiting-point concept was utilised to deduce unique astrophysical conditions for an r-process.
For the first time, a "unified model" (FRDM & RPA) for all nuclear properties was used, aided by the first experimental nuclear data of r-process isotopes:
**N=50** $^{79}$Cu, $^{80}$Zn, $^{81}$Ga,
N=56,57 $^{91,92}$Br,
N=60-63 $^{97\text{-}100}$Rb,
**N=82** $^{130}$Cd, $^{131}$In

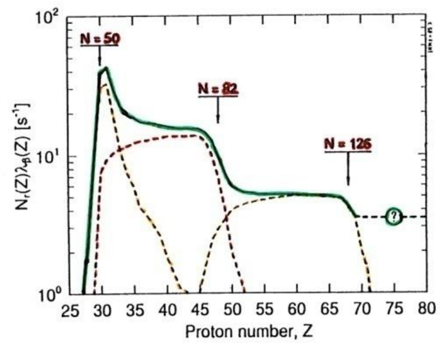
# The FK²L waiting-point approach (II)

Consequences:

- r-process must have several components
  with different n-densities
  and different r-process paths.




- steady-flow is only local,
  breaks down at each $N_r$-peak
  ≙ at $N_{magic}$



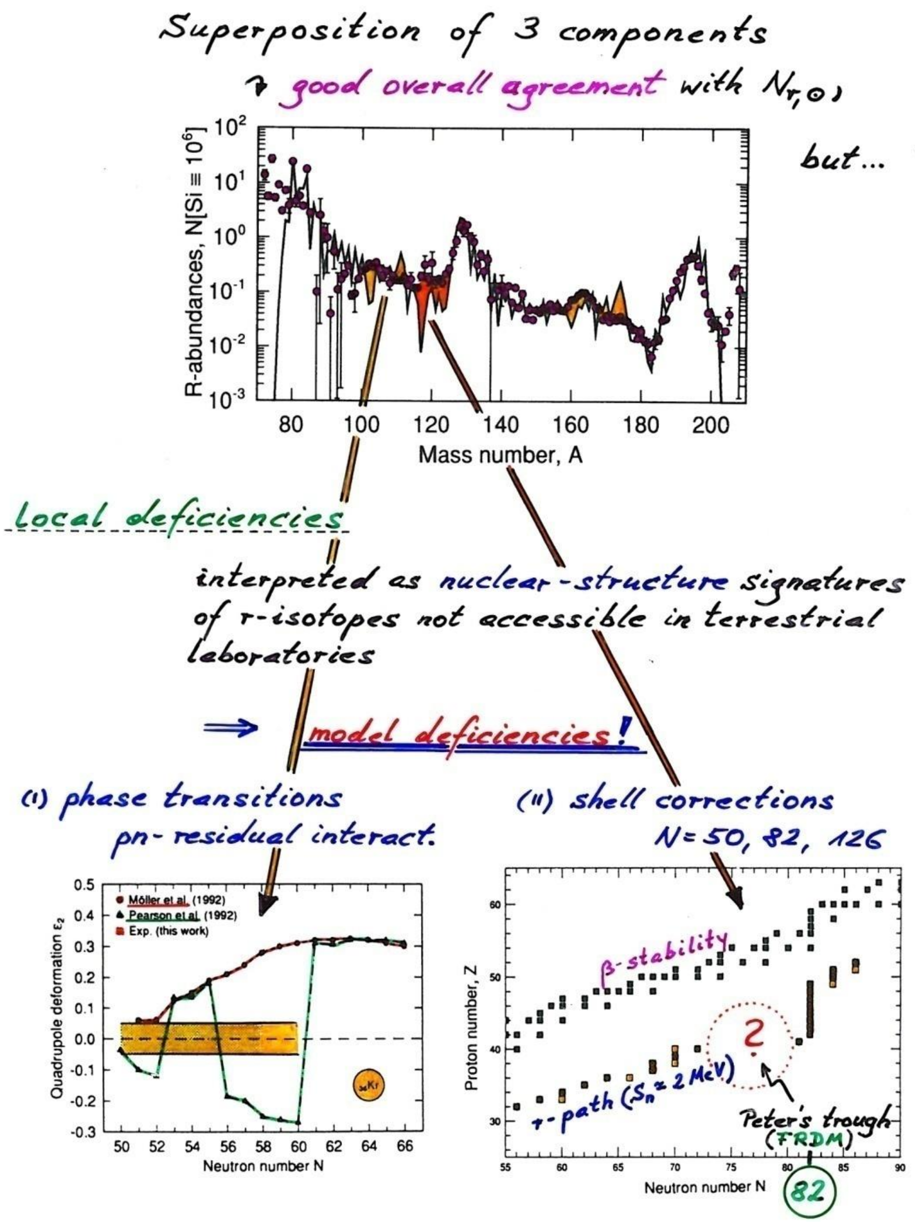

analogous to s-process
with $N_s \sigma = const.$

empirical r-process picture
with superposition of
(minimum) 3 components

$N_r \lambda_\beta = const.$

weighting acc. to
$T_{1/2}$ ($^{80}Zn$, $^{130}Cd$, $^{135}Tm$)

# The FK²L waiting-point approach (III)




first euphoric statement by **W. Hillebrandt**:
"...best $N_{r,\odot}$ fit so far...;
long-standing problem solved..."

birth of N=82
**"shell-quenching"**
idea ...

...this catchword coined by
**W. Nazarewicz** later led to
numerous misinterpretations...

# Consequences of the FK$^2$L waiting-point approach

1. **A unified approach**
   **…for the first time all nuclear properties were studied in a selfconsistent way**

2. **Remaining deficiencies**
   **…missing monopole and quadrupole p–n residual interactions**

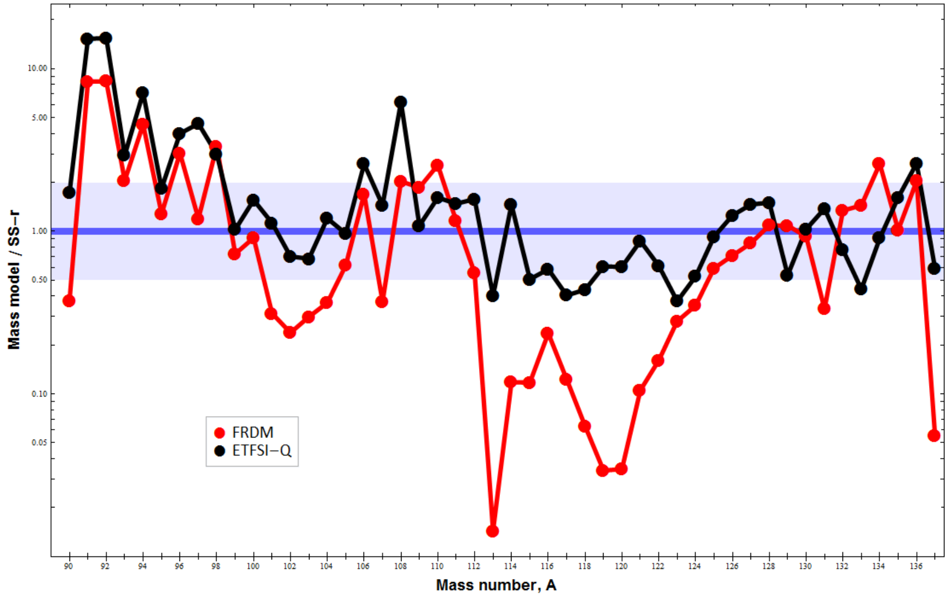
**Consequences:**

**with the filling of the $1g_{9/2}$ proton shell, the $1g_{7/2}$ neutron orbitals are lowered, not contained in the QRPA:**

**the spherical N=56 subshell strength in the QRPA is underestimated, leading to a too early onset of deformation over a too wide Z-range;**

**overestimation of the Z=50 and N=82 shell strengths ⇨**
**r-path moved from (Z,N) = (40,72) to (Z,N) = (41,81) leaving a gap in A of 10 units, where not a single waiting-point isotope will exist; this leads, for example, to the famous A ~ 120 r-abundance trough ("Peter's trough")**

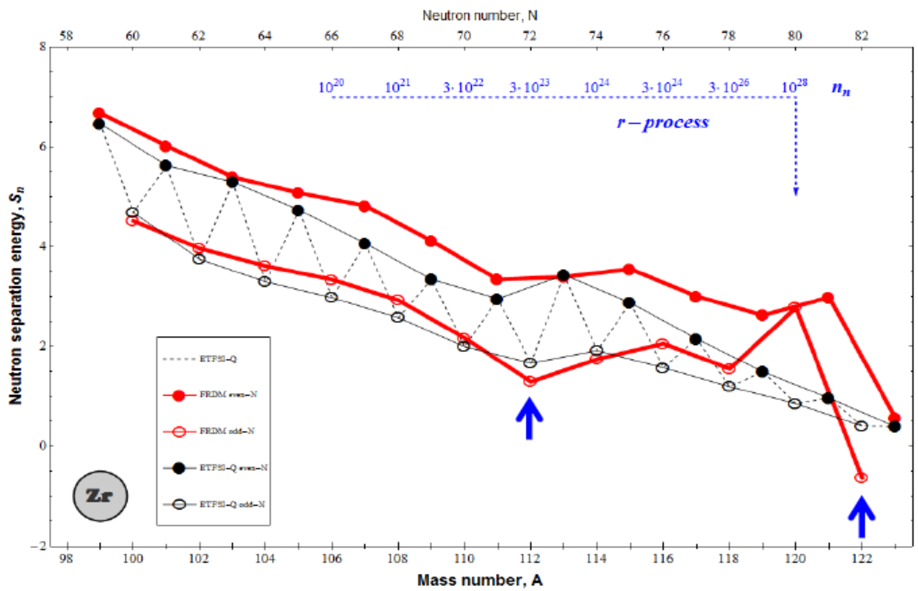
# Deviation from SS-r: FRDM vs. ETFSI-Q

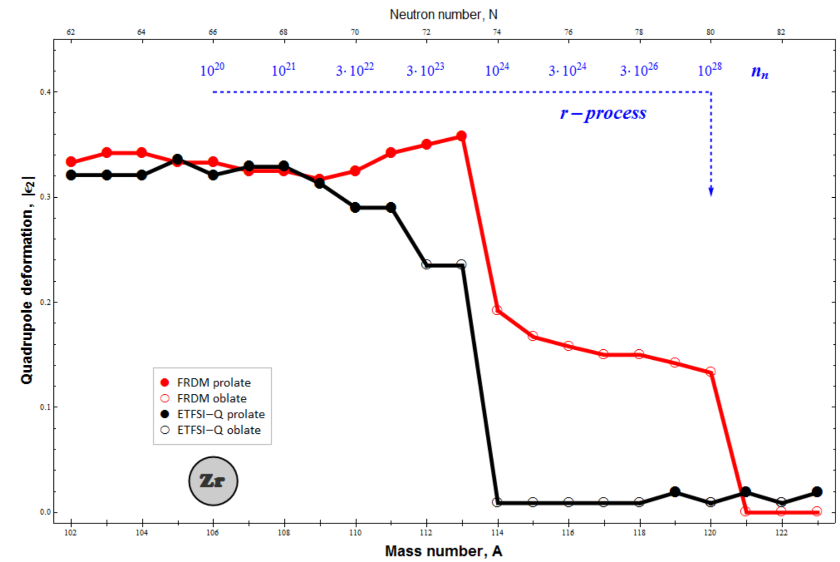



**How to fill up the FRDM A ≈ 115 "trough"?**

**e.g. "tampering" with the $T_{1/2}$ would require completely unrealistic long $T_{1/2}$(w.-p.) of the order 1 – 20 s**

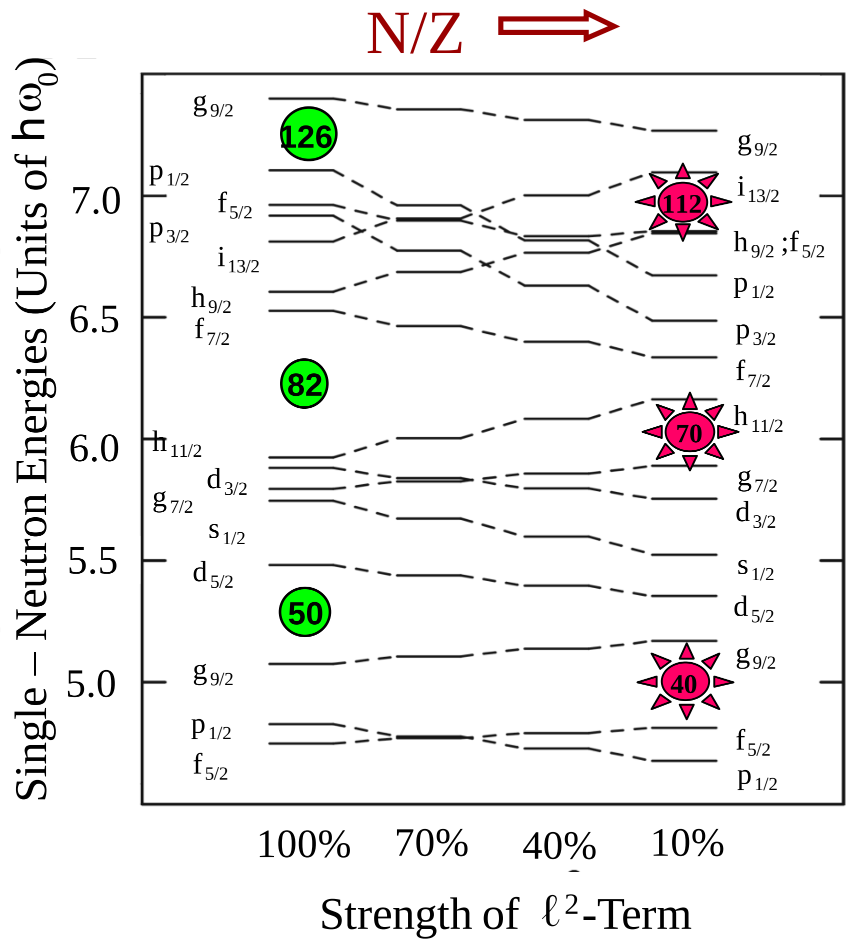
**⇨hence, the solution MUST lie in the masses ($S_n$) and the correlated trend of deformation in this shape-transition region before N=82**

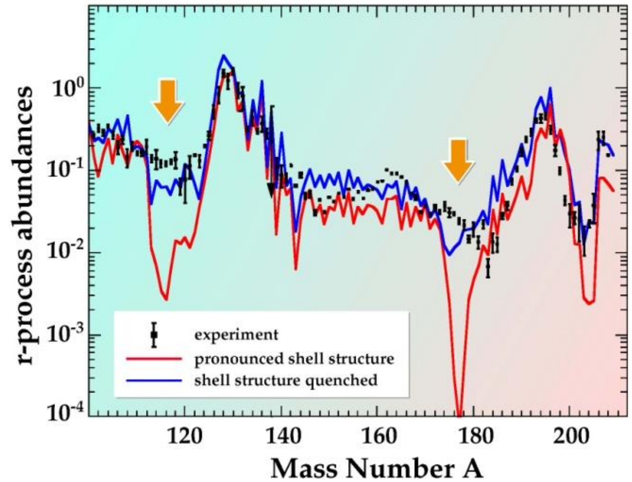


# Effects of N=82 "shell quenching"

…reduction of the spin-orbit coupling strength; caused by interaction between bound and continuum states.




- high-j orbitals ⇑ (e.g. $\nu g_{9/2}$, $\nu h_{11/2}$)
- low-j orbitals ⇓ (e.g. $\nu d_{5/2}$, $\nu f_{7/2}$)
- new "magic" numbers (e.g. 40, 70, 112)

**change of**

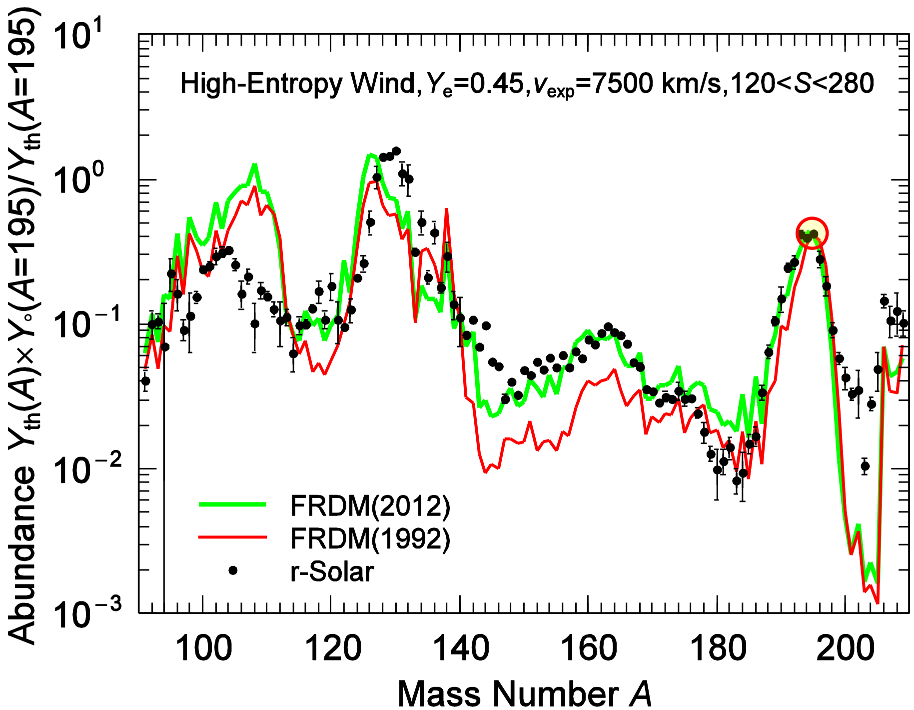
- shell-gaps
- deformation
- r-process path ($S_n$)
- r-matter flow ($\tau_n$)

**…controversial discussions until today !**

# First HEW calculations with FRDM(2012) and QRPA(2012)

**Good news at the end…**

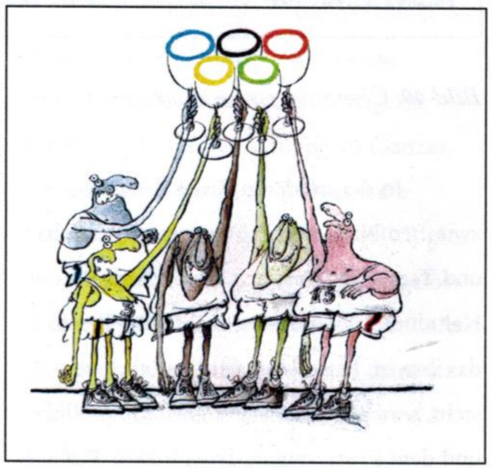
Comparison between $N_{r,\odot}$ and $N_{r,calc}$:
**FRDM(1992)** and **FRDM(2012)**




**Improvements and remaining deficiencies:**

- still overabundances in 80≤A≤110 region
- "abundance trough" at A≈120 removed
- 2nd r-peak slightly improved
- N=82 bottle-neck behavior improved
- REE "pygmy-peak" well reproduced
- shape of 3rd r-peak well reproduced
- shape-transition region above N=126 still imperfect ⇨ deep trough
- Pb, Bi too low ⇨ contribution from α-backday not yet included

**Success !!!**



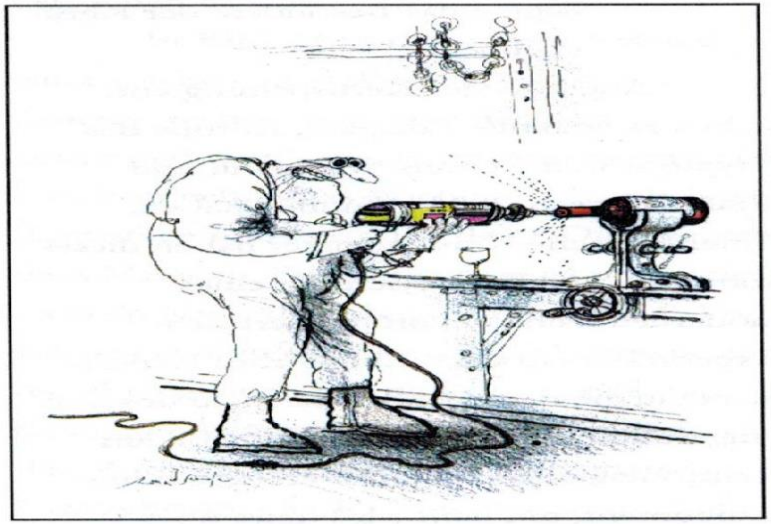
# Conclusion nuclear-structure models

**P. Möller, B. Pfeiffer & K.-L. Kratz, Phys. Rev. C67 (2003)**

"…let us emphasize that **there is no "correct" model in nuclear physics**. Any modeling of nuclear-structure properties involves **approximations**… with the goal to obtain a formulation that can be solved in practice, but that **"retains the essential features"** of the true system under study, so that one can still learn something.

It may well turn out, that when proceeding from a simplistic, macroscopic approach to a more microscopic model the first overall result may be worse just in terms of agreement between calculated and measured data. However, the **disagreements may now be understood** more easily, and further microscopic-based, realistic improvements will become possible."

**…drill to depth**



**… but still, Nature sometimes disagrees with my nice model.**

# Summary and conclusion

**…considerable progress during our 3 decades of collaboration,**

**but still a lot remains to be done**
**for the coming 30 years**
**in all interrelated fields…**

**However, right now**
**let's first celebrate**
**Peter's 70th birthday**

**Happy birthday !**

Bernd, Khalil, Oliver, K.-L.
and Gisela