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The Macroscopic-Microscopic Nuclear-Structure Model
Foundations and Results

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More details about masses, other projects (beta-decay, fission), associated ASCII data files, interactive access to data (type in Z, A and get specific data, contour maps) and figures are at

http://t2.lanl.gov/nis/molleretal/
Global Nuclear-Structure Modeling

Historically success is associated with

- Relatively simple ideas
- Few model parameters
- Consistent application
- Close look at experimental data
What is a model?

- Can be explained(!)

- Can describe new data

- Can describe other types of quantities than those that primarily motivated its development

- Can be generalized to describe new stuff.
Bethe-Weizsäcker Mass Model (1935)

In the first global MACROSCOPIC nuclear-mass model the nuclear ground-state mass is given by

\[ E_{\text{mac}}^{FL}(Z, N, \text{shape}) = \]

\[ M_H Z \quad \text{(Hydrogen – atom mass)} \]

\[ + M_n N \quad \text{(Neutron mass)} \]

\[ - B(N, Z) \quad \text{(Nuclear binding energy)} \]
Nuclear Binding Energy BW (1935)

The nuclear binding energy according to BW is given by

\[ B(N, Z) = \]

\[ + a_v A \quad \text{(Volume energy)} \]

\[ - a_s A^{2/3} \quad \text{(Surface energy)} \]

\[ - a_C \frac{Z^2}{A^{1/3}} \quad \text{(Coulomb energy)} \]

\[ - a_I \frac{(N - Z)^2}{A} \quad \text{(Symmetry energy)} \]

\[ - \delta(A) \quad \text{(Pairing energy)} \]
B(N, Z) =

+ avA \quad \text{(Volume energy)}

- asA^{2/3}Bs(\beta) \quad \text{(Surface energy)}

- ac\frac{Z^2}{A^{1/3}}B_C(\beta) \quad \text{(Coulomb energy)}

- aI\frac{(N - Z)^2}{A} \quad \text{(Symmetry energy)}

- \delta(A) \quad \text{(Pairing energy)}
Nuclear Deformation Energy

Let the nuclear surface be described by

\[ r(\theta, \phi) = R_0 [1 + \alpha_2 P_2(\cos \theta)] \]

The surface energy lowest order Taylor expansion:

\[ E_s = E_s^0 (1 + \frac{2}{5} \alpha_2^2) \]

The Coulomb energy lowest order Taylor expansion

\[ E_C = E_C^0 (1 - \frac{1}{5} \alpha_2^2) \]

The energy at deformation \( \alpha_2 \) relative to spherical shape

\[ E_{\text{def}}(\alpha_2) = E_C(\alpha_2) + E_s(\alpha_2) - (E_C^0 + E_s^0) \]

If \( E_{\text{def}} \) is negative then the system has no barrier wrt fission

\[ E_{\text{def}}(\alpha_2) = \frac{2}{5} \alpha_2^2 E_s^0 - \frac{1}{5} \alpha_2^2 E_C^0 < 0 \]

\[ 1 < \frac{E_C^0}{2E_s^0} = x \]
The surface energy for a sphere

\[ E_s^0 = 17.80 A^{2/3} \]

The Coulomb energy for a sphere

\[ E_C^0 = 0.7103 \frac{Z^2}{A^{1/3}} \]

The fissility parameter \( x \):

\[ x = \frac{Z^2}{50.13 A} \]

<table>
<thead>
<tr>
<th>( Z )</th>
<th>( A )</th>
<th>( x )</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>124</td>
<td>0.402</td>
</tr>
<tr>
<td>82</td>
<td>208</td>
<td>0.645</td>
</tr>
<tr>
<td>92</td>
<td>138</td>
<td>0.709</td>
</tr>
<tr>
<td>100</td>
<td>252</td>
<td>0.792</td>
</tr>
<tr>
<td>114</td>
<td>298</td>
<td>0.870</td>
</tr>
<tr>
<td>125</td>
<td>328</td>
<td>0.950</td>
</tr>
<tr>
<td>130</td>
<td>335</td>
<td>1.006</td>
</tr>
</tbody>
</table>
\[ \sigma_{th} = 0.831 \text{ MeV} \]
Hexadecapole Deformation $\varepsilon_4$

$^{272}\text{110}$  \ $\lambda_p = 34.80, \ a_p = 0.80$ fm

Single-Proton Energy (MeV)

Spheroidal Deformation $\varepsilon_2$
trend is consistent with a straight line, defining \( (Z^2/A)_e = 40.2 \pm 0.7 \). The equation of the line leads to the semiempirical formula,

\[
M_2 - M_1 = 0.090(40.2 \pm 0.7 - Z^2/A)A. \tag{4}
\]

One may combine Eq. (4) with the relation:

\[
M_1 + M_1 = A - \nu \quad (\nu = \text{number of neutrons emitted in fission}),
\]

to predict the positions of the peaks in the yield curves of elements that have not yet been investigated. If an average value \( \nu = 2.8 \) is used, one finds

\[
M_2 = \frac{1}{4}A - 1.4 - 0.045(40.2 \pm 0.7 - Z^2/A)A, \tag{5}
\]

\[
M_1 = \frac{1}{2}A - 1.4 - 0.045(40.2 \pm 0.7 - Z^2/A)A. \tag{6}
\]

The present analysis provides a reason for the empirical observation that in the fission of different elements the position of the heavy peak remains approximately constant. If the degree of asymmetry remained unchanged from nucleus to nucleus, both peaks would move towards higher masses with increasing \( A \). In fact, there is superimposed on this shift a coming together of the peaks with increasing \( Z^2/A \). Since the over-all trend of \( Z^2/A \) is to increase with \( A \), the result is that for the light peak the two shifts add up whereas for the heavy peak they partly cancel. This is illustrated in Table I, where \( M_2 \) and \( M_1 \) calculated according to (5) and (6), are compared with the observed values.

Further measurements of fission asymmetries would be interesting, especially in the region of \( Z^2/A \) close to the critical value, where the present considerations suggest a rapid decrease of \( M_2 - M_1 \).

It is a pleasure to acknowledge stimulating discussions with Professor S. G. Thompson, Dr. A. C. Pappas, and Dr. T. Maris.

2 A. E. S. Green, Phys. Rev. 95, 1006 (1954).
3 W. J. Swiatecki (to be published).

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**Systematics of Spontaneous Fission Half-Lives**

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(Received July 18, 1955)

SEVERAL authors have noted the over-all trend of spontaneous fission half-lives to decrease with increasing \( Z^2/A \) as well as the considerable deviations (by several powers of 10) from any smooth dependence on this parameter. We should like to discuss the close correlation which seems to exist between the half-lives and the finer details in the systematics of the ground-state masses of nuclei.3

A simple way of exhibiting this correlation is to plot the deviation \( \delta \tau \) from a straight line in a plot of \( \tau = \log_{10}(\text{half-life}) \) vs \( Z^2/A \), against deviations \( \delta M \) of the masses \( M \) of the nuclei from a smooth reference surface \( M_{\text{ref}}(A,Z) \). We made such a plot, with \( M_{\text{ref}} \) taken to be the semiempirical mass surface of Green4 (based on the liquid drop model):

\[
\delta M = M - M_{\text{ref}},
\]

\[
M_{\text{ref}} = 1000A - 8.3557A + 19.120A^4 + 0.76275A^2 + 0.25444(N-Z)^2/A + 0.240(N-Z) \text{ millimass units.} \tag{1}
\]

The experimental masses \( M \) were taken from Glass et al.4

In the case of even-even nuclei the plot of \( \delta \tau \) vs \( \delta M \) suggested a series of straight lines, one for each \( Z \), indicating that for the isotopes of one element special stability of a nucleus (small \( \delta M \)) is invariably associated with a longer lifetime (large \( \delta \tau \)). The lines had approximately the same slope, thus defining a spontaneous-fission hindrance factor which corresponds to about 100 times longer lifetime for each millimass unit of extra stability. This suggested that if the observed lifetimes were correct for the variations in stability of the ground states, a more regular dependence of \( \tau \) on \( Z^2/A \) might be discernible.

Figure 1 shows the effect on the plot of \( \tau \) vs \( Z^2/A \) of adding to the observed \( \tau_{\text{exp}} \) an empirical correction \( k\delta M \) (\( k \approx 5 \) if \( \delta M \) in mMU). For even-even nuclei the values of \( \tau_{\text{exp}} + k\delta M \) define a fairly smooth curve, with indications of a similar curve for odd-A nuclei. [In a

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**Table I. Positions of the peaks in the fission yield curves.**

<table>
<thead>
<tr>
<th>Compound nucleus</th>
<th>Position of peaks</th>
<th>Formulas (3), (6)</th>
<th>Remarks</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( M_2 ) \quad</td>
<td>( M_1 ) \quad</td>
<td>( M_2 ) \quad</td>
<td>( M_1 ) \quad</td>
</tr>
<tr>
<td>Th\textsuperscript{232}</td>
<td>140 \quad 91</td>
<td>139.1 \quad 91.1</td>
<td>Low-energy \quad</td>
<td>c \quad</td>
</tr>
<tr>
<td>U\textsuperscript{238}</td>
<td>140 \quad 98</td>
<td>141.1 \quad 95.1</td>
<td>neutron \quad</td>
<td>d \quad</td>
</tr>
<tr>
<td>U\textsuperscript{238}</td>
<td>138.5 \quad 95</td>
<td>138.2 \quad 95.0</td>
<td>fission \quad</td>
<td>b, e</td>
</tr>
<tr>
<td>U\textsuperscript{238}</td>
<td>137 \quad 93</td>
<td>136.2 \quad 95.0</td>
<td>\quad</td>
<td>\quad</td>
</tr>
<tr>
<td>Pu\textsuperscript{239}</td>
<td>138 \quad 99</td>
<td>137.9 \quad 99.3</td>
<td>\quad</td>
<td>\quad</td>
</tr>
<tr>
<td>U\textsuperscript{238}</td>
<td>140 \quad 96</td>
<td>140.2 \quad 95.0</td>
<td>Spontaneous \quad</td>
<td>f, g</td>
</tr>
<tr>
<td>C\textsuperscript{136}</td>
<td>136 \quad 103</td>
<td>134.7 \quad 104.5</td>
<td>fission \quad</td>
<td>g \quad</td>
</tr>
<tr>
<td>C\textsuperscript{136}</td>
<td>139 \quad 108</td>
<td>140.2 \quad 109.0</td>
<td>\quad</td>
<td>\quad</td>
</tr>
</tbody>
</table>

* The uncertainty in the observed values of \( M_2 \) and \( M_1 \) is of the order of \( \pm 1 \) or \( \pm 2 \) mass units (It is more in the cases of U\textsuperscript{238} and U\textsuperscript{238}). No systematic attempt has been made to adjust \( A - M_2 - M_1 \) to agree with available information on the number of emitted neutrons.

3 E. B. Steinberg and M. S. Freedman, Nucl. Phys. 24, 12 (1955).
6 E. B. Steinberg and S. I. Glendenin, Phys. Rev. 95, 867 (1954).
preliminary plot the hindrance factor $k$ was taken to be 5. A small but significant further smoothing of the points resulted from making $k$ vary with $Z^2/A$ according to $k = 5 - (Z^2/A - 37.5)$. This is the case shown in Fig. 1."

The result can be stated in the form of an empirical formula for half-lives; e.g., for even-even nuclei,

$$\tau_{eo} = f(Z^2/A) - b\delta M,$$

where $f$ is the curve defined by the even-even points in Fig. 1. The relation of the points for odd-\(A\) nuclei to the curve obtained from (2) by a shift upwards of 6.6 units is also shown in Fig. 1. The lifetime of the odd-odd nucleus $^{234}\text{E}\text{u}$ (einsteinium, $Z = 99$) is consistent with a further shift of 4.9 units. The curve $f(Z^2/A)$ can be represented for example by a cubic, which leads to the following formulas for the lifetimes:

$$\tau_{eo} = 18.2,$$
$$\tau_{odd \, A} = 24.8 - 7.80 + 0.35\theta + 0.073\theta^2 - (5 - \theta)\delta M,$$

and $\delta M$ is the deviation in mMU of the experimental mass from the surface (1).

Table I compares the observed half-lives with the values calculated by means of (3). The remarkable degree of smoothing achieved by means of the un-sophisticated correction $b\delta M$ is illustrated by the fact that the deviations from (3) rarely exceed 0.5. (Note that a shift in $\tau$ of this amount would be produced by an error of 0.1 mMU in $\delta M$.)

The importance of shell structure in the fission process is suggested by the fact that, according to the present considerations, the oscillations of the masses (associated with individual particle structure) in the range $\delta M = 1 - 3$ mMU shorten the lifetimes by factors of $10^5$ to $10^9$. On the other hand the irregularities in the original plot of $\tau_{exp}$ against $Z^2/A$ are seen to be largely due to irregularities in the ground-state masses, associated with shell structure in the ground-state configuration. The smoothness of the points $\tau_{exp} + b\delta M$ suggests that, after correcting for shell structure in the ground-state configuration, the description of the fission process in terms of a model in which single-particle features are treated in an average way may be useful. Qualitative reasons for the greater validity of such an averaged description for the more strongly deformed nuclear shapes occurring in fission may be found in the disappearance for such shapes of degeneracies in the energy spectrum associated with the proximity to a spherically symmetric configuration.

It is a pleasure to acknowledge discussions with Professor S. G. Thompson and Dr. A. C. Pappas and stimulating contacts with Dr. Aage Bohr and Dr. B. R. Mottelson and members of the C.E.R.N. Theoretical Study Group in Copenhagen.

2 The existence of correlations between nuclear masses, fission thresholds, and half-lives has been considered by Professor D. Frisch, to whom I am greatly indebted for stimulating discussions.
3 A. E. S. Green, Phys. Rev. 95, 1006 (1954).
Potential Energy of Deformation

We use the macroscopic-microscopic method introduced by Swiatecki and Strutinsky:

\[ E_{\text{pot}}(\text{shape}) = E_{\text{macr}}(\text{shape}) + E_{\text{micr}}(\text{shape}) \]  \hspace{1cm} (1)

The macroscopic term is calculated in a liquid-drop type model (for a specific deformed shape).

The microscopic correction is determined in the following steps

1. A shape is prescribed
2. A single-particle potential with this shape is generated. A spin-orbit term is included.
3. The Schrödinger equation is solved for this deformed potential and single-particle levels and wave-functions are obtained
4. The shell correction is calculated by use of Strutinsky’s method.
5. The pairing correction is calculated in the BCS or Lipkin-Nogami method.
Shape Parameterizations

For small distortions we use multipole expansions, for example the $\beta$ parameterization:

$$r(\theta, \phi) = R_0 (1 + \sum_{l=1}^{\infty} \sum_{m=-l}^{l} \beta_{lm} Y_l^m)$$

For large deformations near the outer saddle in the actinide region or beyond we use the three-quadratic-surface parameterization:

$$\rho(z)^2 = \begin{cases} 
  a_1^2 - \frac{a_1^2}{c_1^2} (z - l_1)^2, & l_1 - c_1 \leq z \leq l_1 \\
  a_2^2 - \frac{a_2^2}{c_2^2} (z - l_2)^2, & z_2 \leq z \leq l_2 + c_2 \\
  a_3^2 - \frac{a_3^2}{c_3^2} (z - l_3)^2, & z_1 \leq z \leq z_2 
\end{cases}$$
Model spin and parity compared to experiment

![Graph showing neutron number versus proton number with regions labeled FRDM (1992), Rare earths, A ≈ 80, A ≈ 100. Points indicate agreement and disagreement.]
Model spin and parity compared to experiment

**FRDM (1992)**

Actinides

- Agreement
- Disagreement

Neutron Number $N$ vs. Proton Number $Z$
\[ \beta^- \text{ decay, } \Delta \nu = 2 \text{ transition} \]

\[ \begin{array}{c}
\text{P} \\
\begin{array}{ccc}
\text{n} & \text{n} & \text{n} \\
\text{p} & \text{n} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{Z} - 1 & \text{N} + 1
\end{array}
\end{array} \]

\[ \begin{array}{c}
\begin{array}{ccc}
\text{n} & \text{n} & \text{n} \\
\text{p} & \text{n} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{Z} & \text{N}
\end{array}
\end{array} \]

\[ \begin{array}{c}
\begin{array}{ccc}
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\text{p} & \text{n} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{Z} - 1 & \text{N} + 1
\end{array}
\end{array} \]

\[ \begin{array}{c}
\begin{array}{ccc}
\text{n} & \text{n} & \text{n} \\
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\text{p} & \text{p} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{Z} & \text{N}
\end{array}
\end{array} \]

\[ \beta^- \text{ decay, } \Delta \nu = 0 \text{ transition} \]

\[ \begin{array}{c}
\text{P} \\
\begin{array}{ccc}
\text{n} & \text{n} & \text{n} \\
\text{p} & \text{n} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{Z} - 1 & \text{N} + 1
\end{array}
\end{array} \]

\[ \begin{array}{c}
\begin{array}{ccc}
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\text{p} & \text{p} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{Z} & \text{N}
\end{array}
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\[ \begin{array}{c}
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\text{p} & \text{n} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{Z} - 1 & \text{N} + 1
\end{array}
\end{array} \]

\[ \begin{array}{c}
\begin{array}{ccc}
\text{n} & \text{n} & \text{n} \\
\text{p} & \text{n} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{Z} & \text{N}
\end{array}
\end{array} \]

\[ \beta^- \text{ decay, } \Delta \nu = 2 \text{ transition} \]

\[ \begin{array}{c}
\text{P} \\
\begin{array}{ccc}
\text{n} & \text{n} & \text{n} \\
\text{p} & \text{n} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{Z} - 1 & \text{N} + 1
\end{array}
\end{array} \]

\[ \begin{array}{c}
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\text{p} & \text{p} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{Z} & \text{N}
\end{array}
\end{array} \]

\[ \begin{array}{c}
\begin{array}{ccc}
\text{n} & \text{n} & \text{n} \\
\text{p} & \text{n} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{Z} - 1 & \text{N} + 1
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\begin{array}{ccc}
\text{n} & \text{n} & \text{n} \\
\text{p} & \text{n} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{p} & \text{p} & \text{n} \\
\text{Z} & \text{N}
\end{array}
\end{array} \]
Hexadecapole Deformation $\varepsilon_4$

Spheroidal Deformation $\varepsilon_2$

Single-Proton Energy (MeV)

Single-Neutron Energy (MeV)
CALCULATION OF GAMOW-TELLER $\beta$-STRENGTH FUNCTIONS IN THE RUBIDIUM REGION IN THE RPA APPROXIMATION WITH NILSSON-MODEL WAVE FUNCTIONS

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(Revised 3 August 1983)

Abstract: We calculate allowed Gamow–Teller and, in a few cases, Fermi $\beta$-strength functions in a model that is applicable to studies of nuclei throughout the periodic system. For our first study we have selected a sequence of rubidium isotopes, namely $^{85}$Rb–$^{87}$Rb. We develop a model that uses calculated Nilsson-model wave functions, spherical or deformed, as the case may be, as the starting point for determining the wave functions of the mother and daughter nuclei in the $\beta$-decay. Pairing is treated in the BCS approximation. To account for the retardation of low-energy GT decay rates we add, as is customarily done, a simple residual interaction specific to GT decay, namely $V_{GT} = -\gamma_{1}^{-}\gamma_{1}^{+}$, to the hamiltonian. This residual interaction is treated in the RPA approximation. The strength of the interaction is adjusted to get agreement between the calculated and experimental energy of the giant Gamow–Teller resonance for $^{208}$Pb and $^{144}$Sm. Since the present model is based on calculated wave functions and single-particle levels, studies of nuclei far from stability, where little experimental information is available, are more straightforward relative to calculations where “experimental” levels are used. The model can treat deformed nuclei employing wave functions calculated to desired accuracy, within the framework of the model, for the deformed single-particle well. The calculations show that use of single-particle parameters appropriate to the region studied and taking deformation into account is important. We find good agreement between calculated and experimental spectra over the region studied, provided an appropriate choice of single-particle parameters and deformation is made.

1. Introduction

A theoretical understanding of $\beta$-strength functions is important for the interpretation of the large amount of experimental data that is now being collected on, for instance, the giant Gamow–Teller resonance $^{1-2}$) and on $\beta$-decay spectra of nuclei far from stability $^{3}$. More references on these subjects are found in the conference report $^{4}$) of the 4th International Conference on Nuclei far from Stability and references quoted therein. The $\beta$-strength function must also be known for theoretical studies of phenomena where the $\beta$-strength function cannot be easily measured. Examples of such processes are the decay from the $r$-process line to the line of $\beta$-stability $^{5-7}$), $\beta$-delayed particle emission $^{7}$) and the production of transuranium elements by neutron capture and subsequent decay by $\beta$-emission, fission and neutron emission $^{8,9}$).

A variety of models have been used to calculate $\beta$-strength functions. The gross theory of $\beta$-decay $^{10}$) describes, because of its statistical character, only the average
Fig. 8. Calculated $\beta^-$ GT strength function for $^{95}$Rb with (a) the $A=100$ set of $\kappa$ and $\mu$, and (b) the $N=60$ set of $\kappa$ and $\mu$, in units of $4f^2\text{ MeV}^{-1}$. The peaks are labeled with the quantum numbers of the neutron (first) and proton (last) orbital involved in the transition. (c) Experimental results from ref. 3).
Fig. 9. Calculated $\beta^-$ GT strength function for $^{87}$Rb treated as (a) a spherical nucleus, and (b) a deformed nucleus, in units of $4f^2$ MeV$^{-1}$. The peaks in (b) are labeled with the asymptotic quantum numbers of the neutron (first) and proton (last) orbital involved in the transition. (c) Experimental results from ref. 3.)
Folded-Yukawa potential

\[ P_{1n} = 29.93 \% \quad T_{1/2} = 41.76 \text{ (ms)} \]

\[ {}^{99}_{37}\text{Rb} \rightarrow {}^{99}_{38}\text{Sr} + e^- \]

\[ \varepsilon_2 = 0.317 \quad \Delta_n = 0.99 \text{ MeV} \quad \lambda_n = 33.36 \text{ MeV} \]

\[ \varepsilon_4 = 0.007 \quad \Delta_p = 1.11 \text{ MeV} \quad \lambda_p = 30.48 \text{ MeV} \]

\[ \varepsilon_6 = -0.014 \quad \text{(L-N)} \quad a = 0.80 \text{ fm} \]

\[ Q_{\beta} \]

\[ T_{1/2,\text{exp}} = 50.3 \text{ (ms)} \]

\[ P_{1n,\text{exp}} = 15.9 \% \]
$\beta^-$ decay (Theory: GT)

Total Error = 21.16 for 546 nuclei (13 clipped), $T_{\beta, \text{exp}} < 1000$ s

Total Error = 3.73 for 184 nuclei, $T_{\beta, \text{exp}} < 1$ s

$\beta^-$ decay (Theory: GT + ff)

Total Error = 3.08 for 184 nuclei, $T_{\beta, \text{exp}} < 1$ s

Total Error = 4.82 for 546 nuclei, $T_{\beta, \text{exp}} < 1000$ s
$\beta^{-}$ decay (Th-2012: GT)

Total Error = 2.25 for 118 nuclei, $T_{\beta, \text{exp}} < 100$ ms
Total Error = 2.68 for 272 nuclei, $T_{\beta, \text{exp}} < 1$ s
Total Error = 4.26 for 670 nuclei, $T_{\beta, \text{exp}} < 1000$ s

$\beta^{-}$ decay (Th-2012: GT + ff)

Total Error = 2.25 for 118 nuclei, $T_{\beta, \text{exp}} < 100$ ms
Total Error = 2.68 for 272 nuclei, $T_{\beta, \text{exp}} < 1$ s
Total Error = 4.26 for 670 nuclei, $T_{\beta, \text{exp}} < 1000$ s
Table 1: Analysis of the discrepancy between calculated (with our 1997–2003 models) and measured $\beta^-$-decay half-lives. The experimental data file is Nubase12. The number of 0.1s half-lives increased from 42 to 118.

<table>
<thead>
<tr>
<th>Model</th>
<th>$n$</th>
<th>$M_{r_0}$</th>
<th>$M_{r_0}^{10}$</th>
<th>$\sigma_{r_0}$</th>
<th>$\sigma_{r_0}^{10}$</th>
<th>$\Sigma_{r_0}$</th>
<th>$\Sigma_{r_0}^{10}$</th>
<th>$T_{\beta,exp}^{max}$ (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GT</td>
<td>670</td>
<td>0.38</td>
<td>2.39</td>
<td>1.22</td>
<td>16.47</td>
<td>1.27</td>
<td>18.79</td>
<td>1000.00</td>
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<tr>
<td>GT + FF</td>
<td>670</td>
<td>0.02</td>
<td>1.04</td>
<td>0.64</td>
<td>4.36</td>
<td>0.64</td>
<td>4.36</td>
<td>1000.00</td>
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<tr>
<td>GT</td>
<td>552</td>
<td>0.28</td>
<td>1.89</td>
<td>0.98</td>
<td>9.45</td>
<td>1.01</td>
<td>10.32</td>
<td>100.00</td>
</tr>
<tr>
<td>GT + FF</td>
<td>552</td>
<td>0.02</td>
<td>1.06</td>
<td>0.57</td>
<td>3.73</td>
<td>0.57</td>
<td>3.73</td>
<td>100.00</td>
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<tr>
<td>GT</td>
<td>414</td>
<td>0.20</td>
<td>1.59</td>
<td>0.71</td>
<td>5.16</td>
<td>0.74</td>
<td>5.50</td>
<td>10.00</td>
</tr>
<tr>
<td>GT + FF</td>
<td>414</td>
<td>0.04</td>
<td>1.10</td>
<td>0.51</td>
<td>3.21</td>
<td>0.51</td>
<td>3.22</td>
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<tr>
<td>GT</td>
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<td>0.15</td>
<td>1.42</td>
<td>0.54</td>
<td>3.49</td>
<td>0.56</td>
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<td>1.09</td>
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<tr>
<td>GT</td>
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<td>1.29</td>
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<td>0.49</td>
<td>3.06</td>
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<tr>
<td>GT + FF</td>
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<tr>
<td>GT</td>
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<tr>
<td>GT + FF</td>
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<td>2.44</td>
<td>0.39</td>
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<tr>
<td>GT</td>
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<td>0.04</td>
<td>1.10</td>
<td>0.37</td>
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<tr>
<td>GT + FF</td>
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<td>0.00</td>
<td>1.01</td>
<td>0.36</td>
<td>2.28</td>
<td>0.36</td>
<td>2.28</td>
<td>0.05</td>
</tr>
<tr>
<td>GT</td>
<td>29</td>
<td>0.11</td>
<td>1.29</td>
<td>0.34</td>
<td>2.21</td>
<td>0.36</td>
<td>2.30</td>
<td>0.02</td>
</tr>
<tr>
<td>GT + FF</td>
<td>29</td>
<td>0.07</td>
<td>1.19</td>
<td>0.34</td>
<td>2.17</td>
<td>0.35</td>
<td>2.21</td>
<td>0.02</td>
</tr>
</tbody>
</table>
\[ \beta^- \text{ decay (Theory: GT)} \]

Total Error = 3.52 \times 10^{-2}

Experimental Neutron-Emission Probability \( P_{n,\text{exp}} \) (%)

\[ \beta^- \text{ decay (Theory: GT + ff)} \]

Total Error = 5.54 \times 10^{-3}

\[ \frac{P_{n,\text{calc}}}{P_{n,\text{exp}}} \]

Experimental Neutron-Emission Probability \( P_{n,\text{exp}} \) (%)
β⁻ decay (Th-2012: GT)

Error = 3.10 for 60 nuclei, $T_{\beta,\text{exp}} < 0.1$ s
Error = 4.32 for 184 nuclei, $T_{\beta,\text{exp}} < 100$ s

β⁻ decay (Th-2012: GT+ff)

Error = 2.66 for 60 nuclei, $T_{\beta,\text{exp}} < 0.1$ s
Error = 3.39 for 188 nuclei, $T_{\beta,\text{exp}} < 100$ s
New Masses in Audi 2003 Evaluation, Relative to 1989, Compared to Theory

von Groote et al. (1976)

Proton-rich nuclei only
\[ \sigma_{402} = 0.983 \text{ MeV} \]
\[ \mu_{402} = 0.645 \text{ MeV} \]

Neutron and proton-rich nuclei
\[ \sigma_{1323} = 0.629 \text{ MeV} \]
\[ \sigma_{529} = 1.308 \text{ MeV} \]
\[ \mu_{529} = 0.884 \text{ MeV} \]

Neutron-rich nuclei only
\[ \sigma_{127} = 2.159 \text{ MeV} \]
\[ \mu_{127} = 1.733 \text{ MeV} \]
New Masses in Audi 2003 Evaluation, Relative to 1989, Compared to Theory

Hilf et al. (1976)

Proton-rich nuclei only
\[ \sigma_{402} = 0.605 \text{ MeV} \]
\[ \mu_{402} = 0.081 \text{ MeV} \]

Neutron and proton-rich nuclei
\[ \sigma_{1323} = 0.631 \text{ MeV} \]
\[ \sigma_{529} = 1.069 \text{ MeV} \]
\[ \mu_{529} = 0.478 \text{ MeV} \]

Neutron-rich nuclei only
\[ \sigma_{127} = 2.310 \text{ MeV} \]
\[ \mu_{127} = 1.838 \text{ MeV} \]
Seeger-Howard (1975)

\[ \sigma_{309} = 0.956 \text{ MeV} \]
\[ \sigma_{\text{rms}} = 0.704 \text{ MeV} \]

\[ M_{\text{exp}} - M_{\text{calc}} (\text{MeV}) \]

Neutrons from \( \beta \)-stability
$\sigma_{346} = 0.738$ MeV

$\sigma_{\text{rms}} = 0.276$ MeV

Neutrons from $\beta$-stability

$Liran-Zeldes (1976)$
\[ \sigma_{1654} = 0.669 \text{ MeV} \]
\[ \sigma_{217} = 0.642 \text{ MeV} \]
Successive FRDM enhancements

**Optimization** (2006)
Better search for optimum FRDM parameters.
Accuracy improvement: 0.01 MeV

**New mass data base (AME2003)** (2006)
Better agreement than with AME1989.
Accuracy improvement: 0.04 MeV

**Full 4D energy minimization** (2006–2008)
Full 4D minimization($\epsilon_2, \epsilon_3, \epsilon_4, \epsilon_6$) step=0.01.
Accuracy improvement: 0.02 MeV

Also yields correct SHE gs assignments.
Accuracy improvement: 0.01 MeV

**L variation** (2009–2011)
Accuracy improvement: 0.02 MeV

**Improved gs correlation energies** (2012)
Accuracy improvement: 0.01 MeV
FRDM(1992) adj. to AME1989  Comp. to AME 2011

Discrepancy (Exp. − Calc.)

$\sigma_{1654} = 0.669 \text{ MeV}$

$\sigma_{671} = 0.528 \text{ MeV}$

FRDM(2012)  Compared to AME2011

Discrepancy (Exp. − Calc.)

$\sigma_{2149} = 0.5595 \text{ MeV}$

$\sigma_{154} = 0.5694 \text{ MeV}$

$\mu_{154} = 0.0367 \text{ MeV}$
$^{72}_{36}\text{Kr}_{36}$

Scale 0.20 (MeV)

Spheroidal Deformation $\varepsilon_2$
Number of Minima

Depth > 0.20 MeV, $E_{ex} < 2.0$ MeV, $\varepsilon_2 < 0.45$

Difference (FRDM(1992) − FRDM(2012))

\[ |\Delta E| \text{ (MeV)} \]

Proton Number \( Z \)

Neutron Number \( N \)
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>38</td>
<td>80</td>
<td>-70.308</td>
<td>-70.313</td>
<td>-68.840</td>
<td>-1.473</td>
<td>-70.385</td>
<td>0.072</td>
</tr>
<tr>
<td>38</td>
<td>81</td>
<td>-71.528</td>
<td>-71.528</td>
<td>-70.650</td>
<td>-0.878</td>
<td>-71.688</td>
<td>0.160</td>
</tr>
<tr>
<td>38</td>
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<td>-80.648</td>
<td>-80.880</td>
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<td>-77.971</td>
<td>-77.960</td>
<td>-0.011</td>
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<td>85</td>
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<tr>
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<tr>
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<tr>
<td>43</td>
<td>87</td>
<td>-59.120#</td>
<td>-57.690</td>
<td>-56.540</td>
<td>-1.150</td>
<td>-57.786</td>
<td>0.096</td>
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</tbody>
</table>
Trap Data from Haettner et al. (PRL 106 (2011) 122501)

The graph shows the difference between experimental and theoretical values for various nucleon numbers (A) for elements Sr, Nb, Mo, Zr, and Tc. The experimental data is represented by red dots, and the theoretical predictions by thick black dots.

- **Sr**: The red line and black points indicate a consistent trend with increasing nucleon number, showing a significant deviation from the theoretical prediction.

- **Nb**, **Mo**, **Zr**, and **Tc**: Similar trends are observed, with red dots deviating from the theoretical black points, indicating discrepancies between experiment and theory.

The graph is labeled with the years 1992 and 2012, suggesting the data is compared against predictions from FRDM models from those years.
FRDM (1992)

$\sigma_{th} = 0.6314 \text{ MeV}$

Exp. = AME2003

FRDM (2012)

$\sigma_{th} = 0.5595 \text{ MeV}$

Exp. = AME2003

Discrepancy (Exp. – Calc.) (MeV)

Neutron Number $N$

FRDM (1992)

$\sigma_{th} = 0.6314 \text{ MeV}$

Exp. = AME2003
$\sigma_{th} = 0.5587 \text{ MeV}$

**Exp.** = **AME2003**

### FRDM (2012)

$\sigma_{th} = 0.5595 \text{ MeV}$

**Discrepancy (Exp. – Calc.) (MeV)**

### HFB21

$\sigma_{th} = 0.5587 \text{ MeV}$

**Exp. = AME2003**

**Neutron Number $N$**
\( Q_\alpha \) Deviations beyond \( N = 126 \)

<table>
<thead>
<tr>
<th>Region</th>
<th>Model</th>
<th>Nuclei</th>
<th>RMS (MeV)</th>
</tr>
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<tbody>
<tr>
<td>( Z &gt; 82 )</td>
<td>SkM*</td>
<td>46</td>
<td>2.6</td>
</tr>
<tr>
<td>( Z &gt; 82 )</td>
<td>Sly4</td>
<td>46</td>
<td>2.6</td>
</tr>
<tr>
<td>( Z &gt; 82 )</td>
<td>HFB21</td>
<td>145</td>
<td>0.409</td>
</tr>
<tr>
<td>( Z &gt; 82 )</td>
<td>FRDM(1992)</td>
<td>145</td>
<td>0.463</td>
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<tr>
<td>( Z &gt; 82 )</td>
<td>FRDM(2012)</td>
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<td>0.326</td>
</tr>
<tr>
<td>( Z &gt; 88 )</td>
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<tr>
<td>( Z &gt; 88 )</td>
<td>Sly4</td>
<td>36</td>
<td>2.2</td>
</tr>
<tr>
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<td>HFB21</td>
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<td>0.367</td>
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<tr>
<td>( Z &gt; 88 )</td>
<td>FRDM(1992)</td>
<td>101</td>
<td>0.448</td>
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<tr>
<td>( Z &gt; 88 )</td>
<td>FRDM(2012)</td>
<td>101</td>
<td>0.274</td>
</tr>
</tbody>
</table>
Mass Models Compared to AME2003

HFB(Sly4):
\[ \sigma = 5.11 \text{ (MeV)} \]
\[ \mu = -2.94 \text{ (MeV)} \]

FRDM(1992):
\[ \sigma = 0.67 \text{ (MeV)} \]
\[ \mu = +0.02 \text{ (MeV)} \]
α-decay of $^{278}_{113}$

- OTHER exp.
- FRDM (1992)
- FRLDM (1992)
- HFB8 (Goriely)
- HFB2 (Goriely)

Neutron Number $N$

153 155 157 159 161 163 165 167

Energy Release $Q_{\alpha}$ (MeV)

Z-Proton Number

101 103 105 107 109 111 113 115
$\epsilon_2 > 0.1 \quad \epsilon_2 < 0.1 \Rightarrow$

$\alpha$-Decay Chain from $^{294}_{117}$

Energy Release $Q_\alpha$ (MeV)

Neutron Number $N$

165 167 169 171 173 175 177

Proton Number $Z$

105 107 109 111 113 115 117

FRLDM (1992)
FRDM (1992)
Sobiczewski (2010)
Muntian et al. (2003)
Dubna exp.
Heavy-ion interaction potential

Ground-state microscopic correction

![Diagram of heavy-ion interaction and ground-state correction]
Neutron Separation-Energy Contours (1,2,3,4)

FRDM(2012)

HFB21
INTERMISSION

then

FISSION
Five Essential Fission Shape Coordinates

- \( Q_2 \sim \) Elongation (fission direction)
- \( \alpha_g \sim \) (M1-M2)/(M1+M2) Mass asymmetry
- \( \varepsilon_{f1} \sim \) Left fragment deformation
- \( \varepsilon_{f2} \sim \) Right fragment deformation
- \( d \sim \) Neck

\[ \Rightarrow 5\,315\,625 \text{ grid points} - 306\,300 \text{ unphysical points} \]
\[ \Rightarrow 5\,009\,325 \text{ physical grid points} \]
Fission Barrier and Associated Shapes for $^{228}\text{Ra}$

- Separating ridge
- Symmetric mode
- Asymmetric mode

Nuclear Deformation ($Q_2/b^{(1/2)}$)

Fission-Barrier Height (MeV)

Graphs by Peter Möller
Deficiencies and improvements to fits to $N_{r,\odot}$
The FK²L waiting-point approach (IV)

“...best fit so far...; long-standing problem solved...”

W. Hillebrandt

“...call for a deeper study... before rushing into numerical results... and premature comparisons with the observed abundances”

M. Arnould

...this catchword coined by W. Nazarewicz later led to semantics and misinterpretations
Impact of nuclear masses at $N = 82$

Already FK²L (ApJ 403) concluded from their fits to $N_{r,\odot}$:

"the calculated r-abundance ”trough“ in the $A \approx 120$ region reflects the weakening of the shell strength below $^{132}\text{Sn}_{82}$."

Effect of $S_n$ around $N=82$ shell closure

"static" calculations (Saha equation)
$\Rightarrow$ break-out at $N=82$ $^{130}\text{Cd}$

"time-dependent" calculations (w.-p.)
$\Rightarrow$ r-matter flow to and beyond $A=130$
Use spherical HFB/SkP mass model $\Rightarrow$ FRDM+HFB/SkP “hybrid model” around $N=82$

$\Delta S_n$ as a measure of the $N=82$ shell strength

population of $r$-path

$N_{r,\odot}$ fits
"Shell quenching"

...reduction of the spin-orbit coupling strength; caused by strong interaction between bound and continuum states; due to diffuseness of "neutron-skin" and its influence on the central potential...

- high-j orbitals $\uparrow$ (e.g. $v h_{11/2}$)
- low-j orbitals $\downarrow$ (e.g. $v d_{3/2}$)
- evtl. crossing of orbitals
- new "magic" numbers / shell gaps (e.g. $^{110}\text{Zr}_{70}$, $^{170}\text{Ce}_{112}$)

change of

- shell-gaps
- deformation
- r-process path ($S_n$)
- r-matter flow ($\tau_n$)
r-Process calculations with MHD-SN models

2012 … new “hot r-process topic” → magnetohydrodynamic SNe … but, unfortunately not with the optimum nuclear-physics input…


Impact of new β-decay half-lives on r-process nucleosynthesis

Nobuya Nishimura,1,2* Toshitaka Kajino,3,4 Grant J. Mathews,5 Shunji Nishimura,6 and Toshio Suzuki7

“We investigate the effect of newly measured β-decay half-lives on r-process nucleosynthesis. We adopt … a magnetohydrodynamic supernova explosion model… The \( (T_{1/2}) \) effect slightly alleviates, but does not fully explain, the tendency of r-process models to underproduce isotopes with \( A = 110 – 120 \)…”


MAGNETOROTATIONALLY DRIVEN SUPERNOVAE AS THE ORIGIN OF EARLY GALAXY r-PROCESS ELEMENTS?

C. Winteler1, R. Käppeli2, A. Perего1, A. Arcenes3,4, N. Vassil1, N. Nishimura1, M. Liebendörfer1, and F.-K. Thielemann1

“We examine magnetohydrodynamically driven SNe as sources of r-process elements in the early Galaxy… … the formation of bipolar jets could naturally provide a site for the strong r-process…”
How to fill up the FRDM A ≈ 115 “trough”?

- if via $T_{1/2}$ (as e.g. suggested by Nishimura, Kajino et al.; PRC 85 (2012)), on average all r-progenitors between $^{110}$Zr and $^{126}$Pd should have

$$7.5 \times T_{1/2}^{\text{FRDM}} \approx 350 \text{ ms} \rightarrow 2 \times T_{1/2}^{(^{130}\text{Cd})}$$

- it **must** be the progenitor masses, via $S_n$ (and correlated deformation $\varepsilon_2$)
Reproduction of $N_r,\odot$

Superposition of S-components with $Y_e=0.45$;

**weighting according to** $Y_{\text{seed}}$

![Graphs showing α- and r-Process Yields, $Y_e=0.45$, $V_{\exp}=7500$](image)

No exponential fit to $N_{r,\odot}$!

<table>
<thead>
<tr>
<th>Entropy S</th>
<th>Process duration [ms]</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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<td>ETFSI-Q</td>
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<tr>
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<td>57</td>
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<td>180</td>
<td>209</td>
<td>116</td>
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<td>220</td>
<td>422</td>
<td>233</td>
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<tr>
<td>245</td>
<td>691</td>
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<tr>
<td>260</td>
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<td>2280</td>
<td>710</td>
</tr>
<tr>
<td>300</td>
<td>4310</td>
<td>1395</td>
</tr>
</tbody>
</table>

다고 하는 significant effect of “shell-quenching” below doubly-magic $^{132}\text{Sn}$
What is the origin of the REE r-abundance peak?

Already about 15 years ago, first indications from calculations using two different mass models

⇒ effect of $S_n$

Today, in principle confirmed by new calculations using the “deformed“ FRDM 2012 and two different $T_{1/2}$ & $P_n$ data sets

⇒ effect of $\beta$-decay properties

REE pygmy peak due to deformation, not from fission cycling!
Comparison between $N_{r,\odot}$ and $r$-abundances calculated with FRDM(1992) and FRDM(2012) in both cases normalized to $^{195}$Pt.

Good news at the end...

Improvements and remaining deficiencies:

- still overabundances in the $80 \leq A \leq 110$ mass region
- “abundance trough” at $A \approx 120$ removed
- 2nd $r$-peak slightly improved, but top still too low
- $N=82$ bottle-neck behavior improved
- perfect reproduction of the deformed REE “pygmy-peak”
- shape of 3rd $r$-peak well reproduced
- shape-transition region above $N=126$ still imperfect $\Rightarrow$ deep trough
- $^{208}$Pb,$^{209}$Bi here too low because major contribution from $\alpha$-backdecay not yet included

Summary and conclusion:

promising progress, but still much remains to be done in all interrelated fields