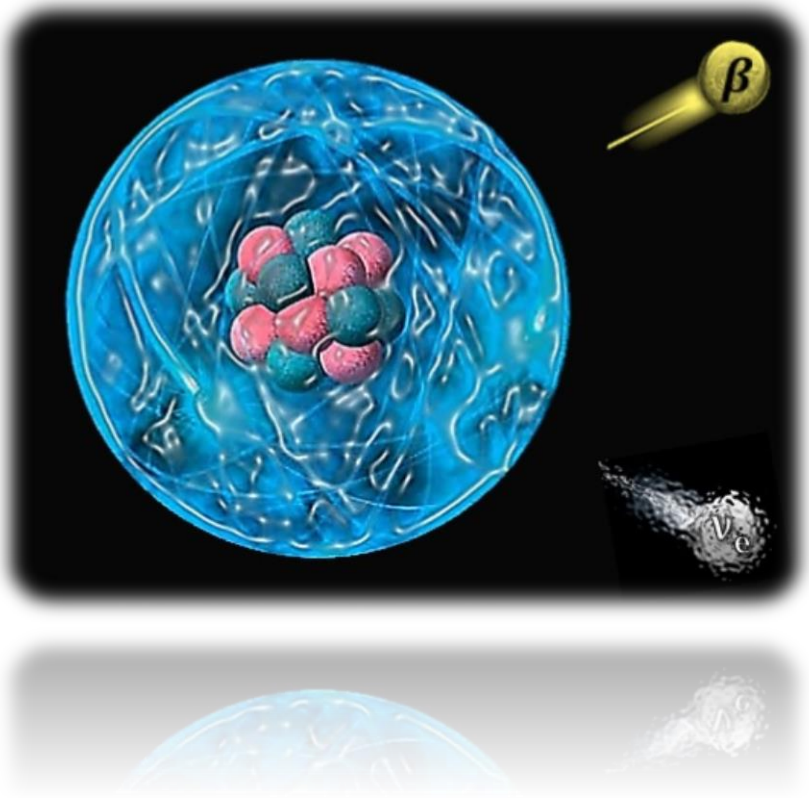

Calculation of weak interaction decays for nuclear data

Nuclear Data Week 2018 | Xavier Mougeot

list
cea tech

LNHB
Laboratoire National Henri Becquerel

LABORATOIRE NATIONAL DE MÉTROLOGIE ET D'ESSAIS
LNE

INSTITUT CARNOT
CEA LIST

université
PARIS-SACLAY

European funding

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Outlines

- Context
- BetaShape
  - Physics modelling
  - Structure of the code
  - Validation
- Past and ongoing developments not implemented in BetaShape
  - Atomic effects in beta decays
  - Electron capture decays
  - Inclusion of nuclear structure

Context

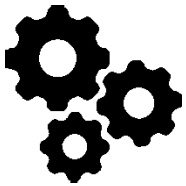
Oriented research

Fundamental research

Nuclear physics

Particle physics

Radiotoxicology



Laboratoire National Henri Becquerel

Ionizing radiation metrology

Radiochemistry

Bq, Gy and Sv units

Activity standards ~ 0.1%

Atomic and nuclear data

Applied research

Industries

Nuclear medicine

Nuclear energy

Instrumentation

Importance of beta decays

Scientific research

- Nuclear astrophysics (r-process)
- Standard Model (CKM matrix unitarity, weak magnetism)
- Beyond Standard Model (Fierz interference, sterile neutrino)
- Neutrino physics (reactor anomaly, reactor monitoring, non-proliferation)
- New detectors ($BrLa_3$)

Ionizing radiation metrology

Activity measurements by Liquid Scintillation Counting

Better knowledge of the beta spectra → **better uncertainties**

IAEA
International Atomic Energy Agency

Atomic and nuclear data

- **ENSDF** nuclear decay data
- **DDEP** (International collaboration)

  Decay Data Evaluation Project
  Atomic and nuclear decay data recommended by the BIPM

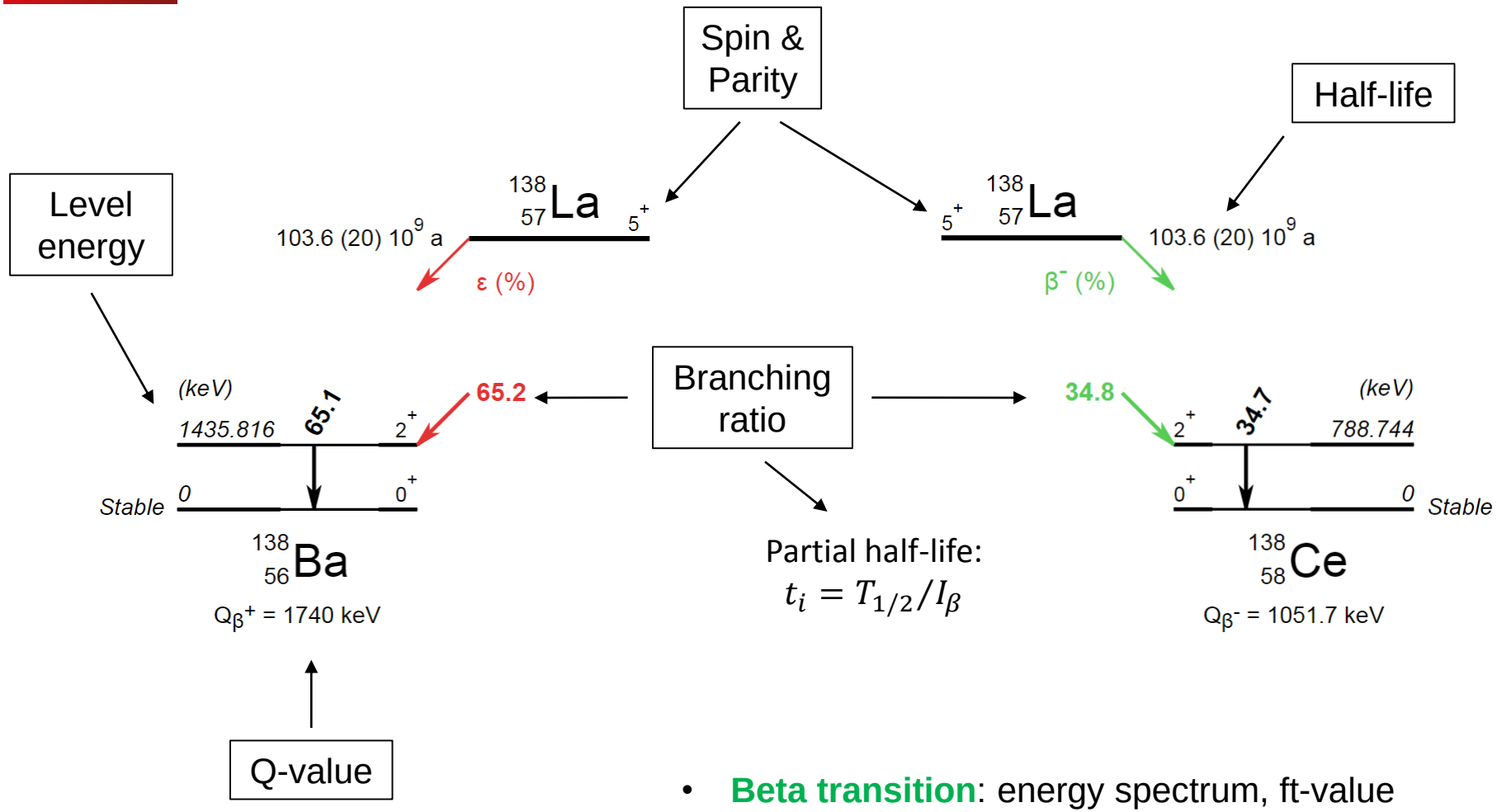
Medical uses

Micro-dosimetry, internal radiotherapy

Nuclear fuel cycle

Decay heat, nuclear waste

Weak interaction decay in nuclear data



- **Beta transition**: energy spectrum, ft-value
- **Electron capture**: capture probability, ft-value

Current situation in nuclear databases

If no experimental data → Theoretical estimates

The LogFT program is widely used in nuclear data evaluations

- Handles β and ε transitions
- Provides mean energies of β spectra, log *ft* values, β^+ and ε probabilities
- Propagates uncertainties from input parameters
- Reads and writes ENSDF files (*Evaluated Nuclear Structure Data File*)

However

- Too simple analytical models → lack of accuracy
- Forbiddenness limitation (allowed, first- and second- forbidden unique)
- Users now require β spectra and correlated ν spectra
- Users now requires detailed information for many subshells in ε

BetaShape

Executables of the BetaShape program for Windows, Linux and OS X are available at
http://www.lnhb.fr/activites-recherche-developpement/logiciels-traitement-spectres/

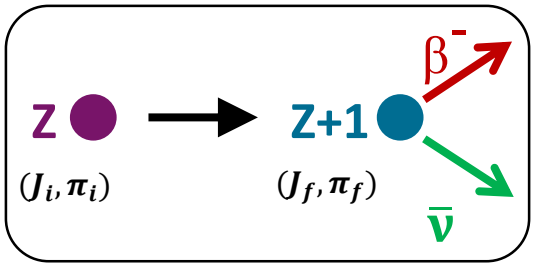
Physics modelling

Beta spectrum $\frac{\mathrm{d}N}{\mathrm{d}W} \propto$ $p\ W\ q^2$ $F_0 L_0$ $C(W)$

Coulomb part (Fermi function)

Phase space

Shape factor



Nuclear current can be **factored out** for **allowed** and **forbidden unique** transitions

$$C(W) = (2L-1)! \sum_{k=1}^{L} \lambda_k \frac{p^{2(k-1)}\ q^{2(L-k)}}{(2k-1)![2(L-k)+1]!}$$

$$F_0 L_0 = \frac{\alpha_{-1}^2 + \alpha_1^2}{2p^2} \qquad \lambda_k = \frac{\alpha_{-k}^2 + \alpha_k^2}{\alpha_{-1}^2 + \alpha_1^2}$$

→ Solving the Dirac equation for the leptons is sufficient with these assumptions

X. Mougeot, Phys. Rev. C 91, 055504 (2015)

Forbidden non-unique transitions calculated according to the ξ **approximation**

if $2\xi = \alpha Z/R \gg E_{\max}$
1st fnu → allowed
applied to 2nd, 3rd, etc.

Assumptions → Corrections

- Analytical screening corrections
- Radiative corrections

Propagation of uncertainty on $E_{\max}$

Reads and writes to/from ENSDF files

Database of experimental shape factors

Relativistic electron wave functions

$$\Psi(\vec{r}) = \begin{pmatrix} S_\kappa f_\kappa(r)\chi^\mu_{-\kappa} \\ g_\kappa(r)\chi^\mu_\kappa \end{pmatrix}$$

Radial component

Spin-angular functions
→ spherical harmonics expansion

Electron wave function
→ spherical symmetry

$$\begin{cases} \dfrac{\mathrm{d}f_\kappa}{\mathrm{d}r} = \dfrac{(\kappa-1)}{r} f_\kappa - [W - 1 - V(r)]g_\kappa \\ \dfrac{\mathrm{d}g_\kappa}{\mathrm{d}r} = [W + 1 - V(r)]f_\kappa - \dfrac{(\kappa+1)}{r} g_\kappa \end{cases}$$

Dirac equation
→ coupled differential equations

Analytical solutions
(approximate)

M.E. Rose, *Relativistic Electron Theory*, Wiley and Sons (1961)

nucleus = point charge + very approximate correction for its spatial extension

} LogFT treatment

Power series expansion
(exact solutions)

$$\begin{Bmatrix} f(r) \\ g(r) \end{Bmatrix} = \frac{(pr)^{k-1}}{(2k-1)!!} \sum_{n=0}^{\infty} \begin{Bmatrix} a_n \\ b_n \end{Bmatrix} r^n$$

nucleus = uniformly charged sphere
→ fast computation of the solutions

H. Behrens, W. Bühring, *Electron Radial Wave functions and Nuclear Beta Decay*, Oxford Science Publications (1982)

} BetaShape treatment

Excellent agreement with all the parameters tabulated in

H. Behrens, J. Jänecke, Landolt-Börnstein, New Series, Group I, vol. 4, Springer Verlag, Berlin (1969)

Analytical screening corrections

Rose

M.E. Rose, Phys. Rev. 49, 727 (1936)

Thomas-Fermi $V_0(Z, \beta^{\pm})$

$\Rightarrow W \rightarrow W' = W \pm V_0$ in all quantities except in neutrino energy

→ **non-physical discontinuity** for β^- spectrum

→ **identical for all transitions**

N.B. Gove and M.J. Martin, Nucl. Data Tables 10, 205 (1971)

Bühring

W. Bühring, Nucl. Phys. A 430, 1 (1984)

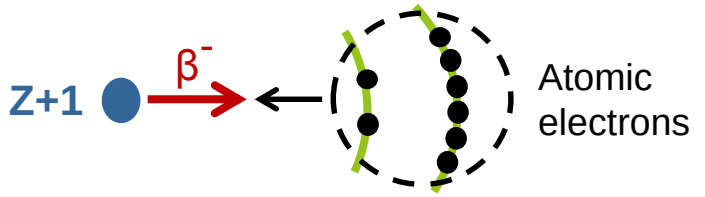
All quantities depend on the normalization of electron wave functions

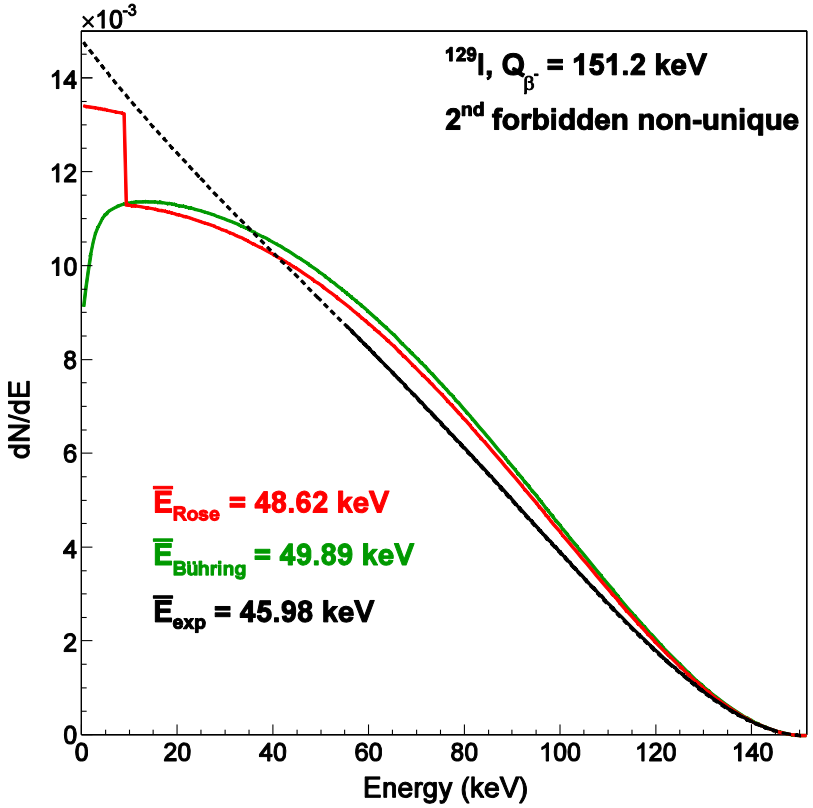
⇒ **Analytical solutions** and **leading order** at the nucleus + **asymptotic** solutions

Hulthén screened potentials → **Salvat's preferred**

F. Salvat *et al.*, Phys. Rev. A 36, 467 (1987)

→ **acting on Fermi function and λ_k parameters, thus different according to the forbiddenness**





More precise + no breakdown at low energy

Radiative corrections

Electrons – Old correction

A. Sirlin, Phys. Rev. 164, 1767 (1967)
W. Jaus, Phys. Lett. 40, 616 (1972)

Electrons – New correction

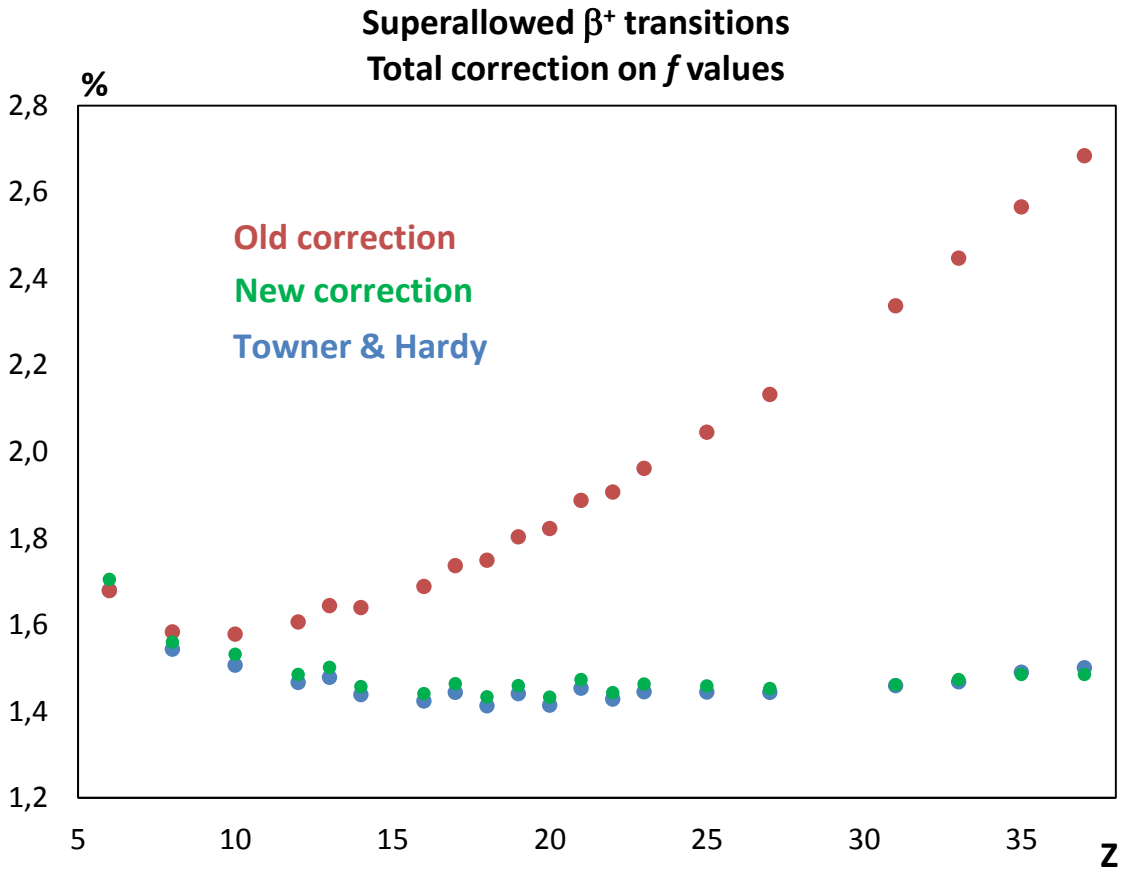
I.S. Towner, J.C. Hardy, PRC 77, 025501 (2008)
A. Czarnecki et al., PRD 70, 093006 (2004)

Neutrinos

A. Sirlin, Phys. Rev. D 84, 014021 (2011)

First version of BetaShape

New version of BetaShape



Calculated quantities

- **Single and total β^+/β^- and $\nu_e/\bar{\nu}_e$ spectra**

- **Mean energy** $\bar{E} = \int_0^{E_0} E \cdot N(E)\mathrm{d}E \Big/ \int_0^{E_0} N(E)\mathrm{d}E$

- **Log *ft* value** ☑ $f_{\beta^-} = \int_1^{W_0} N(W)\mathrm{d}W$

  ☒ $f_{\varepsilon/\beta^+} = f_\varepsilon + f_{\beta^+}$

  } + partial half-life from data: $t_i = T_{1/2}/P_\beta$

For allowed and forbidden unique transitions

$$\frac{I_\varepsilon}{I_{\beta^+}} = \frac{\lambda_\varepsilon}{\lambda_{\beta^+}} = \frac{C_{\mathrm{ns}} \sum_x n_x C_x f_x}{C_{\mathrm{ns}} \int_1^{W_0} N(W)\mathrm{d}W} \approx \frac{f_\varepsilon}{f_{\beta^+}}$$

C_x: lepton dynamics

C_{ns}: nuclear structure (allowed, forbidden unique)

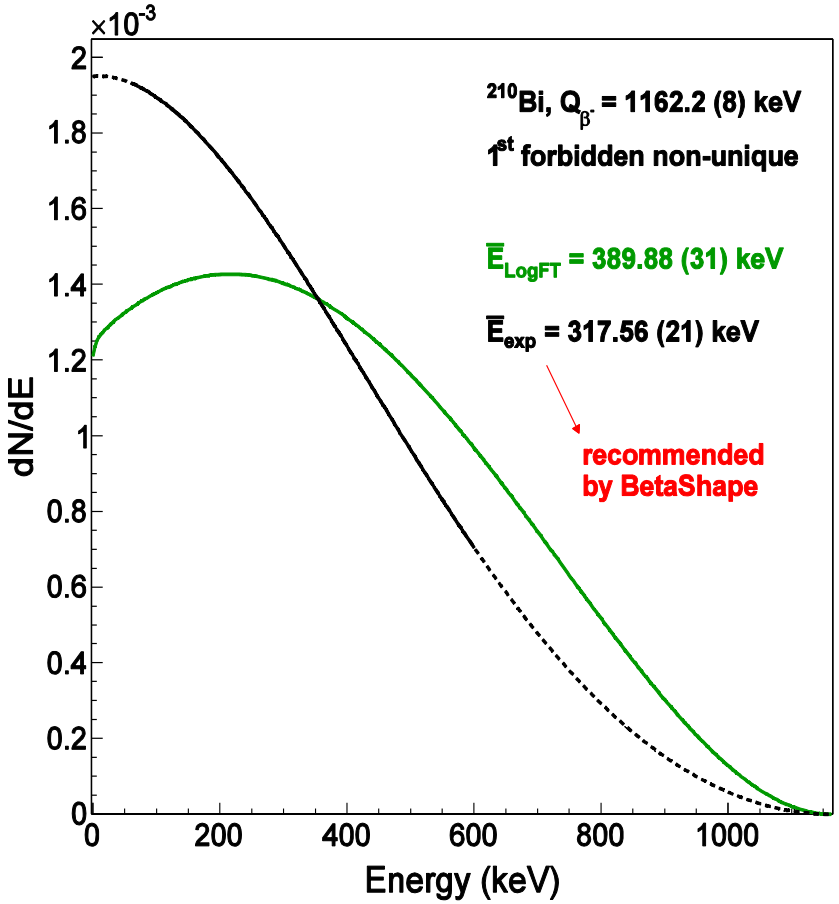
n_x: relative occupation number of the orbital, not accounted for in the LogFT program

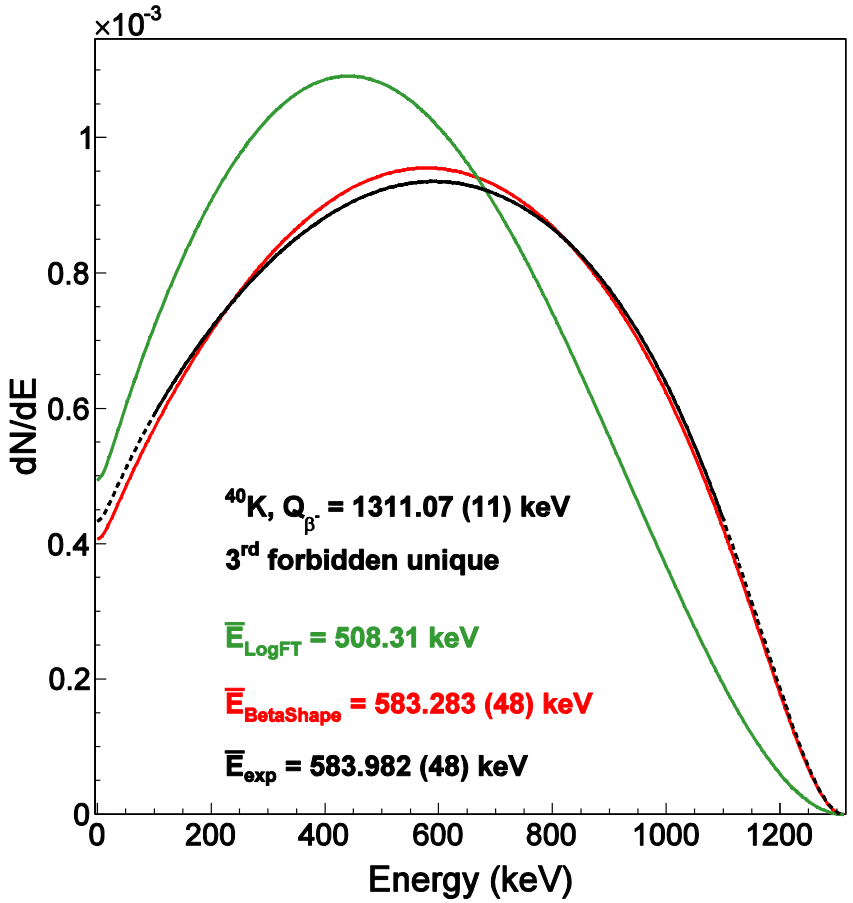
$$\rightarrow \log ft = \log\left(\frac{f_\varepsilon + f_{\beta^+}}{I_\varepsilon + I_{\beta^+}} T_{1/2}\right)$$

$$= \log\left(\frac{f_{\beta^+}}{I_{\beta^+}} T_{1/2}\right) + \log\left(\frac{1 + f_\varepsilon/f_{\beta^+}}{1 + I_\varepsilon/I_{\beta^+}}\right)$$

$$\approx \log\left(\frac{f_{\beta^+}}{I_{\beta^+}} T_{1/2}\right)$$

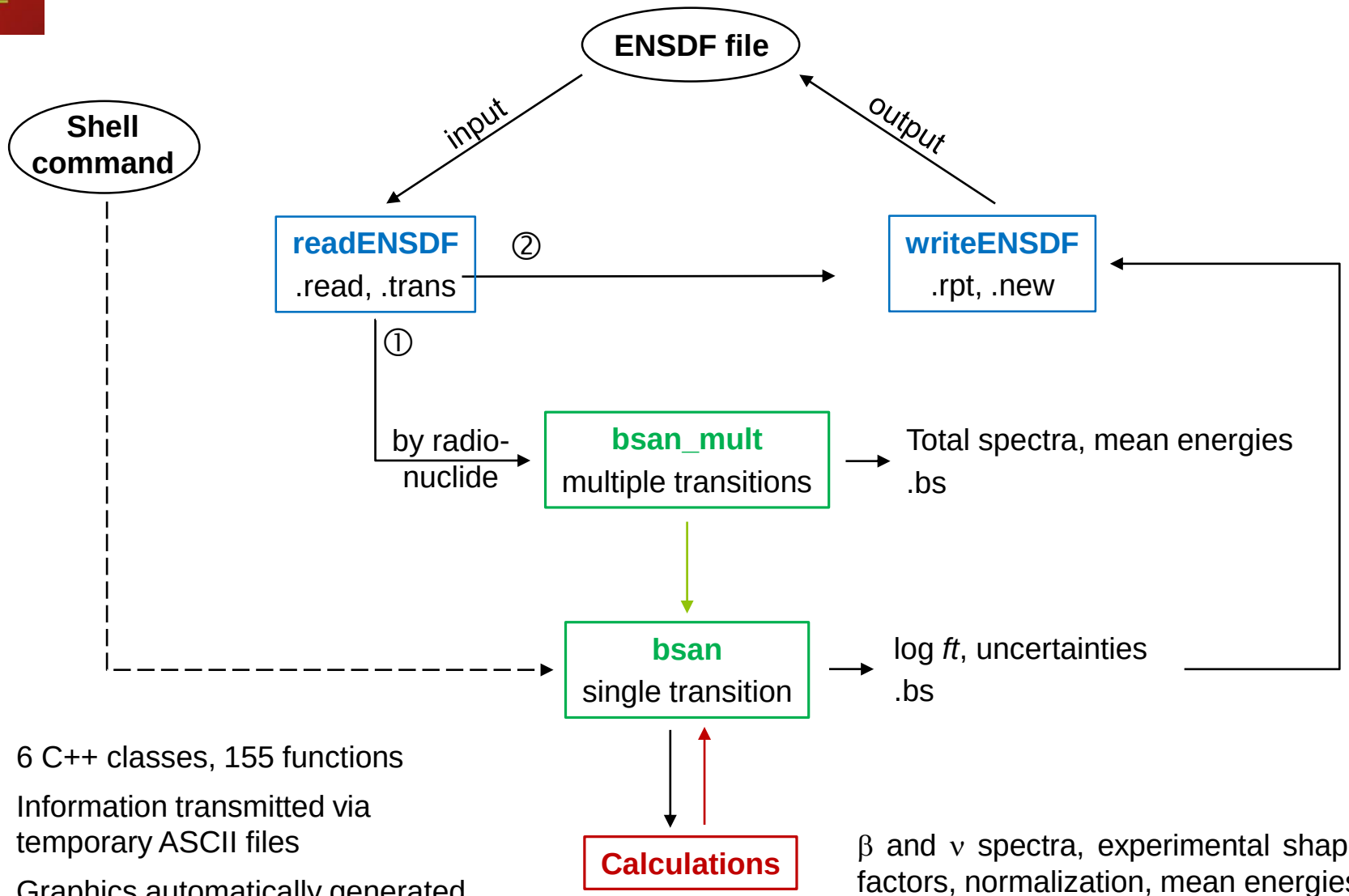
Examples of improved calculations





These two transitions are calculated as allowed by the LogFT program.

Structure of the code



- 6 C++ classes, 155 functions
- Information transmitted via temporary ASCII files
- Graphics automatically generated via ROOT (*not distributed*)

From input parameters

.read

```
Information read from the input file: /mnt/hgfs/Donnees/Beta/NNDC/m041.ensdf

####################################

Identification record has been found
Daughter Z: 15    Daughter A: 41    Symbol: P
Transition type: B-
Estimated parent nuclide from identification record: Z 14, A 41

Parent record has been found
Parent Z: 14     Parent A: 41    Symbol: Si
Parent energy of the initial level: G.S.
Spin and parity of the parent level undefined. Allowed transition will be assumed.
Parent half-life: 20.0 (25) MS or 0.0200 (25) S
Parent Q-value: 1.710E4 (38) keV

Normalization record has been found
Total branching ratio: 1

------------------------------------
Level record has been found
Daughter energy of the final level: G.S.
Level spin and parity | Read: (1/2+)       | Treated as: 1/2+
Spin and parity of the daughter level not clearly defined.
Level half-life not given.

####################################

Identification record has been found
Daughter Z: 16    Daughter A: 41    Symbol: S
Transition type: B-
Estimated parent nuclide from identification record: Z 15, A 41

Parent record has been found
Parent Z: 15     Parent A: 41    Symbol: P
Parent energy of the initial level: G.S.
Spin and parity of the parent level undefined. Allowed transition will be assumed.
Parent half-life: 150 (15) MS or 0.150 (15) S
Parent Q-value: 1.374E4 (24) keV

Normalization record has been found
Total branching ratio: 1
```

.trans

```
####################################

Transitions that have been found.
Only beta +/- transitions will be calculated.


------------------------------------
Parent nucleus: 17-Cl-41 [1/2+] g.s.  -->  Daughter nucleus: 18-Ar-41 [5/2-] 1.7E2 (10) keV
Half-life of the parent nuclide: 38.4 (8) s
Beta - transition. Order: 1st forbidden unique
Given transition order different. Determined order from spins and parities kept.
Transition energy calculated from Q-value and level energies: 5.56E3 (12) keV.
Global normalization of the beta - decay: 1
Normalization of this transition: 0 %
Warning: this decay is uncertain or questionable.
Warning: information about this decay is not totally sure.

------------------------------------
Parent nucleus: 17-Cl-41 [1/2+] g.s.  -->  Daughter nucleus: 18-Ar-41 [3/2-] 5.2E2 (30) keV
Half-life of the parent nuclide: 38.4 (8) s
Beta - transition. Order: 1st forbidden non-unique
Given transition order different. Determined order from spins and parities kept.
Transition energy calculated from Q-value and level energies: 5.21E3 (30) keV.
Global normalization of the beta - decay: 1
Normalization of this transition: 0 %
Warning: this decay is uncertain or questionable.
Warning: information about this decay is not totally sure.

⋮                ⋮                ⋮

####################################

Summary

5 nuclei and 115 transitions have been read.

Parent nucleus: 17-Cl-41
19 transitions have been read (19 B-).

Parent nucleus: 18-Ar-41
3 transitions have been read (3 B-).

Parent nucleus: 20-Ca-41
1 transition has been read (1 EC).

Parent nucleus: 21-Sc-41
6 transitions have been read (3 EC, 3 B+).

Parent nucleus: 22-Ti-41
86 transitions have been read (43 EC, 43 B+).


####################################
```

⋮ ⋮ ⋮

From input parameters

```
####################################

Identification record has been found
Daughter Z: 15   Daughter A: 41   Symbol: P
Transition type: B-
Estimated parent nuclide from identification record: Z 14, A 41

Parent record has been found
Parent Z: 14    Parent A: 41   Symbol: Si
Parent energy of the initial level: G.S.
Spin and parity of the parent level undefined. Allowed transition will be assumed.
Parent half-life: 20.0 (25) MS or 0.0200 (25) S
Parent Q-value: 1.710E4 (38) keV

Normalization record has been found
Total branching ratio: 1

-------------------------------------
Level record has been found
Daughter energy of the final level: G.S.
Level spin and parity | Read: (1/2+)      | Treated as: 1/2+
Spin and parity of the daughter level not clearly defined.
Level half-life not given.
```

.read

From input parameters

.read

```
Information read from the input file: /mnt/hgfs/Donnees/Beta/NNDC/m041.ensdf

###################################

Identification record has been found
Daughter Z: 15    Daughter A: 41    Symbol: P
Transition type: B-
Estimated parent nuclide from identification record: Z 14, A 41

Parent record has been found
Parent Z: 15     Parent A: 41    Symbol: P
Parent energy of the initial level: G.S.
Spin and parity of the parent level undefined. Allowed transition will be assumed.
Parent half-life: 150 (15) MS or 0.150 (15) S
Parent Q-value: 1.374E4 (24) keV

Normalization record has been found
Total branching ratio: 1
```

.trans

```
###################################

Transitions that have been found.
Only beta +/- transitions will be calculated.


-----------------------------------
Parent nucleus: 17-Cl-41 [1/2+] g.s.  -->  Daughter nucleus: 18-Ar-41 [5/2-] 1.7E2 (10) keV
Half-life of the parent nuclide: 38.4 (8) s
Beta - transition. Order: 1st forbidden unique
Given transition order different. Determined order from spins and parities kept.
Transition energy calculated from Q-value and level energies: 5.56E3 (12) keV.
```


.trans

```
-----------------------------------
Parent nucleus: 17-Cl-41 [1/2+] g.s.  -->  Daughter nucleus: 18-Ar-41 [5/2-] 1.7E2 (10) keV
Half-life of the parent nuclide: 38.4 (8) s
Beta - transition. Order: 1st forbidden unique
Given transition order different. Determined order from spins and parities kept.
Transition energy calculated from Q-value and level energies: 5.56E3 (12) keV.
```


```
Global normalization of the beta - decay: 1
Normalization of this transition: 0 %
Warning: this decay is uncertain or questionable.
Warning: information about this decay is not totally sure.
```

```
5 nuclei and 115 transitions have been read.

Parent nucleus: 17-Cl-41
19 transitions have been read (19 B-).

Parent nucleus: 18-Ar-41
3 transitions have been read (3 B-).

Parent nucleus: 20-Ca-41
1 transition has been read (1 EC).

Parent nucleus: 21-Sc-41
6 transitions have been read (3 EC, 3 B+).

Parent nucleus: 22-Ti-41
86 transitions have been read (43 EC, 43 B+).


###################################
```

From input parameters

```
Information read from the input file: /m

###################################

Identification record has been found
Daughter Z: 15   Daughter A: 41   Symbol
Transition type: B-
Estimated parent nuclide from identifica

Parent record has been found
Parent Z: 14    Parent A: 41    Symbol: S
Parent energy of the initial level: G.S.
Spin and parity of the parent level unde
Parent half-life: 20.0 (25) MS or 0.0200
Parent Q-value: 1.710E4 (38) keV

Normalization record has been found
Total branching ratio: 1

-----------------------------------
Level record has been found
Daughter energy of the final level: G.S.
Level spin and parity | Read: (1/2+)
Spin and parity of the daughter level no
Level half-life not given.

###################################

Identification record has been found
Daughter Z: 16   Daughter A: 41   Symbol
Transition type: B-
Estimated parent nuclide from identifica

Parent record has been found
Parent Z: 15    Parent A: 41    Symbol: P
Parent energy of the initial level: G.S.
Spin and parity of the parent level unde
Parent half-life: 150 (15) MS or 0.150 (
Parent Q-value: 1.374E4 (24) keV

Normalization record has been found
Total branching ratio: 1
```

⋮

```
#####################################

Summary

5 nuclei and 115 transitions have been read.

Parent nucleus: 17-Cl-41
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3 transitions have been read (3 B-).

Parent nucleus: 20-Ca-41
1 transition has been read (1 EC).

Parent nucleus: 21-Sc-41
6 transitions have been read (3 EC, 3 B+).

Parent nucleus: 22-Ti-41
86 transitions have been read (43 EC, 43 B+).


#####################################
```

.trans

```
ucleus: 18-Ar-41 [5/2-] 1.7E2 (10) keV

om spins and parities kept.
nergies: 5.56E3 (12) keV.

sure.

ucleus: 18-Ar-41 [3/2-] 5.2E2 (30) keV

om spins and parities kept.
nergies: 5.21E3 (30) keV.

sure.
```

⋮

```
1187
1188 ###################################
```

Report

Check of the consistency of the new ENSDF file

Summary

Report of the calculations and new values for each transition

.rpt

```
Input file:  /mnt/hgfs/Donnees/Beta/NNDC/m041.ensdf
Output file: /mnt/hgfs/Donnees/Beta/NNDC/m041.new

Input file: 12828 lines
Output file: 12828 lines
--> Output file is consistent.

################################################  B- DECAYS  ################################################

--------------------------------------------------------------------------------------------------------------  1

 41CL  P 0           (1/2+,3/2+)       38.4 S    8                 5728  65    - PARENT
 41AR  N                       1.0                                             - NORMALIZATION
 41AR  L 1868        1/2+                                                      - LEVEL

***** Daughter level energy without uncertainty: estimated uncertainty (~60%) from a flat distribution in [0,2*Energy] *****
***** Intensity without uncertainty: estimated uncertainty (~60%) from a flat distribution in [0,2*Intensity] *****
***** BR*NB from PN record *****

From calculated spectrum
Emean 1.7E3 (5) keV   |   log ft 5.1 (9)

*    log ft
 41AR  B 3.80E3    15  80    GT             5.0  LT                    C    - OLD CARD
 41AR  B 3.80E3    15  80    GT          5.1      9                    C    - NEW CARD

*    Mean energy
 41ARS B EAV=1717 32                                                       - OLD CARD
 41ARS B EAV=1.7E3 5                                                       - NEW CARD

--------------------------------------------------------------------------------------------------------------  2

 41AR  P 0           7/2-            109.61 M  4             2491.61   67    - PARENT
 41K   N  0.9916   2          1.0       1.0                                  - NORMALIZATION
 41K   PN                                                    3    - PRODUCTION NORMALIZATION
 41K   L 0           3/2+                                                    - LEVEL

***** BR and NB from N record *****

                    ⋮                         ⋮                         ⋮
--------------------------------------------------------------------------------------------------------------

-------- Total: 4
-------- Added lines: 0

################################################  B+ DECAYS  ################################################

--------------------------------------------------------------------------------------------------------------  1

 41SC  P 0           7/2-            596.3 MS  17              6495.28  27    - PARENT
 41CA  N  1.0                  1.0       1.0                                  - NORMALIZATION
 41CA PN                                                     4    - PRODUCTION NORMALIZATION
```

Report

Check of the consistency of the new ENSDF file

Summary

Report of the calculations and new values for each transition

.rpt

```
Input file:  /mnt/hgfs/Donnees/Beta/NNDC/m041.ensdf
Output file: /mnt/hgfs/Donnees/Beta/NNDC/m041.new

Input file: 12828 lines
Output file: 12828 lines
--> Output file is consistent.
```

```
*    log ft
 41AR  B 3.80E3    15  80    GT            5.0  LT                    C   - OLD CARD
 41AR  B 3.80E3    15  80    GT          5.1      9                   C   - NEW CARD

*    Mean energy
 41ARS B EAV=1717 32                                                    - OLD CARD
 41ARS B EAV=1.7E3 5                                                    - NEW CARD

-----------------------------------------------------------------------------------------------------------------------

 41AR  P 0           7/2-            109.61 M  4            2491.61   67    - PARENT
 41K   N  0.9916   2          1.0       1.0                                 - NORMALIZATION
 41K   PN                                                          3   - PRODUCTION NORMALIZATION
 41K   L 0           3/2+                                                  - LEVEL

***** BR and NB from N record *****

-----------------------------------------------------------------------------------------------------------------------

-------- Total: 4
-------- Added lines: 0

#################################################  B+ DECAYS  ##################################################

-----------------------------------------------------------------------------------------------------------------------

 41SC  P 0           7/2-            596.3 MS  17           6495.28   27    - PARENT
 41CA  N  1.0                 1.0       1.0                                 - NORMALIZATION
 41CA  PN                                                            4   - PRODUCTION NORMALIZATION
```

Report

```
Input file:  /mnt/hgfs/Donnees/Beta/NNDC/m041.ensdf
Output file: /mnt/hgfs/Donnees/Beta/NNDC/m041.new
```

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```
################################################  B- DECAYS  ################################################

-------------------------------------------------------------------------------------------------------------  1

 41CL  P 0          (1/2+,3/2+)       38.4 S    8                 5728  65    - PARENT
 41AR  N                        1.0                                            - NORMALIZATION
 41AR  L 1868       1/2+                                                       - LEVEL

***** Daughter level energy without uncertainty: estimated uncertainty (~60%) from a flat distribution in [0,2*Energy] *****
***** Intensity without uncertainty: estimated uncertainty (~60%) from a flat distribution in [0,2*Intensity] *****
***** BR*NB from PN record *****

From calculated spectrum
Emean 1.7E3 (5) keV   |   log ft 5.1 (9)

*    log ft
 41AR  B 3.80E3    15  80    GT             5.0  LT                    C    - OLD CARD
 41AR  B 3.80E3    15  80    GT          5.1      9                    C    - NEW CARD

*    Mean energy
 41ARS B EAV=1717 32                                                        - OLD CARD
 41ARS B EAV=1.7E3 5                                                        - NEW CARD
```

```
35  41K  N  0.9916  2          1.0       1.0                                - NORMALIZATION
36  41K  PN                                                    3  - PRODUCTION NORMALIZATION
```

```
################################################  B+ DECAYS  ################################################

-------------------------------------------------------------------------------------------------------------  1

 41SC  P 0          7/2-            596.3 MS  17              6495.28  27    - PARENT
 41CA  N  1.0                  1.0       1.0                                 - NORMALIZATION
 41CA PN                                                          4  - PRODUCTION NORMALIZATION
 41CA  L 0          7/2-                                                     - LEVEL

***** BR and NB from N record *****

From calculated spectrum
```

Output file

.bs
single transition

Transition parameters and options for calculation

Experimental shape factor

Mean energies, log *ft* values, analysis parameters

β and ν spectra

```
--------------------------------------------------------------------------------

BetaShape
Analytical version: 1.0 (10/06/2016)
Author: X. Mougeot (xavier.mougeot@cea.fr)
CEA, LIST, Laboratoire National Henri Becquerel (LNHB), Gif-sur-Yvette F-91191, France
Please cite: X. Mougeot, Physical Review C 91, 055504; Erratum Phys. Rev. C 92, 059902 (2015)

--------------------------------------------------------------------------------

Parent nucleus: 18-Ar-41 [7/2*] g.s.  -->  Daughter nucleus: 19-K-41 [3/2+] g.s.
Calculation of the 1st forbidden unique transition from the beta - decay of Ar-41

Bühring's screening correction is considered.

End-point energy: 2491.60 (40) keV     Energy step: 8 keV     Intensity: 0.00784 (19)

An experimental shape factor has been found: (q^2 + l_2*p^2)
Energy range of the measurement: 1330 - 2420 keV
From [1961KA19] G.R. Kartashov, N.A. Burgov, A.V. Davydov,  Izvest. Akad. Nauk SSSR, Ser. Fiz. 25, 189 (1961) or Columbia Tech. Transl. 25, 184 (1962)

Input mean energy: 1076.60 (20) keV
Mean energy from the calculated spectrum: 1072.92 (19) keV
Mean energy from the experimental shape factor: 1076.05 (19) keV
Mean energy from the calculated spectrum if lk=1: 1076.0 (33) keV

Input log ft value: 9.72
Log ft value from the calculated spectrum: log ft 9.735 (11)   with components: log f 3.81177 (42) and log partial T1/2 5.924 (11)
Log ft value from the experimental shape factor: log ft 9.728 (11)   with component: log f 3.80453 (42)
Log ft value from the calculated spectrum if lk=1: log ft 9.740 (12)   with component: log f 3.816 (5)

Agreement of the experimental and calculated spectra in [1330,2420] keV: 99.98 %
Corresponding disagreement: 1.75e-02 %
Variation of the mean energies: -2.91e-01 %

E(keV)      dN/dE calc.     unc.            dN/dE exp.      unc.            dN/dE lk=1      unc.
     0      1.37491e-06     4.56604e-10     1.36282e-06     4.54479e-10     1.35951e-06     1.58534e-08
     8      1.41489e-06     4.67613e-10     1.40958e-06     4.67776e-10     1.39901e-06     1.63497e-08
    16      1.46578e-06     4.82021e-10     1.46404e-06     4.83425e-10     1.44933e-06     1.69282e-08
    24      1.52758e-06     4.99830e-10     1.52621e-06     5.01425e-10     1.51049e-06     1.75890e-08
                ⋮                               ⋮                               ⋮
  2472      6.09655e-09     2.46104e-10     6.32780e-09     2.54503e-10     6.12687e-09     2.71767e-10
  2480      2.15057e-09     1.49183e-10     2.24064e-09     1.54856e-10     2.16118e-09     1.54915e-10
  2488      2.07631e-10     4.86465e-11     2.18157e-10     5.09102e-11     2.08648e-10     4.76298e-11
 2491.6     0.00000e+00     0.00000e+00     0.00000e+00     0.00000e+00     0.00000e+00     0.00000e+00


-------------------------
Antineutrino spectrum
-------------------------

Mean energy from the calculated spectrum: 1416.48 (29) keV
Mean energy from the experimental shape factor: 1416.24 (29) keV
Mean energy from the calculated spectrum if lk=1: 1413.4 (34) keV

E(keV)      dN/dE calc.     unc.            dN/dE exp.      unc.            dN/dE lk=1      unc.
     0      0.00000e+00     0.00000e+00     0.00000e+00     0.00000e+00     0.00000e+00     0.00000e+00
     8      1.06916e-09     5.37713e-13     1.07023e-09     5.37166e-13     1.07440e-09     5.77388e-12
    16      4.23052e-09     2.12127e-12     4.23474e-09     2.11910e-12     4.25140e-09     2.30004e-11
    24      9.41583e-09     4.70705e-12     9.42521e-09     4.70220e-12     9.46266e-09     5.15326e-11
                ⋮                               ⋮                               ⋮
```

Output file

.bs
single transition

Transition parameters and options for calculation

```
--------------------------------------------------------------------------------

BetaShape
Analytical version: 1.0 (10/06/2016)
Author: X. Mougeot (xavier.mougeot@cea.fr)
CEA, LIST, Laboratoire National Henri Becquerel (LNHB), Gif-sur-Yvette F-91191, France
Please cite: X. Mougeot, Physical Review C 91, 055504; Erratum Phys. Rev. C 92, 059902 (2015)

--------------------------------------------------------------------------------

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Calculation of the 1st forbidden unique transition from the beta - decay of Ar-41

Bühring's screening correction is considered.

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Energy range of the measurement: 1330 - 2420 keV
From [1961KA19] G.R. Kartashov, N.A. Burgov, A.V. Davydov,  Izvest. Akad. Nauk SSSR, Ser. Fiz. 25, 189 (1961) or Columbia Tech. Transl. 25, 184 (1962)

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Bühring's screening correction is considered.

End-point energy: 2491.60 (40) keV     Energy step: 8 keV     Intensity: 0.00784 (19)
```


```
      8     1.41489e-06     4.67613e-10     1.40958e-06     4.67776e-10     1.39901e-06     1.63497e-08
     16     1.46578e-06     4.82021e-10     1.46404e-06     4.83425e-10     1.44933e-06     1.69282e-08
     24     1.52758e-06     4.99830e-10     1.52621e-06     5.01425e-10     1.51049e-06     1.75890e-08
                ⋮               ⋮               ⋮

   2472     6.09655e-09     2.46104e-10     6.32780e-09     2.54503e-10     6.12687e-09     2.71767e-10
   2480     2.15057e-09     1.49183e-10     2.24064e-09     1.54856e-10     2.16118e-09     1.54915e-10
   2488     2.07631e-10     4.86465e-11     2.18157e-10     5.09102e-11     2.08648e-10     4.76298e-11
 2491.6     0.00000e+00     0.00000e+00     0.00000e+00     0.00000e+00     0.00000e+00     0.00000e+00


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     0      0.00000e+00     0.00000e+00     0.00000e+00     0.00000e+00     0.00000e+00     0.00000e+00
     8      1.06916e-09     5.37713e-13     1.07023e-09     5.37166e-13     1.07440e-09     5.77388e-12
    16      4.23052e-09     2.12127e-12     4.23474e-09     2.11910e-12     4.25140e-09     2.30004e-11
    24      9.41583e-09     4.70705e-12     9.42521e-09     4.70220e-12     9.46266e-09     5.15326e-11
                ⋮               ⋮               ⋮
```

Output file

.bs
single transition

Experimental shape factor

```
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Energy range of the measurement: 1330 - 2420 keV
From [1961KA19] G.R. Kartashov, N.A. Burgov, A.V. Davydov,  Izvest. Akad. Nauk SSSR, Ser. Fiz. 25, 189 (1961)
```

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-------------------------------------------------------------------------------

BetaShape
Analytical version: 1.0 (10/06/2016)
Author: X. Mougeot (xavier.mougeot@cea.fr)
CEA, LIST, Laboratoire National Henri Becquerel (LNHB), Gif-sur-Yvette F-91191, France
Please cite: X. Mougeot, Physical Review C 91, 055504; Erratum Phys. Rev. C 92, 059902 (2015)

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Bühring's screening correction is considered.

End-point energy: 2491.60 (40) keV     Energy step: 8 keV     Intensity: 0.00784 (19)

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Energy range of the measurement: 1330 - 2420 keV
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Log ft value from the calculated spectrum if lk=1: log ft 9.740 (12)   with component: log f 3.816 (5)

Agreement of the experimental and calculated spectra in [1330,2420] keV: 99.98 %
Corresponding disagreement: 1.75e-02 %
Variation of the mean energies: -2.91e-01 %

E(keV)      dN/dE calc.     unc.            dN/dE exp.      unc.            dN/dE lk=1      unc.
     0      1.37491e-06     4.56604e-10     1.36282e-06     4.54479e-10     1.35951e-06     1.58534e-08
     8      1.41489e-06     4.67613e-10     1.40958e-06     4.67776e-10     1.39901e-06     1.63497e-08
    16      1.46578e-06     4.82021e-10     1.46404e-06     4.83425e-10     1.44933e-06     1.69282e-08
    24      1.52758e-06     4.99830e-10     1.52621e-06     5.01425e-10     1.51049e-06     1.75890e-08
                ⋮                               ⋮                               ⋮

  2472      6.09655e-09     2.46104e-10     6.32780e-09     2.54503e-10     6.12687e-09     2.71767e-10
  2480      2.15057e-09     1.49183e-10     2.24064e-09     1.54856e-10     2.16118e-09     1.54915e-10
  2488      2.07631e-10     4.86465e-11     2.18157e-10     5.09102e-11     2.08648e-10     4.76298e-11
 2491.6     0.00000e+00     0.00000e+00     0.00000e+00     0.00000e+00     0.00000e+00     0.00000e+00


-------------------------
Antineutrino spectrum
-------------------------

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Mean energy from the calculated spectrum if lk=1: 1413.4 (34) keV

E(keV)      dN/dE calc.     unc.            dN/dE exp.      unc.            dN/dE lk=1      unc.
     0      0.00000e+00     0.00000e+00     0.00000e+00     0.00000e+00     0.00000e+00     0.00000e+00
     8      1.06916e-09     5.37713e-13     1.07023e-09     5.37166e-13     1.07440e-09     5.77388e-12
    16      4.23052e-09     2.12127e-12     4.23474e-09     2.11910e-12     4.25140e-09     2.30004e-11
    24      9.41583e-09     4.70705e-12     9.42521e-09     4.70220e-12     9.46266e-09     5.15326e-11
                ⋮                               ⋮                               ⋮
```

Output file

.bs
single transition

```
------------------------------------------------------------------------------------------

BetaShape
Analytical version: 1.0 (10/06/2016)
Author: X. Mougeot (xavier.mougeot@cea.fr)
CEA, LIST, Laboratoire National Henri Becquerel (LNHB), Gif-sur-Yvette F-91191, France
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Mean energy from the calculated spectrum if lk=1: 1076.0 (33) keV

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Log ft value from the experimental shape factor: log ft 9.728 (11)   with component: log f 3.80453 (42)
Log ft value from the calculated spectrum if lk=1: log ft 9.740 (12)   with component: log f 3.816 (5)

Agreement of the experimental and calculated spectra in [1330,2420] keV: 99.98 %
Corresponding disagreement: 1.75e-02 %
Variation of the mean energies: -2.91e-01 %
```

Mean energies, log *ft* values, analysis parameters

363	16	4.23052e-09	2.12127e-12	4.23474e-09	2.11910e-12	4.25140e-09	2.30004e-11
364	24	9.41583e-09	4.70705e-12	9.42521e-09	4.70220e-12	9.46266e-09	5.15326e-11

Output file

.bs
single transition

```
------------------------------------------------------------------------------------------

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Analytical version: 1.0 (10/06/2016)
Author: X. Mougeot (xavier.mougeot@cea.fr)
CEA, LIST, Laboratoire National Henri Becquerel (LNHB), Gif-sur-Yvette F-91191, France
Please cite: X. Mougeot, Physical Review C 91, 055504; Erratum Phys. Rev. C 92, 059902 (2015)

------------------------------------------------------------------------------------------
```

E(keV)	dN/dE calc.	unc.	dN/dE exp.	unc.	dN/dE lk=1	unc.
0	1.37491e-06	4.56604e-10	1.36282e-06	4.54479e-10	1.35951e-06	1.58534e-08
8	1.41489e-06	4.67613e-10	1.40958e-06	4.67776e-10	1.39901e-06	1.63497e-08
16	1.46578e-06	4.82021e-10	1.46404e-06	4.83425e-10	1.44933e-06	1.69282e-08
24	1.52758e-06	4.99830e-10	1.52621e-06	5.01425e-10	1.51049e-06	1.75890e-08
32	1.59207e-06	5.18314e-10	1.59014e-06	5.19795e-10	1.57433e-06	1.82615e-08

```
Mean energy from the calculated spectrum: 1072.92 (19) keV
Mean energy from the experimental shape factor: 1076.05 (19) keV
```

```
-------------------------
Antineutrino spectrum
-------------------------

Mean energy from the calculated spectrum: 1416.48 (29) keV
Mean energy from the experimental shape factor: 1416.24 (29) keV
Mean energy from the calculated spectrum if lk=1: 1413.4 (34) keV
```

E(keV)	dN/dE calc.	unc.	dN/dE exp.	unc.	dN/dE lk=1	unc.
0	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00
8	1.06916e-09	5.37713e-13	1.07023e-09	5.37166e-13	1.07440e-09	5.77388e-12
16	4.23052e-09	2.12127e-12	4.23474e-09	2.11910e-12	4.25140e-09	2.30004e-11

β and ν spectra


```
-------------------------
Antineutrino spectrum
-------------------------

Mean energy from the calculated spectrum: 1416.48 (29) keV
Mean energy from the experimental shape factor: 1416.24 (29) keV
Mean energy from the calculated spectrum if lk=1: 1413.4 (34) keV
```


E(keV)	dN/dE calc.	unc.	dN/dE exp.	unc.	dN/dE lk=1	unc.
0	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00
8	1.06916e-09	5.37713e-13	1.07023e-09	5.37166e-13	1.07440e-09	5.77388e-12
16	4.23052e-09	2.12127e-12	4.23474e-09	2.11910e-12	4.25140e-09	2.30004e-11
24	9.41583e-09	4.70705e-12	9.42521e-09	4.70220e-12	9.46266e-09	5.15326e-11
⋮	⋮	⋮	⋮	⋮	⋮	⋮

Output file

```
Mean energy from the total beta - spectrum: 461.24 (29) keV
Mean energy from the total antineutrino spectrum: 746.94 (46) keV
```

E(keV)	dNtot/dE b-	unc.
0	6.46345e-04	4.33494e-07
2	6.48384e-04	4.34182e-07
4	6.51291e-04	4.35438e-07
6	6.55064e-04	4.37264e-07
8	6.59705e-04	4.39659e-07
10	6.65079e-04	4.42530e-07

dNtot/dE nu	unc.
0.00000e+00	0.00000e+00
3.06131e-08	3.42335e-11
1.21807e-07	1.36066e-10
2.73582e-07	3.05496e-10
4.85147e-07	5.41442e-10
7.56347e-07	8.43690e-10

Mean energies of total spectra

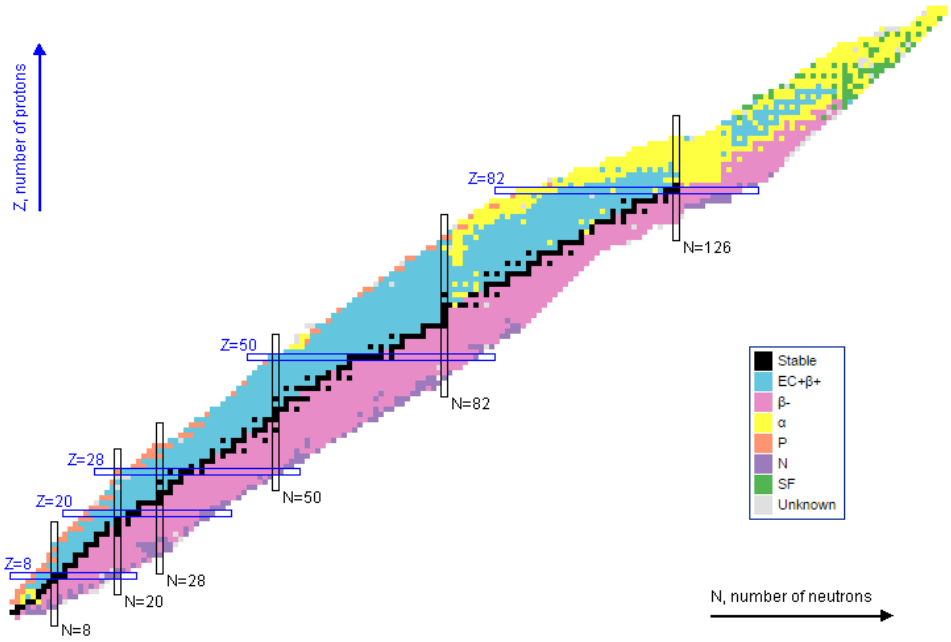
Total β spectrum

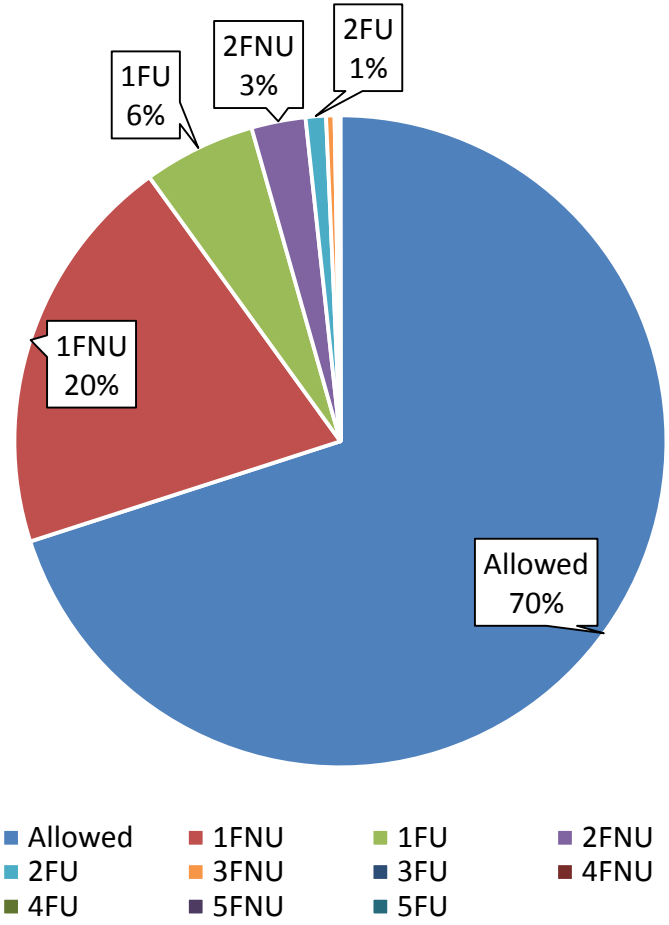
Total ν spectrum

.bs

total spectra

Analysis of ENSDF database (2015)

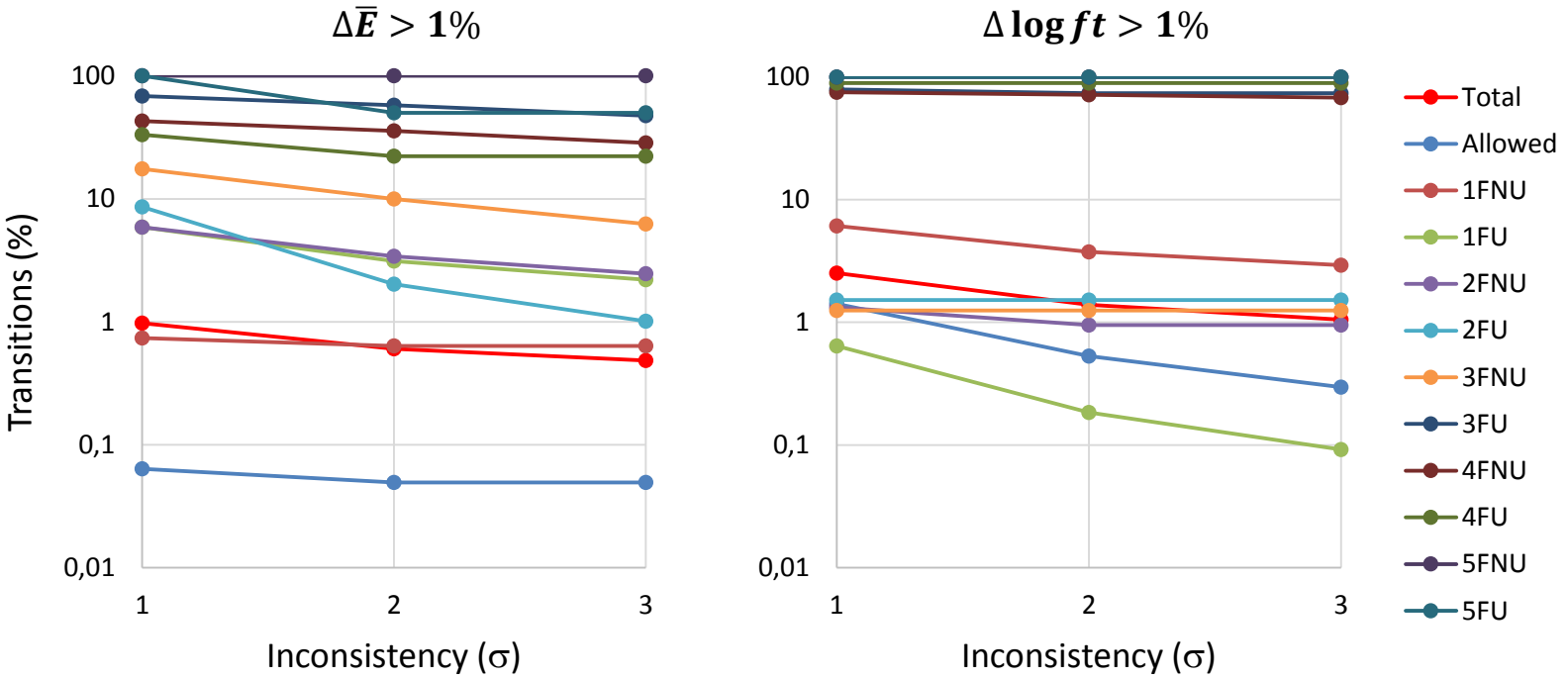




- 21 768 $\beta^{\pm}$ transitions read in ENSDF database
- 19 602 $\beta^{\pm}$ transitions with $I_{\beta} \geq 0$ and $E_{\max} \geq 0$ keV
- 4 529 transitions calculated as allowed due to lack of spins and parities

Study of the consistency of the results from LogFT and BetaShape at 1σ, 2σ, 3σ (68.3%, 95.4%, 99.7% C.L.) → Validation of BetaShape

BetaShape vs LogFT



For allowed and forbidden unique β^+/ε transitions

$$\log ft \approx \log\left(\frac{f_{\beta^+}}{I_{\beta^+}} T_{1/2}\right) \; ?$$

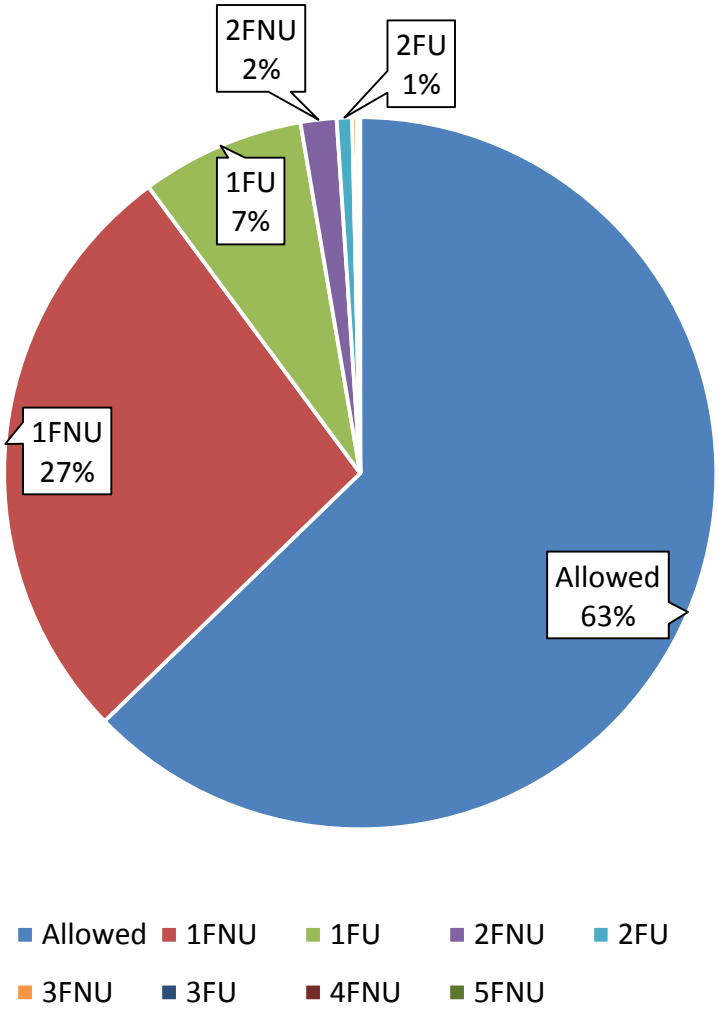
→ 21 of 8 506 β^+ transitions with inconsistent log *ft* at 1σ (experimental shape factors, no uncertainty on intensities, disagreement ≤ 2.5%)

This approximation leads to consistent results with LogFT for β^+/ε transitions at the precision level of current nuclear data.

Well-defined transitions

- Well-defined forbiddenness: spins and parities firmly assigned.
- Well-defined Q-values, parent half-life, energies, intensities and their uncertainties.
- Ionized or excited atomic states, uncertain or questionable states and decays, and decays with more than one parent (mixed source) are not considered.
- Pandemonium radionuclides are still present.

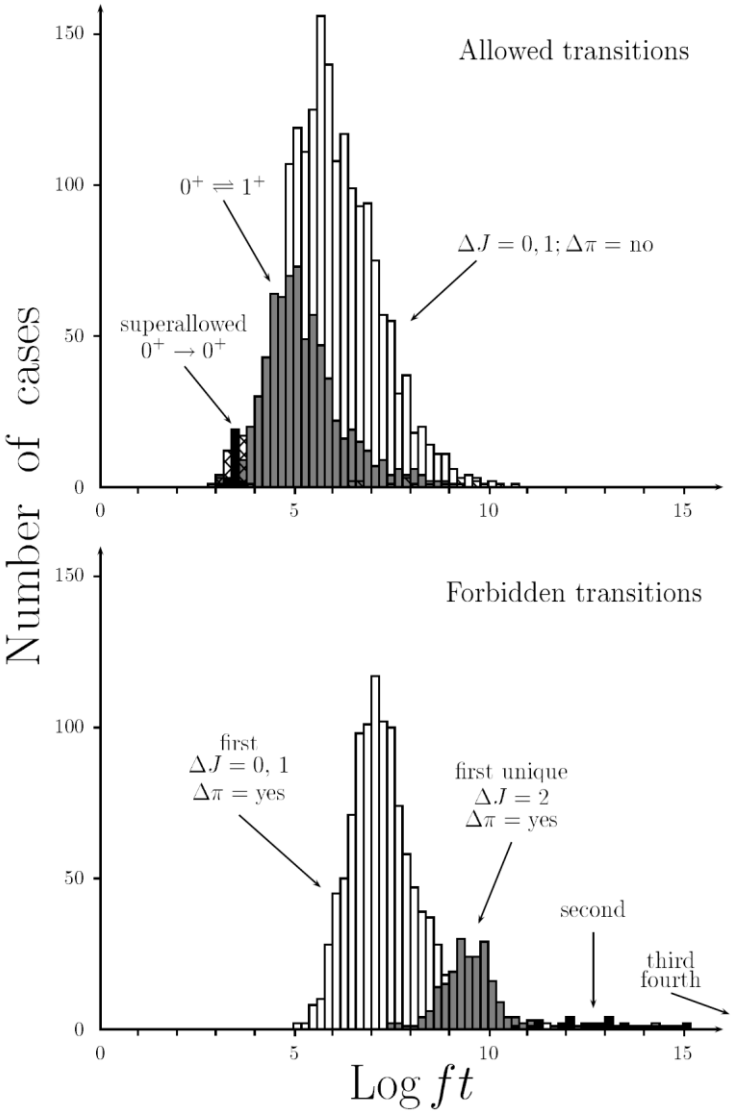
Type	Transitions
Total	3868
Allowed	2427
1FNU	1049
1FU	288
2FNU	63
2FU	27
3FNU	8
3FU	2
4FNU	3
5FNU	1

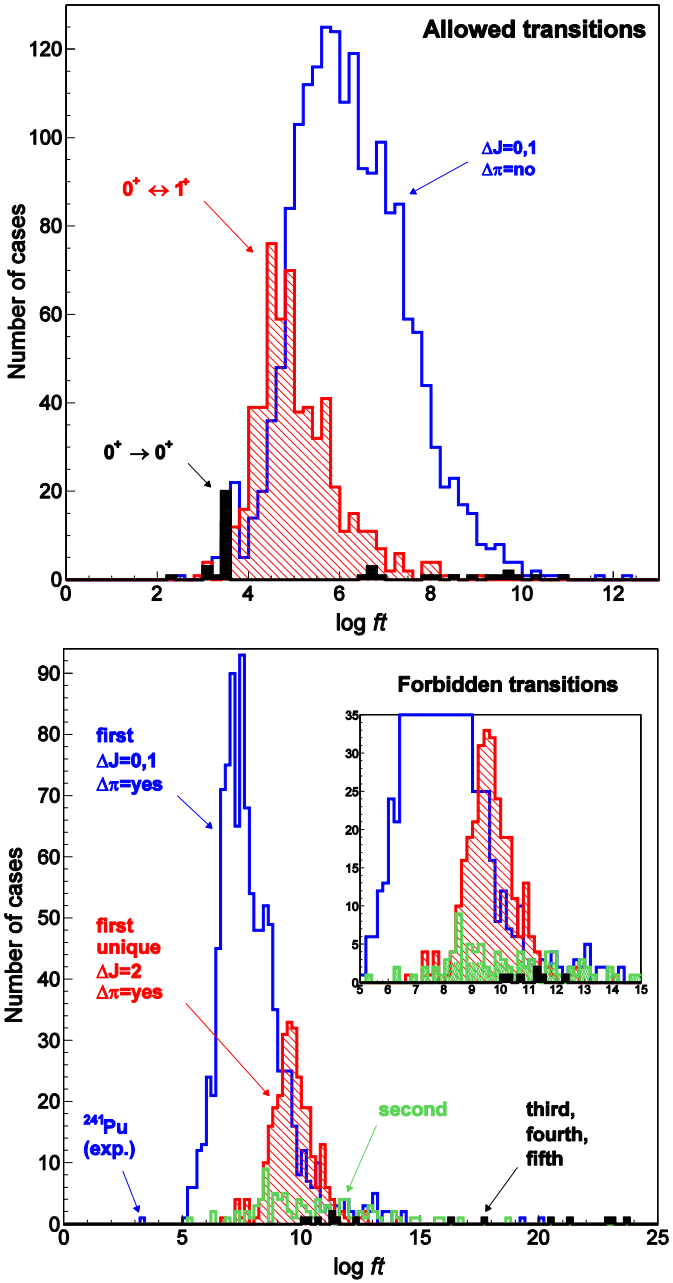


BetaShape results

B. Singh *et al.*, *Review Of Logft Values In β Decay*, Nuclear Data Sheets 84, 487 (1998)

(with electron capture transitions)

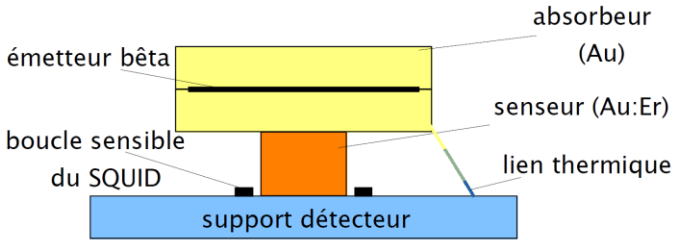


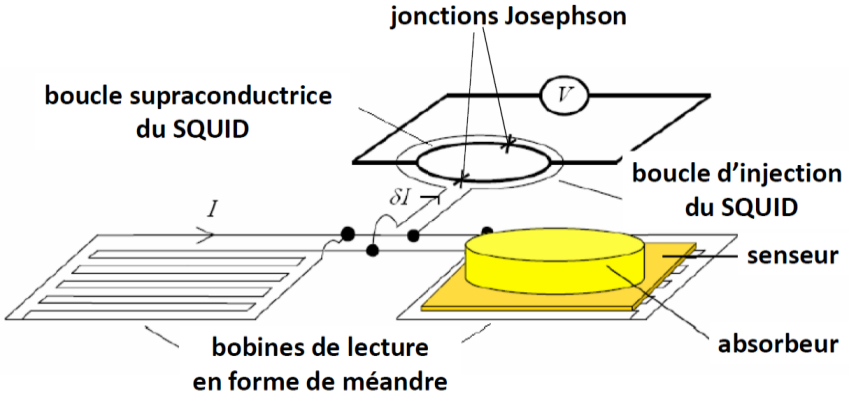


Atomic effects in beta decays

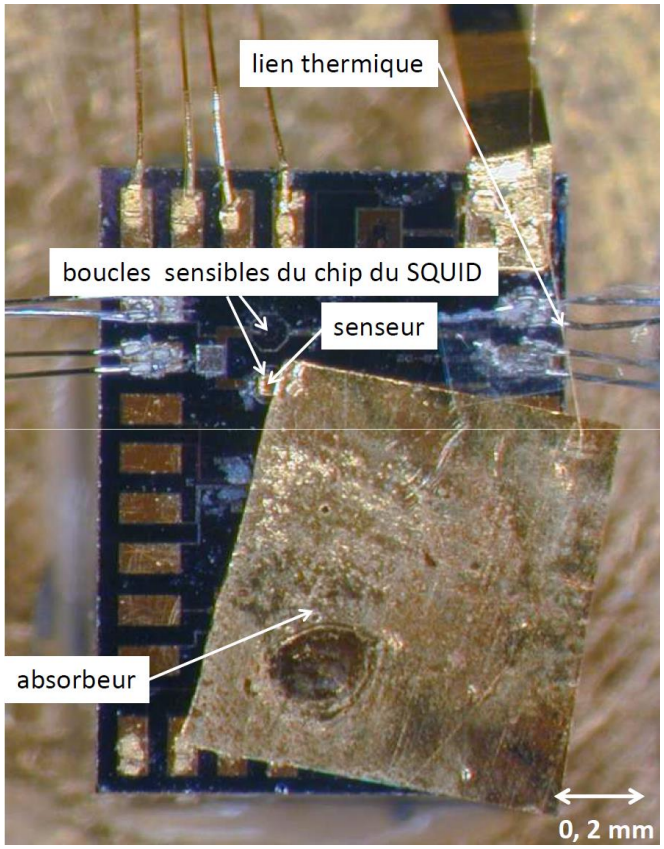
Metallic magnetic calorimetry at LNHB

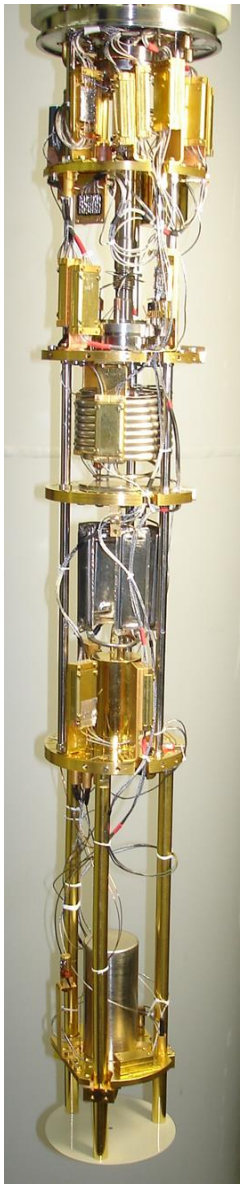
Direct magnetic coupling





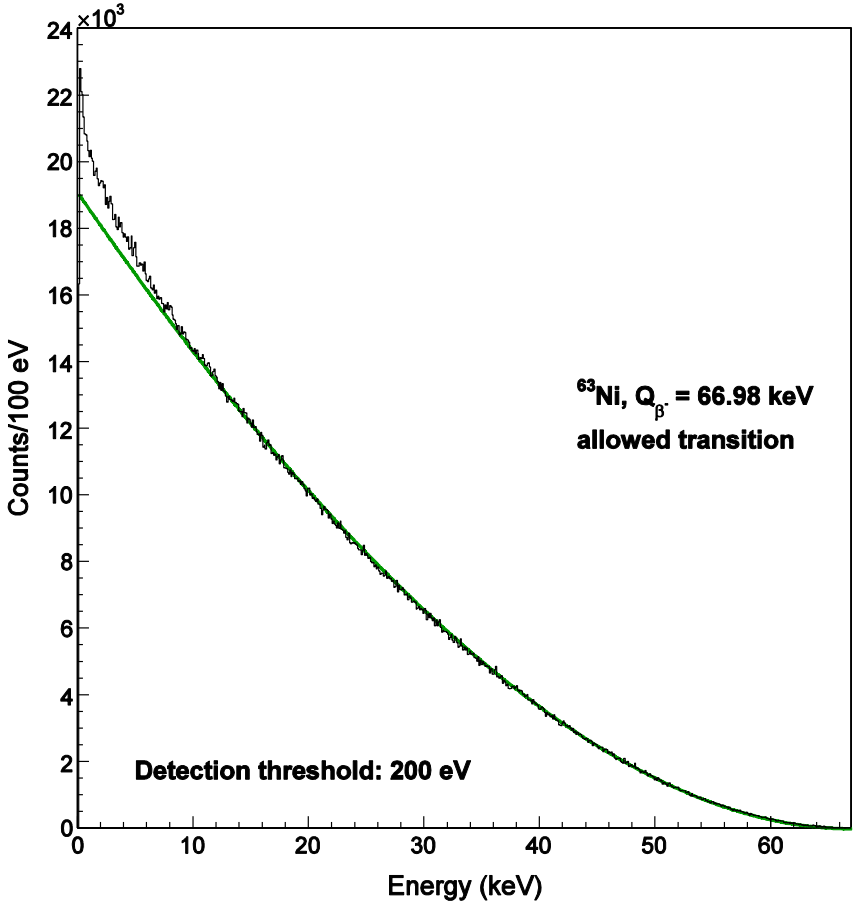
Indirect magnetic coupling

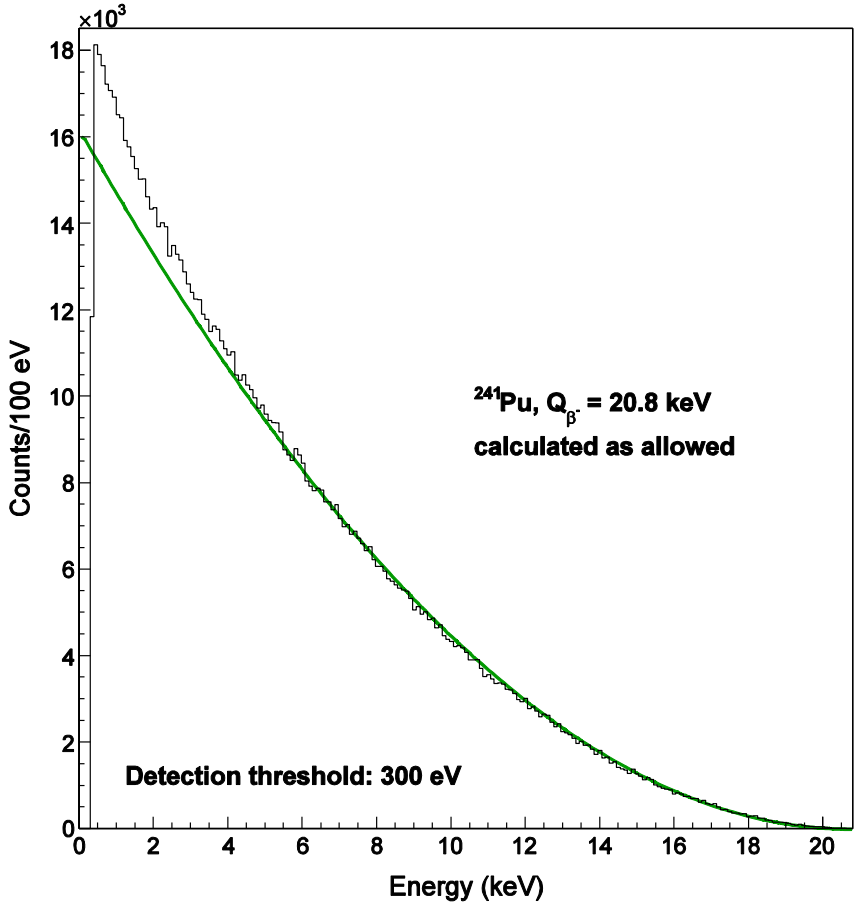




System cooled down to 10 mK

^{63}Ni and ^{241}Pu beta spectra





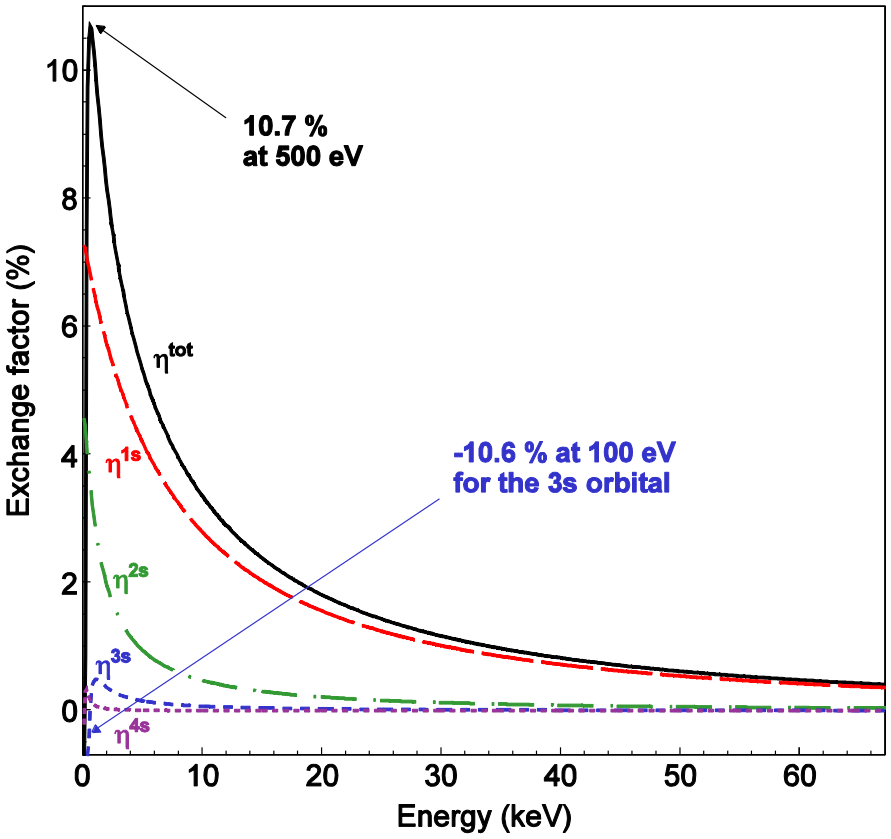
Classical beta calculations fail to reproduce these “simple” spectra

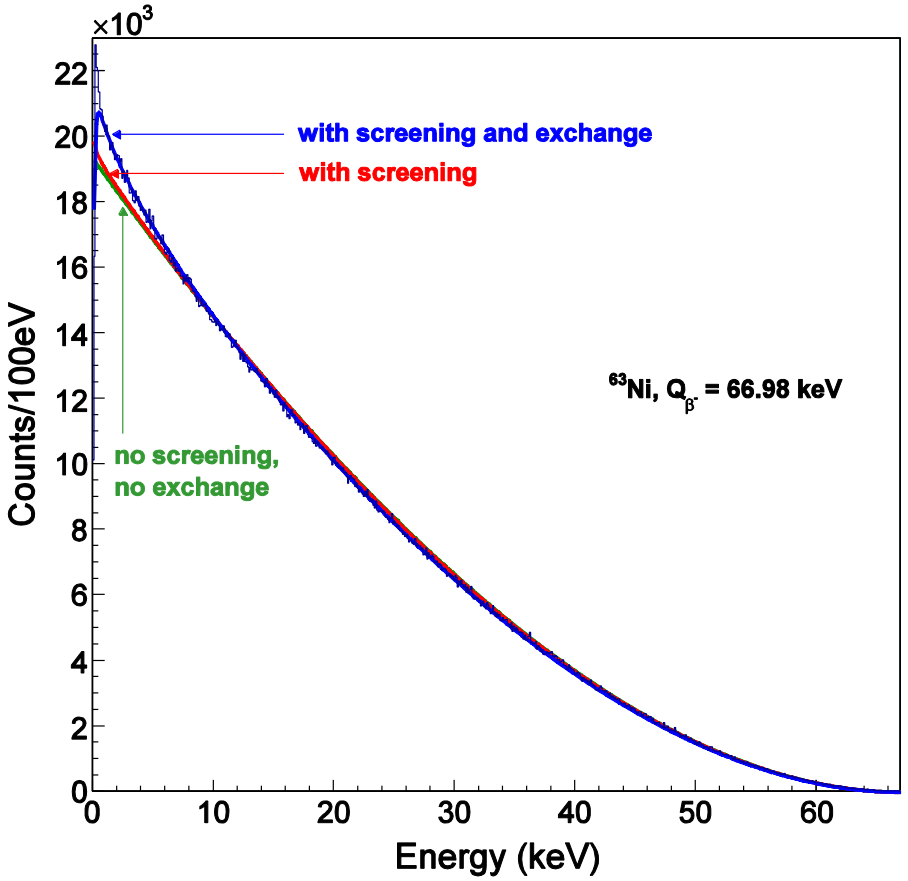
1st forbidden non-unique transition calculated as **allowed**

$2\xi = \alpha Z/R \gg E_0$ = 20.8 keV $\ll$ 19.8 MeV

^{63}Ni

X. Mougeot, C. Bisch, Phys. Rev. A 90, 012501 (2014)





Analytic: $\bar{E} = 17.45$ keV

With screening: $\bar{E} = 17.40$ keV

With screening and exchange: $\bar{E} = 17.14$ keV

Mean energy of the spectrum decreased by **1.8 %**

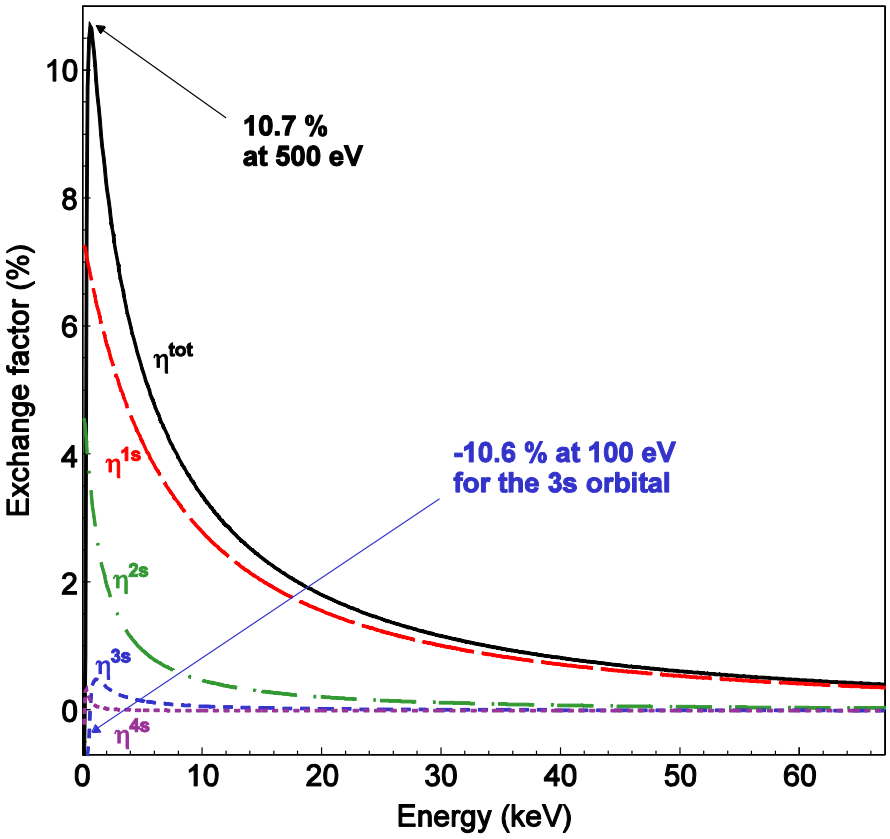
Allowed transition

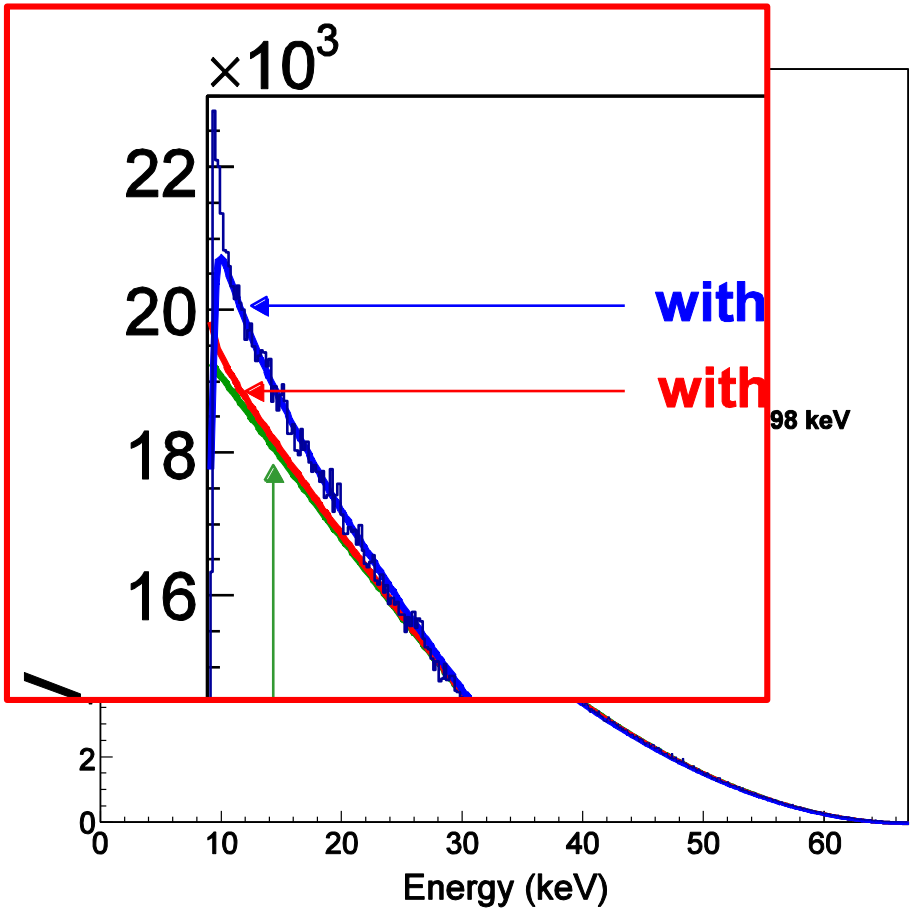
Experimental spectrum

C. Le-Bret, PhD thesis, Université Paris 11 (2012)

^{63}Ni

X. Mougeot, C. Bisch, Phys. Rev. A 90, 012501 (2014)





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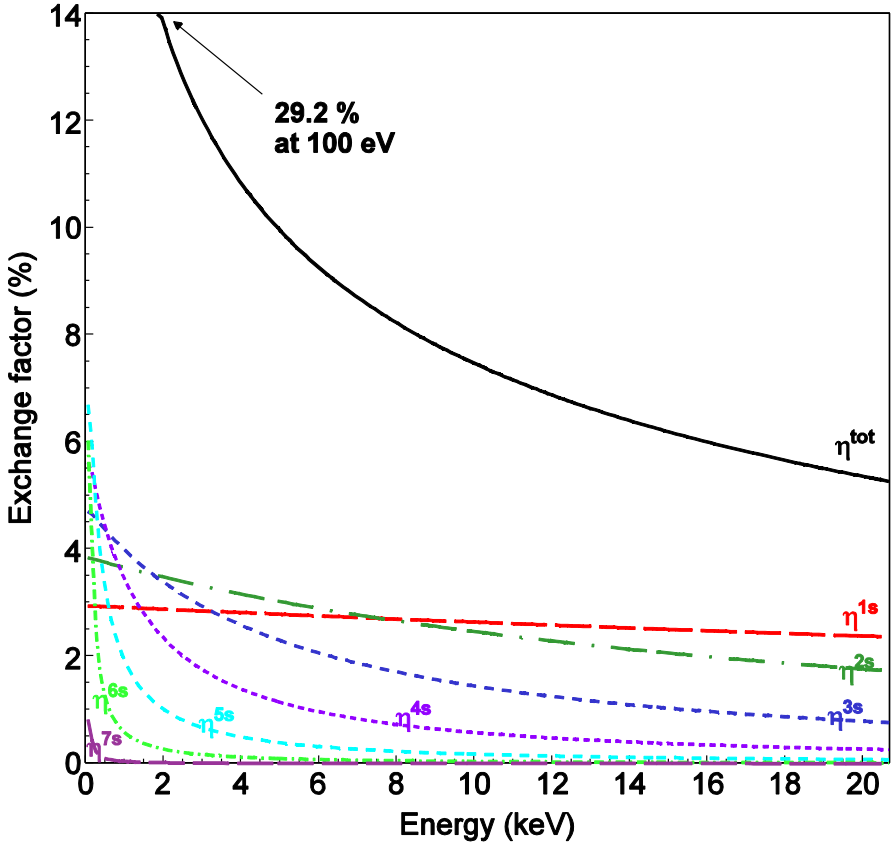
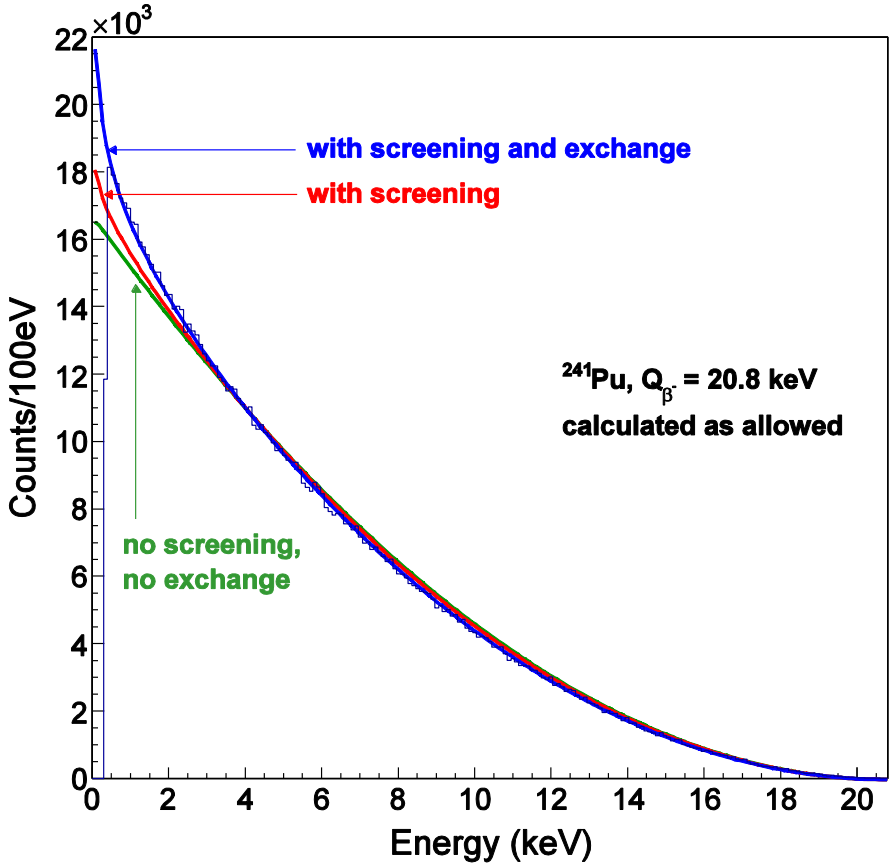




Analytic: $\bar{E} = 5.24$ keV

With screening: $\bar{E} = 5.18$ keV

With screening and exchange: $\bar{E} = 5.03$ keV

Mean energy of the spectrum decreased by **4** %

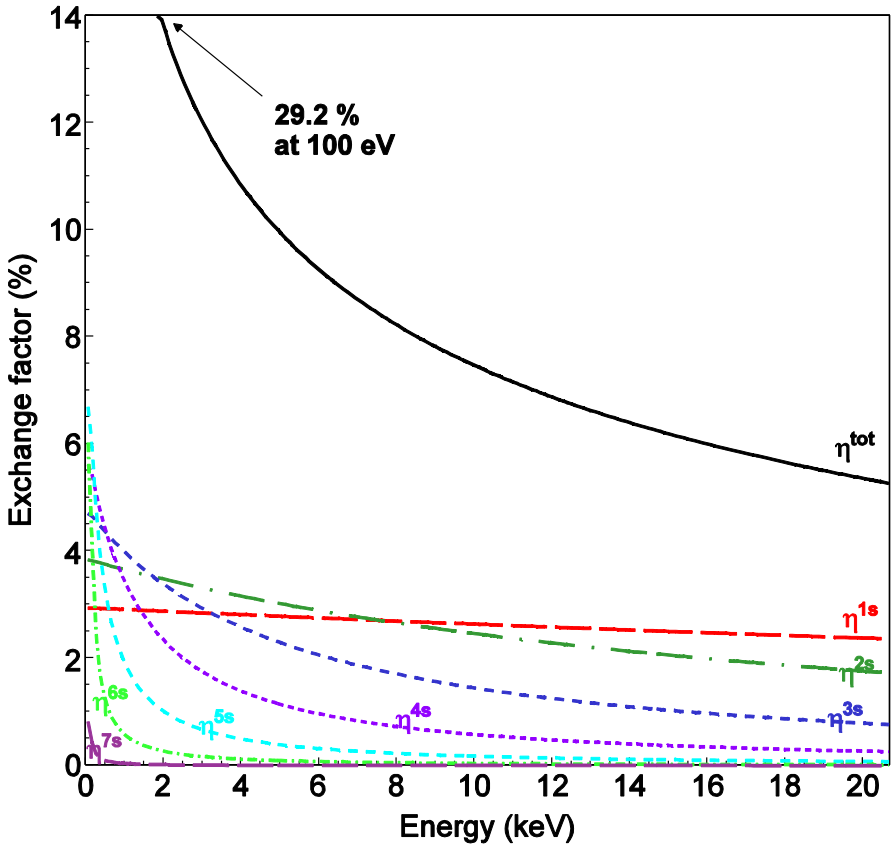
Calculated as **allowed**

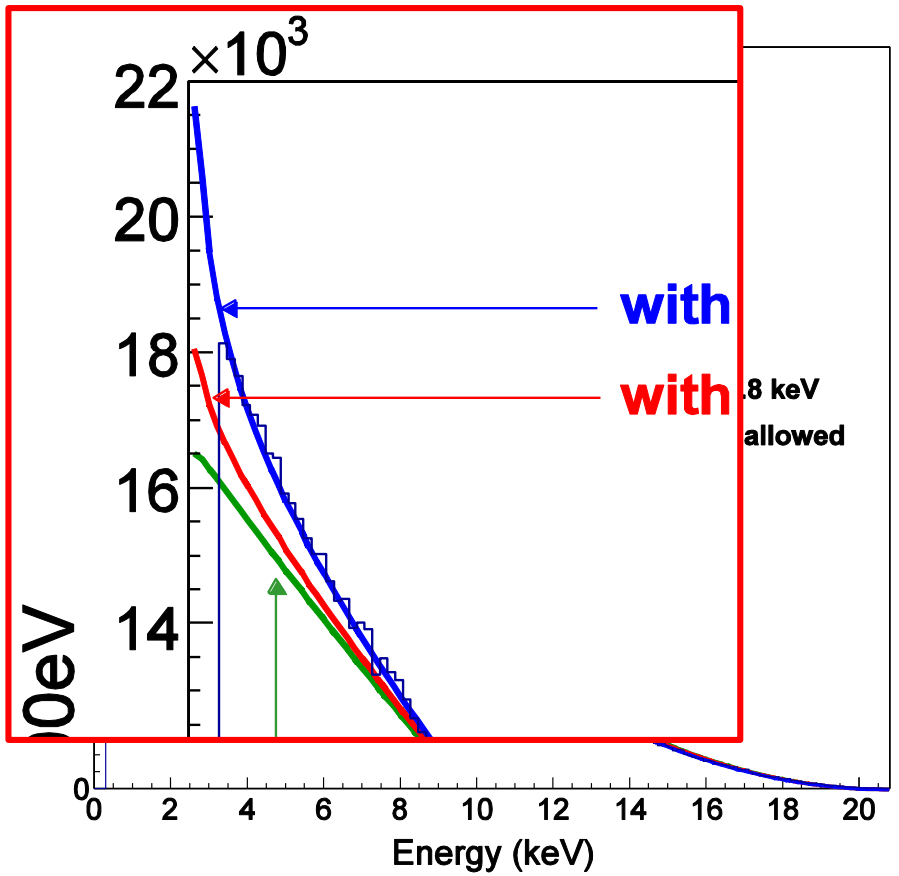
Experimental spectrum

M. Loidl *et al.*, App. Radiat. Isot. 68, 1454 (2010)

^{241}Pu

X. Mougeot, C. Bisch, Phys. Rev. A 90, 012501 (2014)





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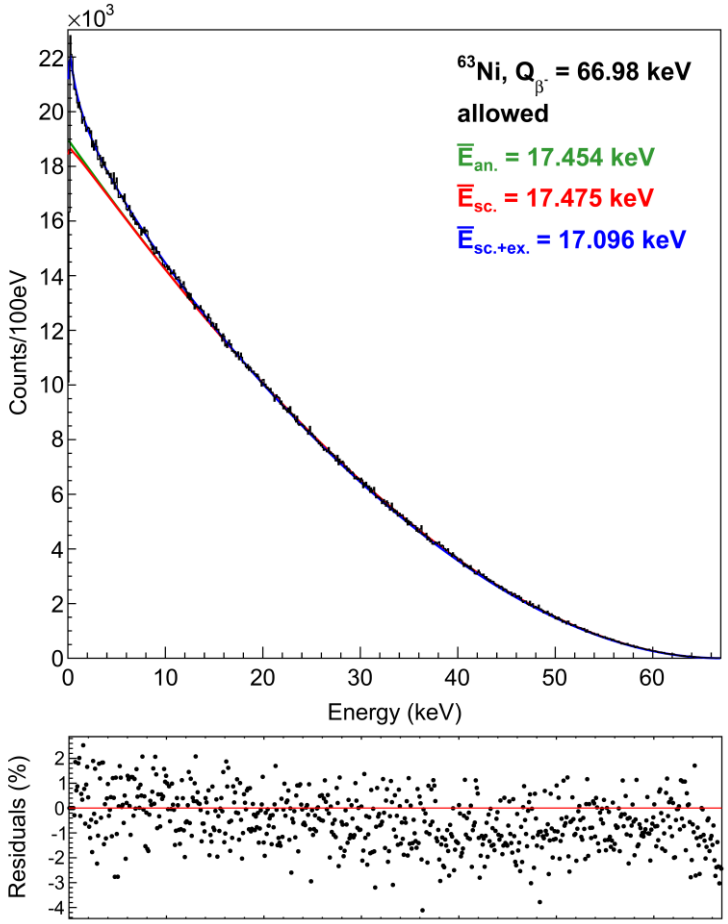
Influence of orbital energies: ^{63}Ni



Past study on atomic effects in allowed beta decays, with inclusion of the **atomic exchange effect for $s_{1/2}$ orbitals** and an ad hoc new screening correction.

X. Mougeot, C. Bisch, Phys. Rev. A 90, 012501 (2014)

Formalism has been revised to **include the $p_{1/2}$ orbitals**, initially expected to be negligible → ad hoc screening correction not necessary anymore.

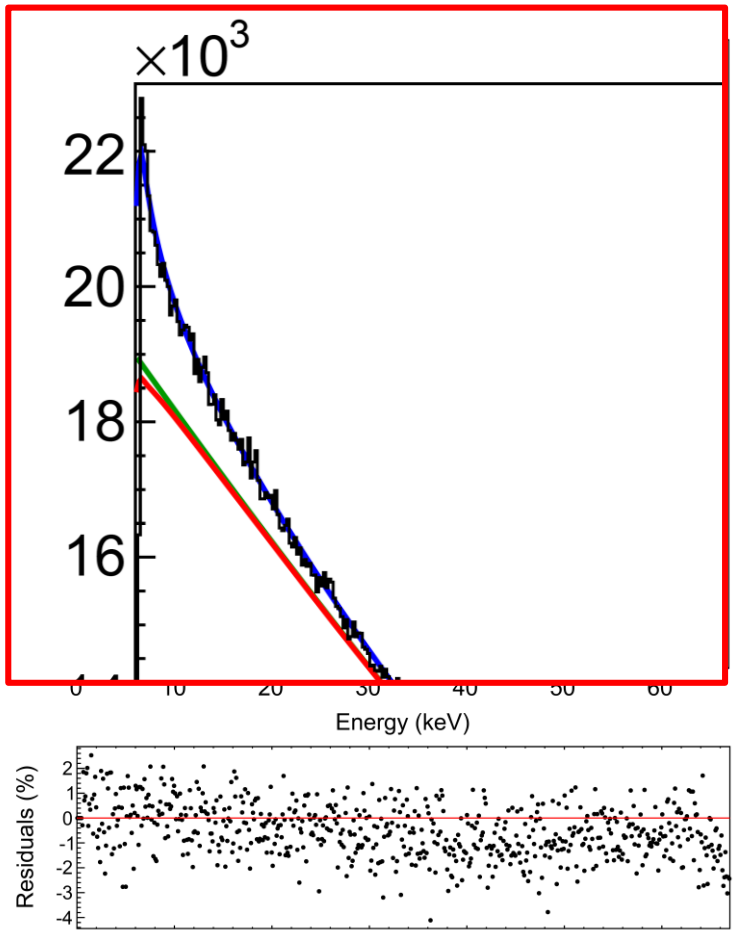
L. Hayen et al., Rev. Mod. Phys. 90, 015008 (2018)

In addition, **new radiative correction** and **new orbital energies** have been considered.

The relativistic local-density approximation (RLDA) approximates the electron correlations and self-consistently solves a set of single particle equations.

Eigenvalues obtained for the ground-state configuration of atoms from H to U are available on NIST website. Claimed accuracy is 0.05 meV.

Influence of orbital energies: ^{63}Ni



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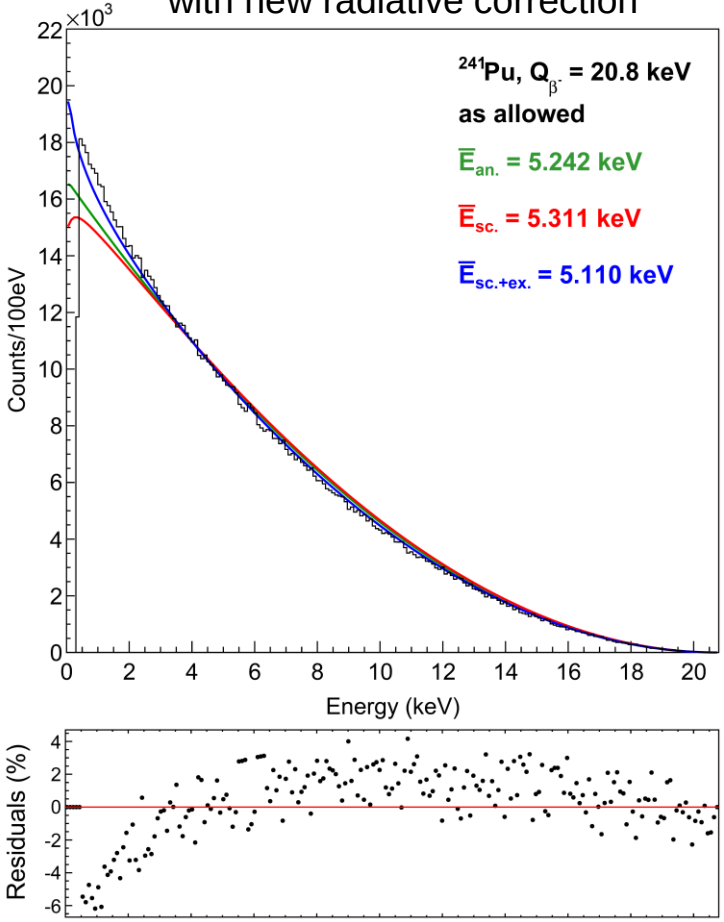
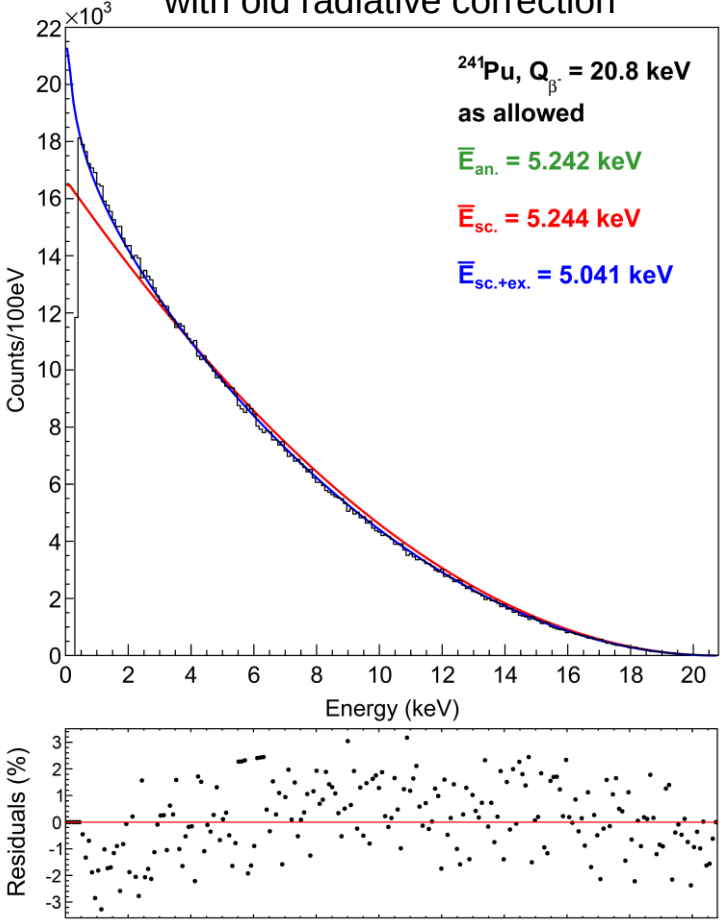
Influence of orbital energies: ^{241}Pu

with new radiative correction



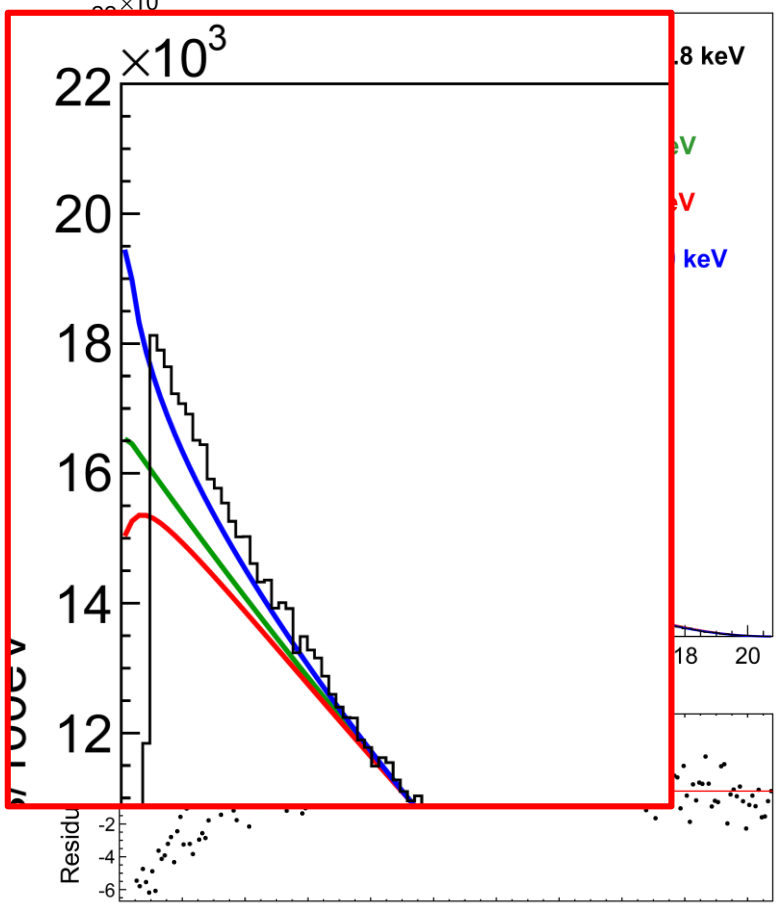
with old radiative correction



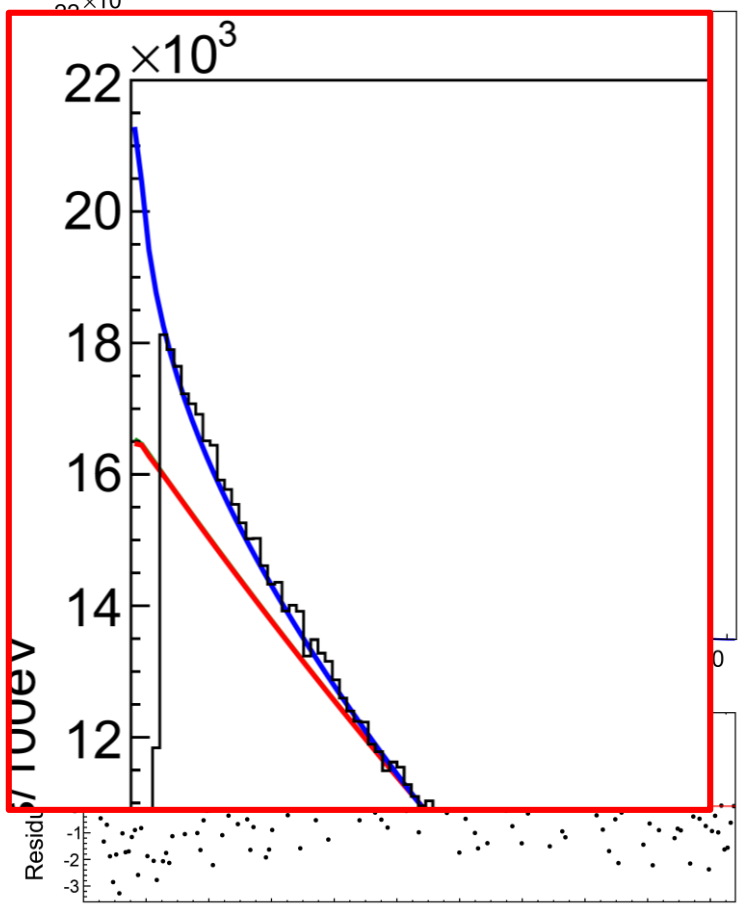
Orbital energies have been interpolated from NIST values with lower Z.

Influence of orbital energies: ^{241}Pu

with new radiative correction



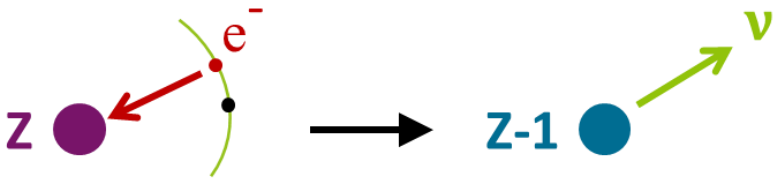
with old radiative correction



Orbital energies have been interpolated from NIST values with lower Z.

Electron capture decays

Basics of electron capture decay



Allowed and forbidden unique transitions can be calculated without any nuclear structure.

If transition energy $\geq 2m_e$

→ competition with a β^+ transition

Total capture probability

$$\lambda_\varepsilon \propto \sum_{\kappa_x} n_{\kappa_x} C_{\kappa_x} q^2_{\kappa_x} \beta^2_{\kappa_x} B_{\kappa_x} \left(1 + \sum_{m,\kappa} P_{m\kappa}\right)$$

- n_{κ_x}: relative occupation number
- $q^2_{\kappa_x}$: ν momentum
- $\beta^2_{\kappa_x}$: amplitude of wave function
- κ_x: shell quantum number
- C_{κ_x}: "shape" factor similar to $C(W)$ in β decay
- B_{κ_x}: overlap and exchange corrections
- $\left(1 + \sum_{m,\kappa} P_{m\kappa}\right)$: shaking effects

W. Bambynek *et al.*, Rev. Mod. Phys. 49, 77 (1977)

Atomic wave functions

Relativistic electron wave functions for the atomic bound states are needed.

The method used was initially developed for the atomic exchange effect in β^- decay calculations.

X. Mougeot, C. Bisch, Phys. Rev. A 90, 012501 (2014)

Dirac equation is solved numerically

- Local power series expansion $$\begin{Bmatrix} f(r) \\ g(r) \end{Bmatrix} = \frac{(pr)^{k-1}}{(2k-1)!!} \sum_{n=0}^{\infty} \begin{Bmatrix} a_n \\ b_n \end{Bmatrix} r^n$$

- **Coulomb potential** = **extended nucleus** (uniformly charged sphere)
  + **screened potential** (Coulomb influence of electrons)
  + **exchange potential** (indistinguishability of fermions)

- Iterative procedure to reach atomic energies from a multi-configurational Dirac-Fock code.

J.P. Desclaux, At. Data Nucl. Data Tab. 12, 311 (1973)

Overlap and exchange corrections

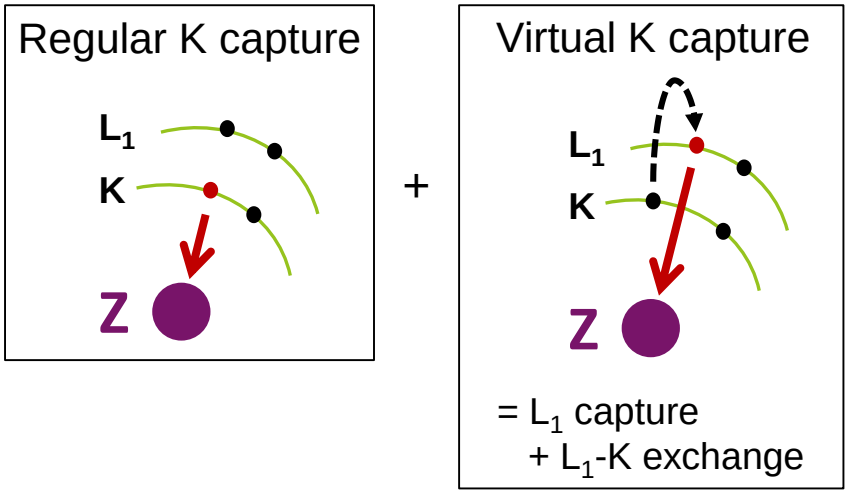
Overlap effect

Variation of nuclear charge: the **spectator electrons** contribute to the total decay rate.

→ Imperfect overlap between initial and final atomic wave functions

Exchange effect

Vacancy in the K shell?



+ M_1, etc.

Two approaches for overlap and exchange corrections

J.N. Bahcall, Phys. Rev. 129, 2683 (1963)	E. Vatai, Nucl. Phys. A 156, 541 (1970)

- **Bahcall**: only K, L_1 and M_1 shells
- **Vatai**: up to N_1 shell; other shells taken into account for overlap
- No multiple exchange process

Extension to every subshell

Generalization of the two approaches from Bahcall and Vatai

$$B_{n\kappa} = \left| \frac{b_{n\kappa}}{\beta_{n\kappa}} \right|^2 \quad \text{with}$$

Exchange

$$b_{n\kappa} = t_{n\kappa} \left[\prod_{m \neq n} \langle (m,\kappa)' | (m,\kappa) \rangle \right] \left[\beta_{n\kappa} - \sum_{m \neq n} \beta_{m\kappa} \frac{\langle (m,\kappa)' | (n,\kappa) \rangle}{\langle (m,\kappa)' | (m,\kappa) \rangle} \right]$$

Overlap

Bahcall

$$t_{n\kappa} = 1$$

Shake-up and shake-off roughly included, but **underestimation** of some probabilities and **overestimation** of others

Vatai

$$t_{n\kappa} = \langle (n,\kappa)' | (n,\kappa) \rangle^{n_{n\kappa} - 1/2|\kappa|} \left[\prod_{m \neq n} \langle (m,\kappa)' | (m,\kappa) \rangle^{n_{m\kappa}-1} \right] \left[\prod_{\substack{m,\mu \\ \mu \neq \kappa}} \langle (m,\mu)' | (m,\mu) \rangle^{n_{m\mu}} \right]$$

No shake-up and shake-off, but **more comprehensive** approach

Shaking effects

Each electron has only three possible final states

- **Spectator**: same original quantum numbers
- **Shake-up**: excitation to an unoccupied bound state
- **Shake-off**: ionization to a continuum state

Creation of a **secondary vacancy**

Original state preserved

Pauli principle
→ No transition to occupied bound states

$$P_{m\kappa} = 1 - |\langle (m,\kappa)'|(m,\kappa)\rangle|^{2n_{m\kappa}} - \sum_{l\neq m} n'_{l\kappa} n_{m\kappa} |\langle (l,\kappa)'|(m,\kappa)\rangle|^2$$

number of electrons in the subshell

B. Crasemann *et al.*, Phys. Rev. C 19, 1042 (1979)

For a given captured electron, **sum of shaking probability for each atomic electron**

$$\lambda_{n\kappa} \longrightarrow \lambda_{n\kappa}\left(1 + \sum_{m,\kappa} P_{m\kappa}\right)$$

Hole effect

The **capture** process induces that the **daughter** atom is in an **excited state**

→ Influence of the hole on the bound wave functions

First order perturbation theory $(\mathcal{H}_0 + \mathcal{H}')|(i,\kappa)'\rangle = (E_0 + E')|(i,\kappa)'\rangle$

Initial: parent atom **Perturbation**: the electron (n,κ) is captured

$$\mathcal{H}' = \frac{\alpha}{r} - \langle(n,\kappa)|\frac{\alpha}{|\overrightarrow{r_{n\kappa}} - \vec{r}|}|(n,\kappa)\rangle \quad \rightarrow \quad |(i,\kappa)'\rangle = |(i,\kappa)\rangle - \sum_{j\neq i}\frac{\langle(j,\kappa)|\mathcal{H}'|(i,\kappa)\rangle}{W_j - W_i}|(j,\kappa)\rangle$$

The correction of the hole effect is thus only applied through the **asymmetric overlaps**

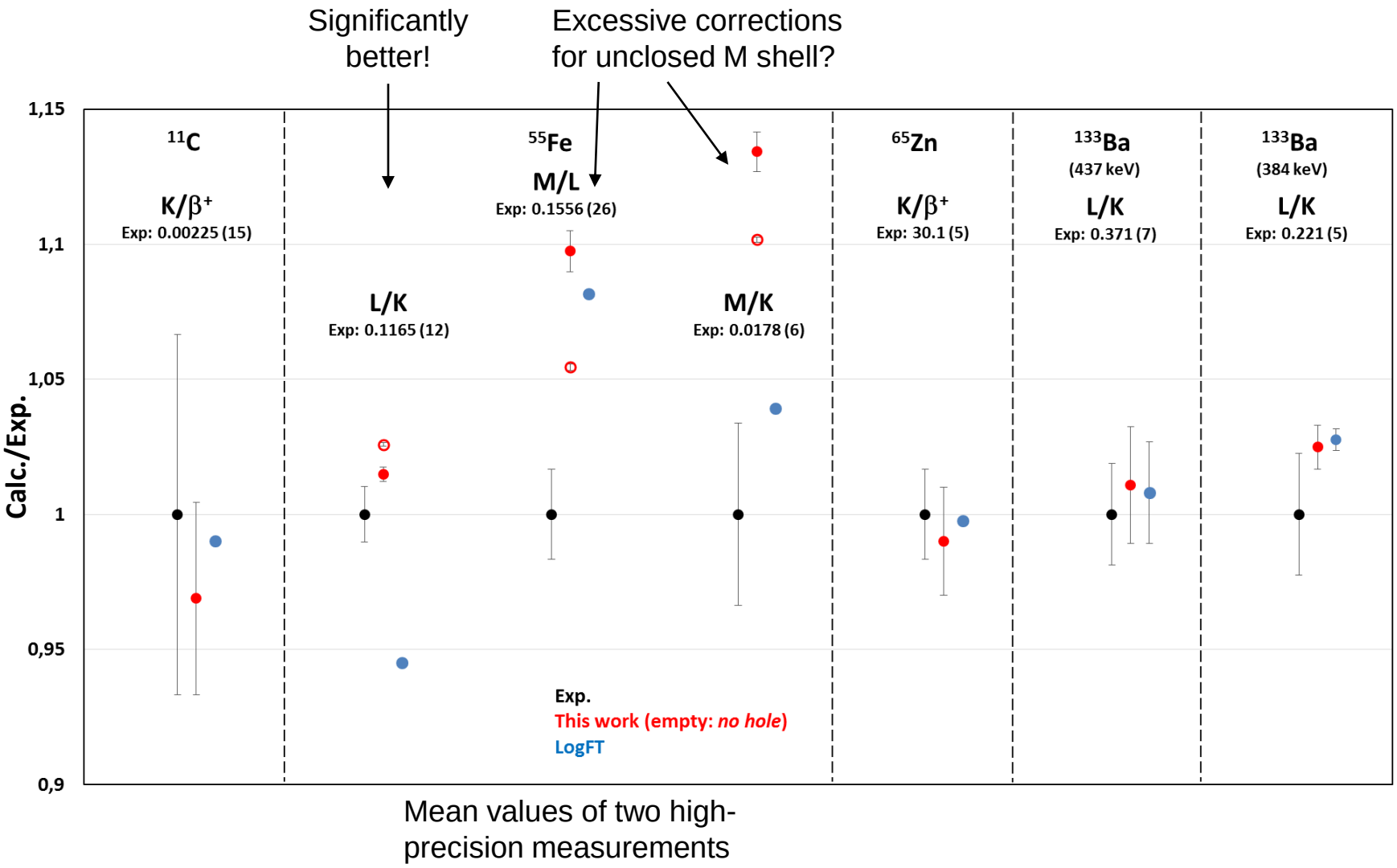
$$\langle(j,\kappa)'|(i,\kappa)\rangle = \frac{\langle(j,\kappa)|\mathcal{H}'|(i,\kappa)\rangle}{W_j - W_i}$$

with

$$\langle(j,\kappa)|\mathcal{H}'|(i,\kappa)\rangle = \int_0^\infty (\alpha r)\left[f_{j\kappa}(r)f_{i\kappa}(r) + g_{j\kappa}(r)g_{i\kappa}(r)\right] \times$$

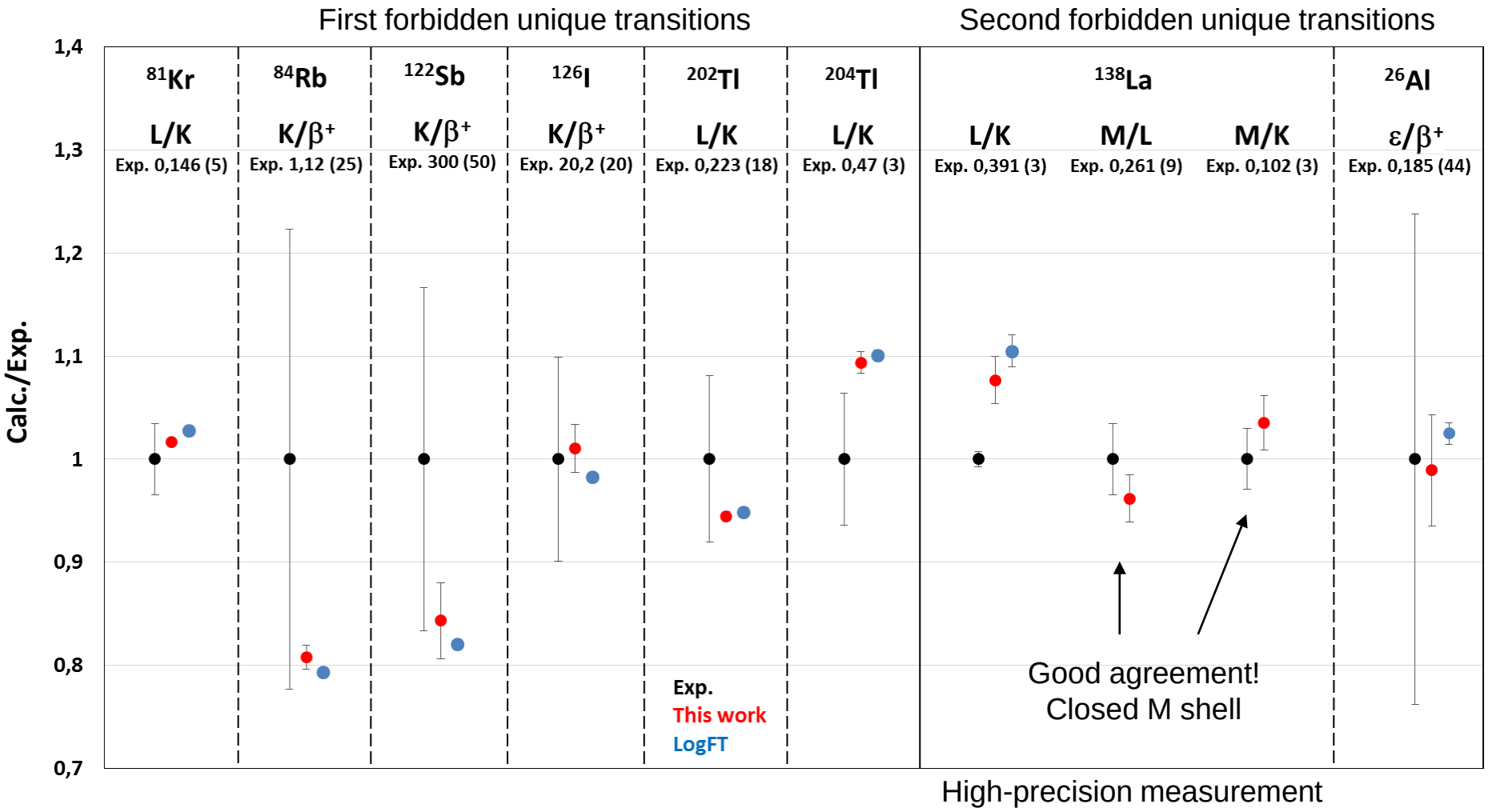
$$\left\{1 - \int_0^r x^2[g_{n\kappa}^2(x) + f_{n\kappa}^2(x)]\mathrm{d}x - r\int_r^\infty x[g_{n\kappa}^2(x) + f_{n\kappa}^2(x)]\,\mathrm{d}x\right\}\mathrm{d}r$$

Allowed transitions



Mean values of two high-precision measurements

Forbidden unique transitions



Influence of orbital energies (preliminary study)

The relativistic local-density approximation (RLDA) approximates the electron correlations and self-consistently solves a set of single particle equations.

Eigenvalues obtained for the ground-state configuration of atoms from H to U are available on NIST website. Claimed accuracy is 0.05 meV.

		Previous calculation			With RLDA energies		
^{55}Fe	**Experiment**	**Final**	Bahcall	Vatai	**Final**	Bahcall	Vatai
L/K	**0.1165 (12)**	**0.1182 (3)**	0.1185	0.1179	**0.1166 (3)**	0.1169	0.1163
M/L	**0.1556 (26)**	**0.1708 (12)**	0.1714	0.1701	**0.1577 (11)**	0.1583	0.1570
M/K	**0.0178 (6)**	**0.0202 (1)**	0.0203	0.0201	**0.0184 (1)**	0.0185	0.0183

→ Now results are compatible with measurements.

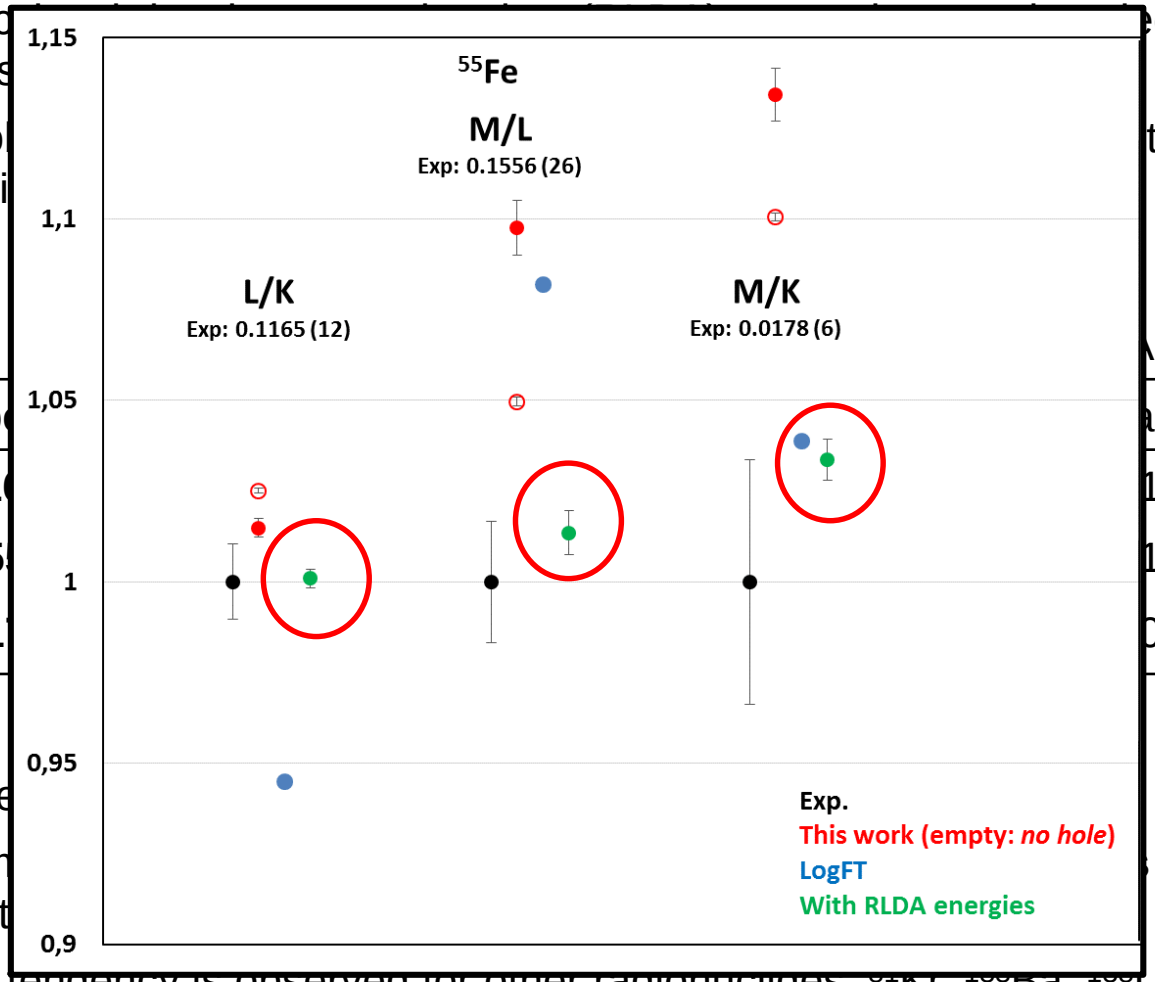
→ It seems also possible to see the better predictive power of Vatai's approach, as expected from a pure theoretical point of view.

→ Same tendency is observed for other radionuclides: ^{81}Kr, ^{133}Ba, ^{138}La, ^{202}Tl, ^{204}Tl.

Influence of orbital energies (preliminary study)

The relativistic [illegible] ectron correlations and self-consis[illegible]

Eigenvalues o[illegible] to U are available on NIST websi[illegible]



[illegible] energies

^{55}Fe	Exp[illegible]	[illegible]ahcall	Vatai
L/K	**0.11[illegible]**	[illegible]1169	0.1163
M/L	**0.15[illegible]**	[illegible]1583	0.1570
M/K	**0.01[illegible]**	[illegible]0185	0.0183

→ Now re[illegible]

→ It seen[illegible] approach, as expect[illegible]

→ Same tendency is observed for other radionuclides: ^{81}Kr, ^{133}Ba, ^{139}La, ^{202}Tl, ^{204}Tl.

Capture-to-positron ratios (preliminary study)

- Precise measurements, with relative uncertainty < 5%, are scarce.
- Radiative corrections are different as β^+ transition competes.

	Hagberg et al., Nucl. Phys. A 357, 365 (1981)				This work with RLDA energies		
^{130}Cs	**Experiment**	Theory	Rad. Corr.	**Total Theory**	Theory	Rad. Corr.	**Total Theory**
K/β^+	**1.025 (22)**	1.063 (23)	1.3%	**1.077 (23)**	1.025 (18)	1.24%	**1.038 (18)**

→ Now results are compatible with measurements.

→ Still difficult to distinguish between Bahcall's and Vatai's approaches.

→ Difficult also to be conclusive with other radionuclides due to the precision of the measurements. Tested: ^{11}C, ^{22}Na, ^{26}Al, ^{65}Zn, ^{84}Rb, ^{122}Sb, ^{126}I.

→ New measurements would be very interesting.

Inclusion of nuclear structure

Beta transition probability per beta particle energy

$$P(W_e)\mathrm{d}W_e = \frac{G_\beta^2}{2\pi^3} F_0 L_0 C(W_e) p_e W_e (W_0 - W_e)^2 \mathrm{d}W_e$$

Phase space

Fermi function

Shape factor

H. Behrens, W. Bühring, *Electron Radial Wave functions and Nuclear Beta Decay*, Oxford Science Publications (1982)

Theoretical shape factor

$$C(W_e) = \sum_{K k_e k_\nu} \lambda_{k_e} \left[M_K^2(k_e, k_\nu) + m_K^2(k_e, k_\nu) - \frac{2\mu_{k_e}\gamma_{k_e}}{k_e W_e} M_K(k_e, k_\nu) m_K(k_e, k_\nu) \right]$$

This formulation allows the calculation of **beta transition of every nature** (allowed, forbidden unique and forbidden non-unique).

Decay constants, partial half-lives, branching ratios and log *ft* values are integrated quantities of the beta spectrum.

$M_K(k_e, k_\nu)$ and $m_K(k_e, k_\nu)$ couple the nuclear component with the lepton component.

M_K for beta minus transitions

Spherical Bessel functions from multipole expansion

$$M_K(k_e,k_\nu) = \frac{2}{\pi}\frac{1}{\sqrt{2K+1}}\sum_{Ls}(-1)^{K-L}\int_0^\infty q^2\mathrm{d}q\int_0^\infty r^2\mathrm{d}r\frac{(qR)^L}{(2L+1)!!}j_L(qr)$$

Form factors with nuclear matrix elements

$$\times F_{KLs}(q^2)\frac{(p_e r)^{k_e-1}}{(2k_e-1)!!}\{H_{k_e}(r)[j_{k_\nu-1}(p_\nu r)G_{KLs}(-k_e,-k_\nu)$$

$$-j_{k_\nu}(p_\nu r)G_{KLs}(-k_e,k_\nu)] + \frac{r}{R}D_{k_e}(r)[j_{k_\nu-1}(p_\nu r)G_{KLs}(k_e,-k_\nu)$$

$$-j_{k_\nu}(p_\nu r)G_{KLs}(k_e,k_\nu)]\}$$

Depend on relativistic electron wave functions

Spherical Bessel functions for neutrino wave functions

Geometrical coefficients

Geometrical coefficients

These coefficients come from the coupling of the angular momenta of many particles

→ 2 particles: Clebsch-Gordan coefficient (or 3j-symbol)

→ 3 particles: 6j-symbol

→ 4 particles: 9j-symbol

$$G_{KLs}(\kappa_e,\kappa_\nu) = i^{l_e+l_\nu+L}(-1)^{j_e-j_\nu} \times \sqrt{(2s+1)(2K+1)(2j_e+1)(2j_\nu+1)} \times \sqrt{(2l_e+1)(2l_\nu+1)} \times C(l_e\ l_\nu\ L;00) \begin{Bmatrix} K & s & L \\ j_e & \frac{1}{2} & l_e \\ j_\nu & \frac{1}{2} & l_\nu \end{Bmatrix}$$

Racah's formulas allow the calculation of 3j-symbols, Clebsch-Gordan coefficients and 6j-symbols. 9j-symbols can be linked to a combination of 3j- or 6j-symbols.

The geometrical coefficients ensure the consistency of the formalism between the angular momenta of nucleons and leptons.

Nuclear matrix elements

Nuclear matrix elements are embedded within M_K quantities.

In the case of single-particle matrix elements, an analytical integration over the transferred momentum q in the M_K quantities can be conducted.

This procedure is mathematically consistent with the usual statement for allowed transitions, namely that electron wave functions can be approximated by their value at the nucleus surface.

$$^{V}\mathcal{M}_{KK0}(q^2) = \frac{\sqrt{2}}{\sqrt{2J_i+1}} \cdot \frac{(2K+1)!!}{(qR)^K}$$

Geometrical coefficients

$$\times \Big[G_{KK0}(\kappa_f,\kappa_i) \int_0^\infty g_f(r,\kappa_f) j_K(qr) g_i(r,\kappa_i) r^2 \mathrm{d}r$$

$$+ S_{\kappa_f} S_{\kappa_i} G_{KK0}(-\kappa_f,-\kappa_i) \int_0^\infty f_f(r,\kappa_f) j_K(qr) f_i(r,\kappa_i) r^2 \mathrm{d}r \Big]$$

Relativistic single-particle wave functions of the nucleons in their bound states.

→ Input from a nuclear structure model is necessary here.

Relativistic nucleon wave functions

Two simple tests in spherical symmetry

1. Non-relativistic harmonic oscillator

$$V(r) = -V_0 + \frac{1}{2}(\hbar\omega_0)^2 r^2$$

No Coulomb potential: only nucleons, proton = neutron

Relativistic small component estimated from non-relativistic (large) component

$$f_\kappa(r) = \frac{\mathrm{sign}(\kappa)}{2m}\left(\frac{\mathrm{d}}{\mathrm{d}r} + \frac{\kappa+1}{r}\right) g_\kappa(r)$$

2. Relativistic harmonic oscillator

Introduction of a purely imaginary vector potential: $\vec{p} \longrightarrow \vec{p} + i\beta m\omega\vec{r}$

This approach induces a very strong spin-orbit coupling ($\omega/\hbar$)

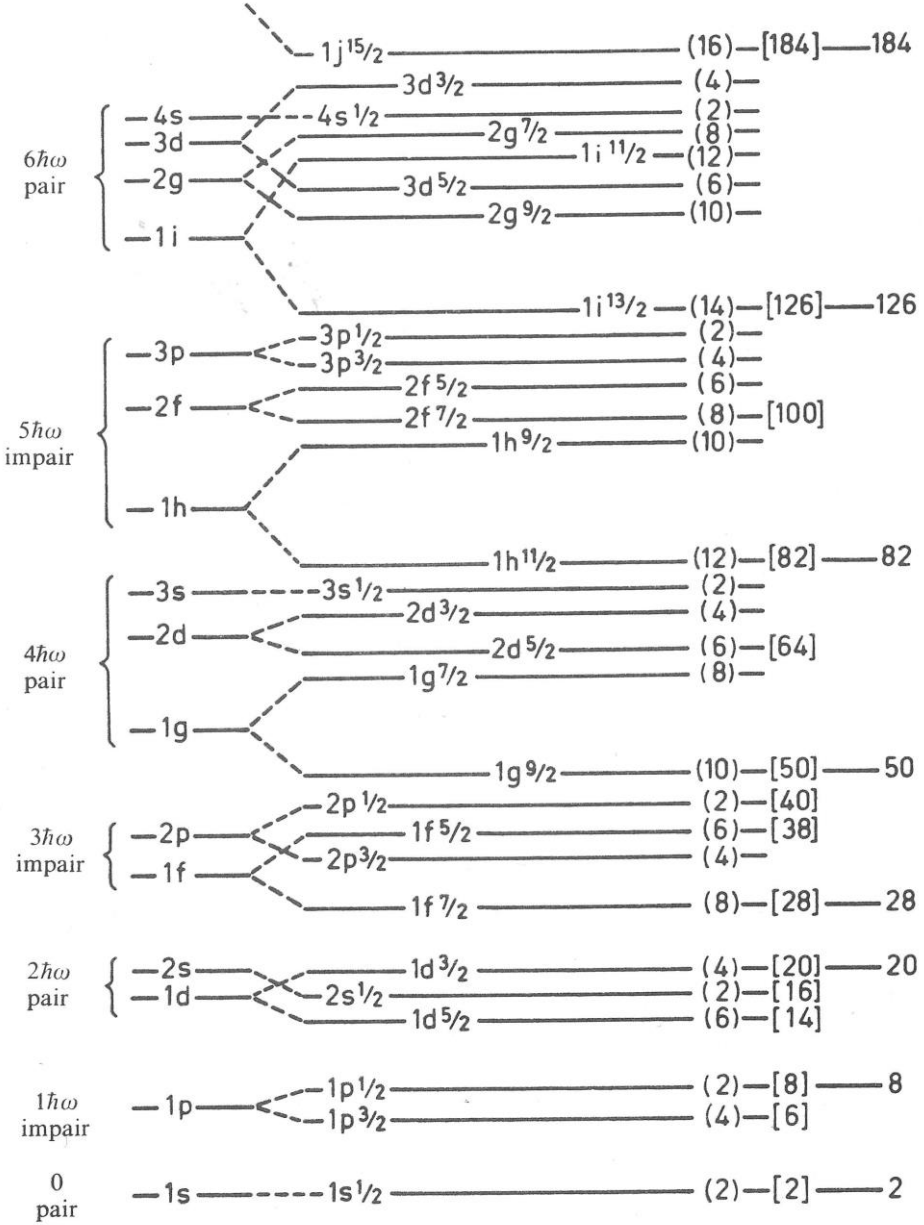
Protons ≠ neutrons: introduction of a quadratic Coulomb potential

→ only a shift in the harmonic oscillator frequency

Naive shell model

In the present study, a naive shell model has been used to determine the nucleon configurations.

L. Valentin, *Noyaux et particules : modèles et symétries*, Paris Hermann (1989)



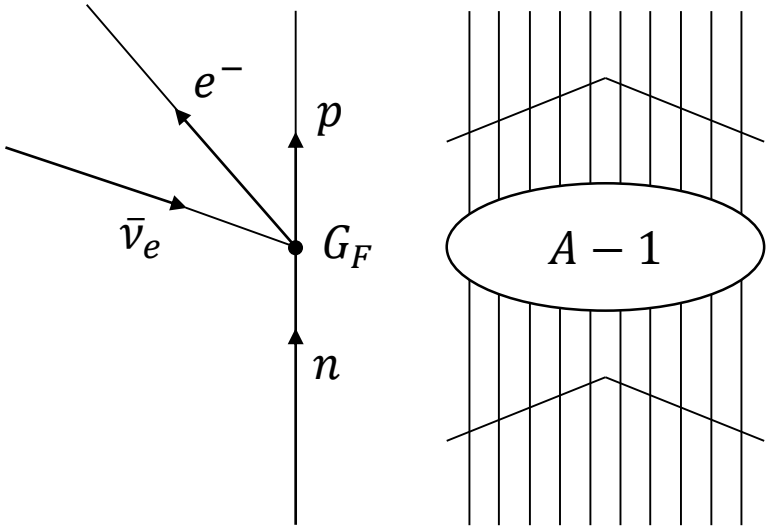
Description of the weak decay process

In the present study, **impulse approximation** is considered:

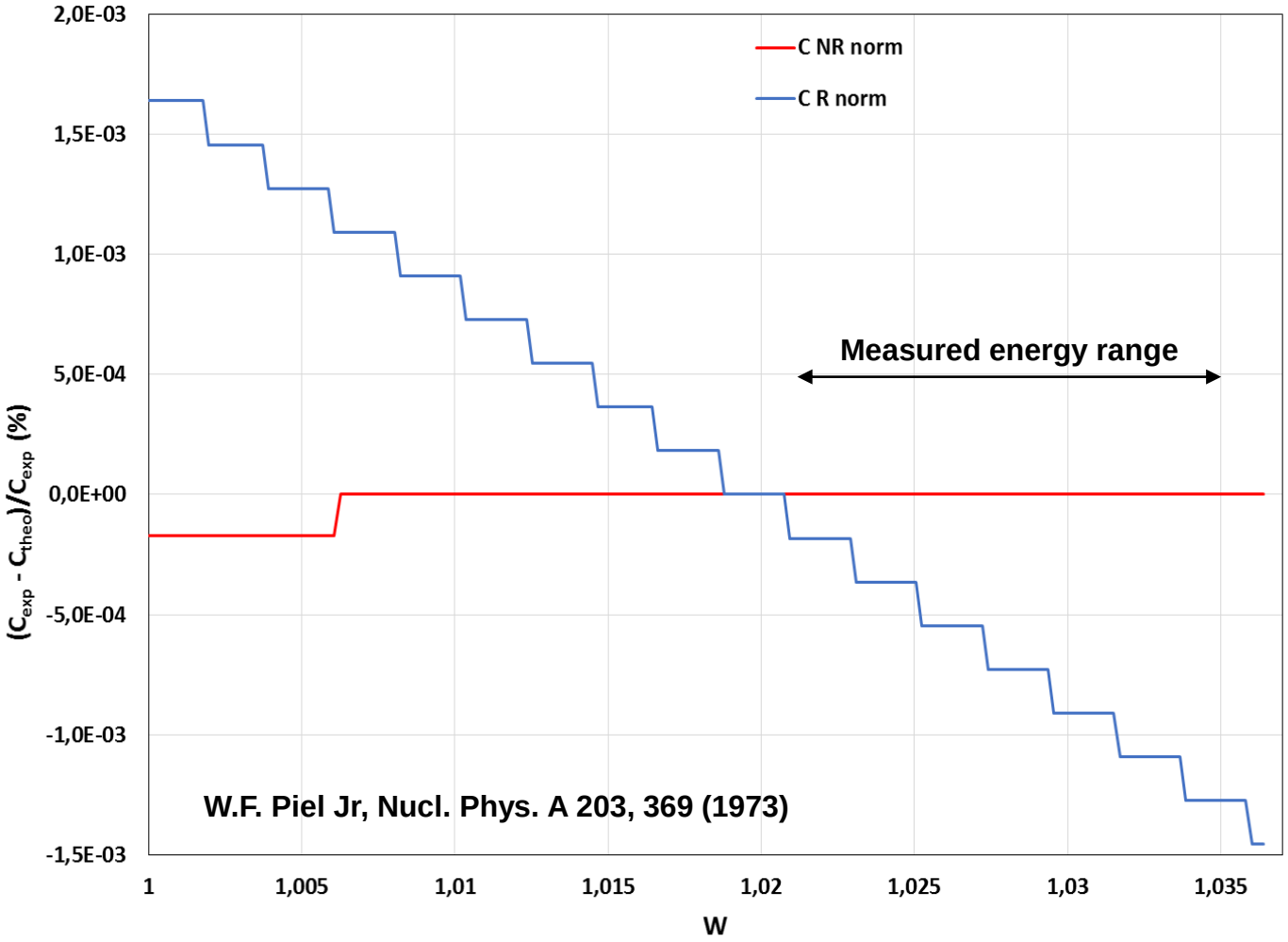
- At the moment of the decay, the nucleon is assumed to feel only the weak interaction.
- Other nucleons are assumed to be spectators with respect to the weak decay process.

Fermi theory is also considered:

- Vertex of the weak interaction is assumed to be pointlike.
- No $W^{\pm}$ boson is propagated.
- The effective coupling constant G_F is used.



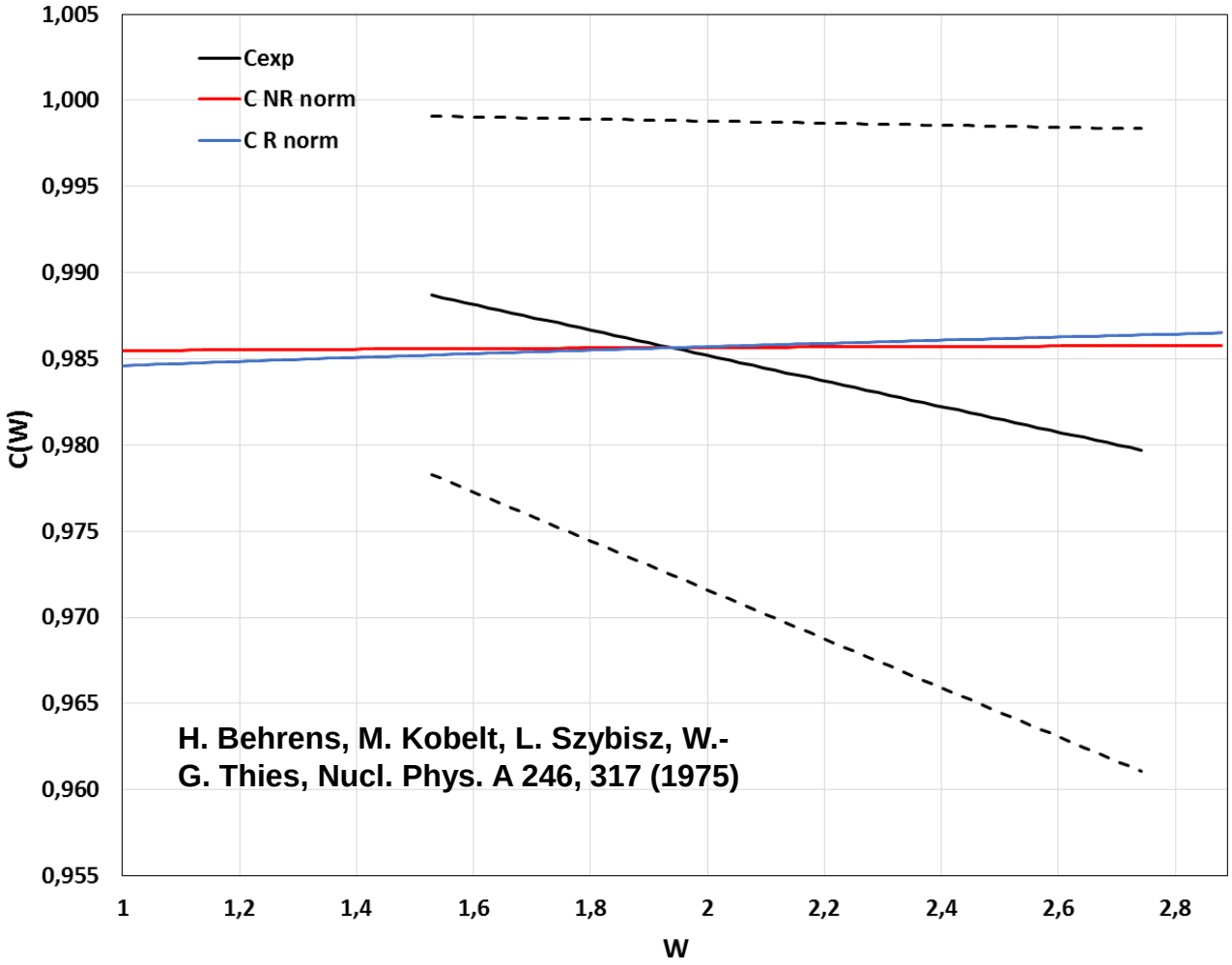
Theoretical shape factor: ^{3}H



Allowed

Initial state	Final state
$\left\|\pi^{-1}, 1s_{1/2}\right\rangle$	$\left\|\nu^{-1}, 1s_{1/2}\right\rangle$

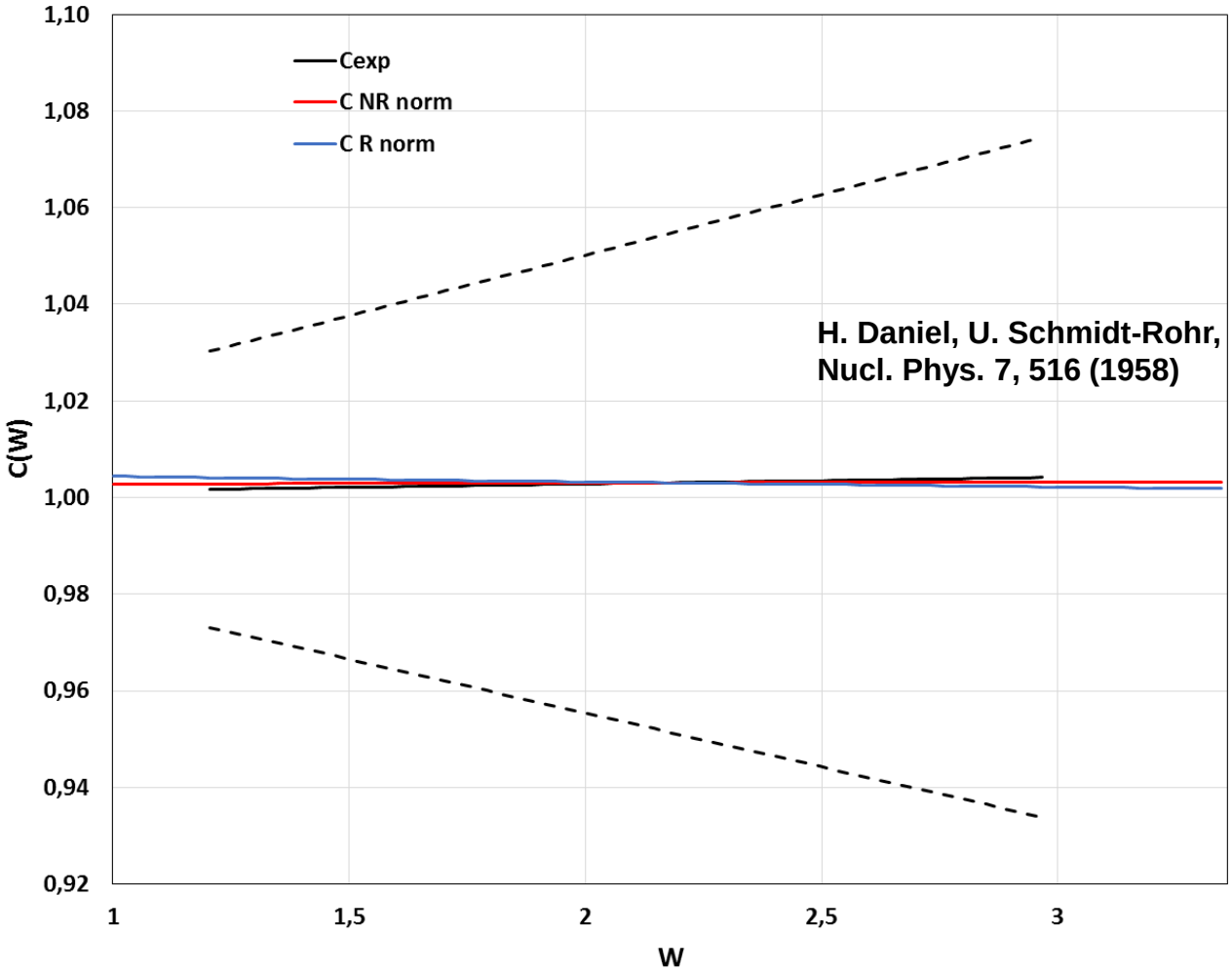
Theoretical shape factor: ^{11}C



Allowed

Initial state	Final state
$\left\|\nu^{-1}, 1p_{3/2}\right\rangle$	$\left\|\pi^{-1}, 1p_{3/2}\right\rangle$

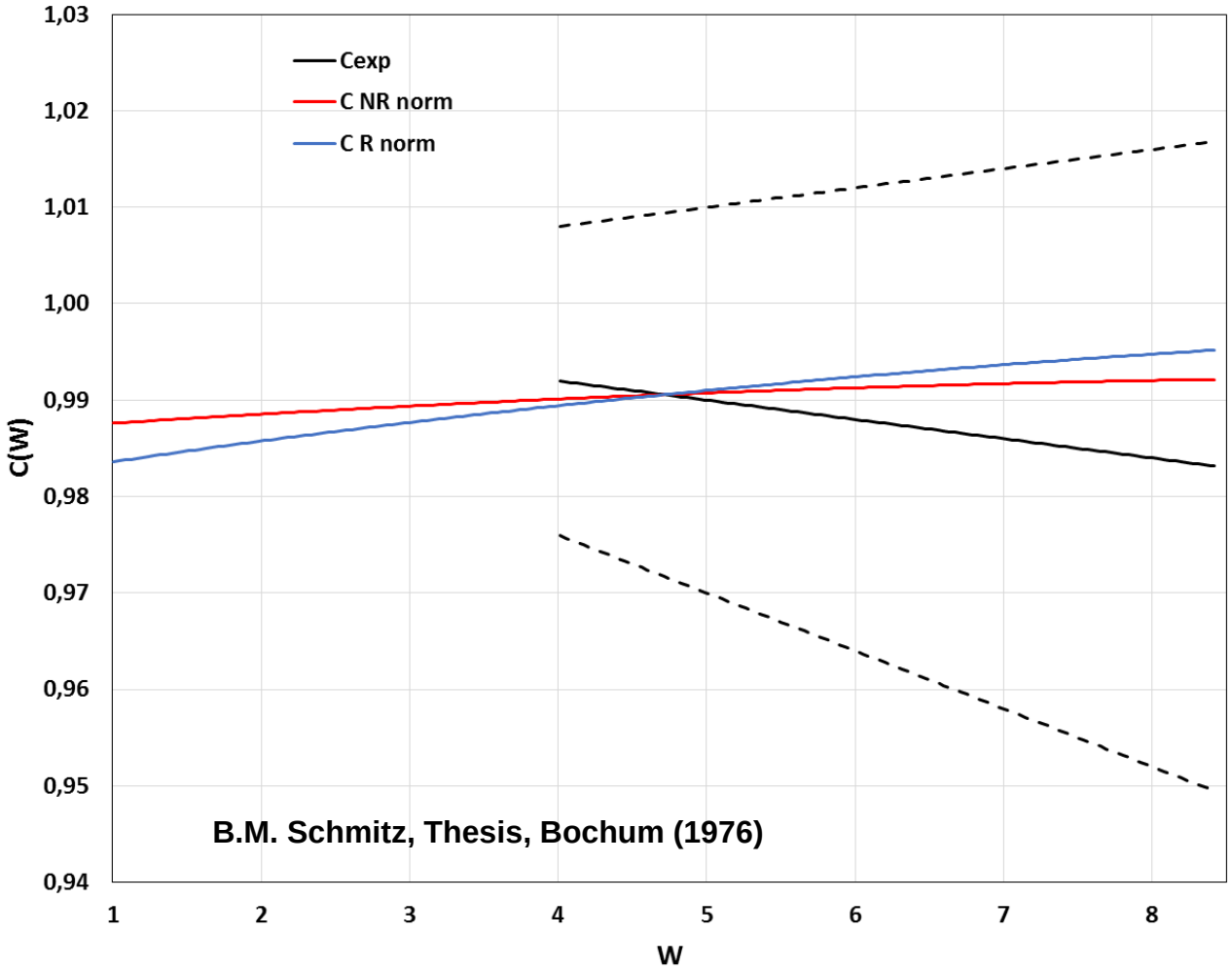
Theoretical shape factor: ^{13}N



Allowed

Initial state	Final state
$\|\pi, 1p_{1/2}\rangle$	$\|\nu, 1p_{1/2}\rangle$

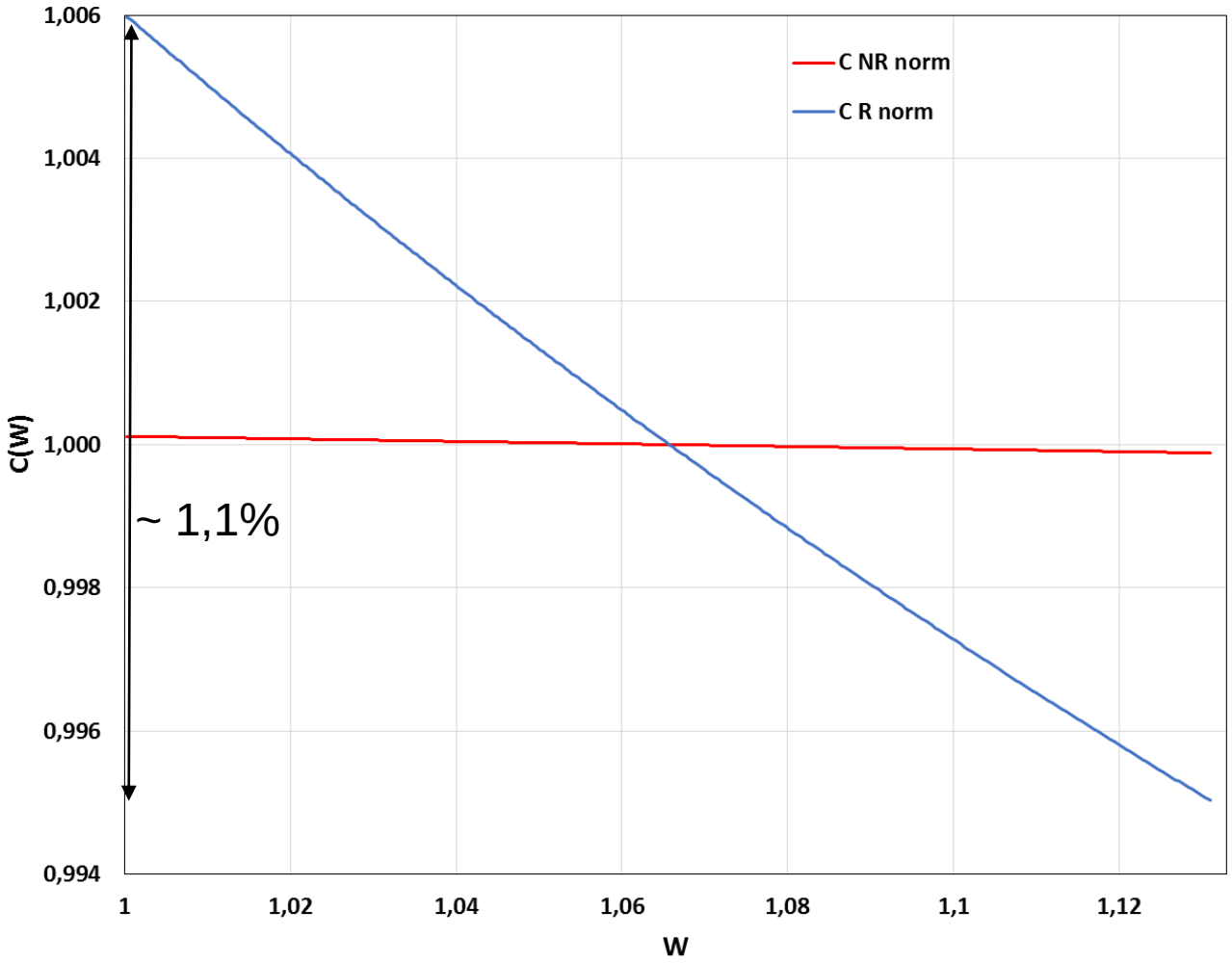
Theoretical shape factor: ^{27}Si



Allowed

Initial state	Final state
$\left\|\nu^{-1}, 1d_{5/2}\right\rangle$	$\left\|\pi^{-1}, 1d_{5/2}\right\rangle$

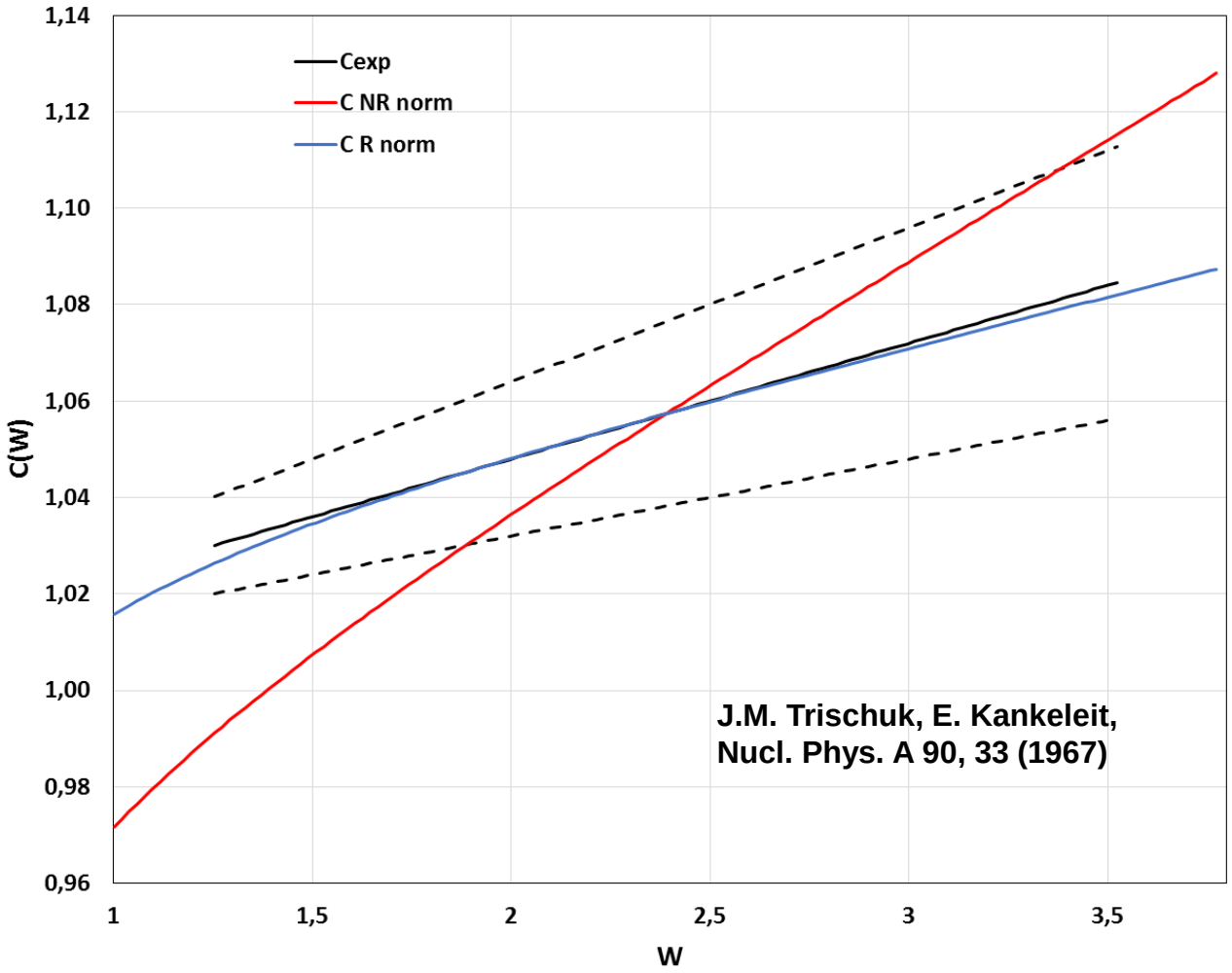
Theoretical shape factor: ^{63}Ni



Allowed

Initial state	Final state
$\lvert\nu, 2p_{1/2}\rangle$	$\lvert\pi, 2p_{3/2}\rangle$

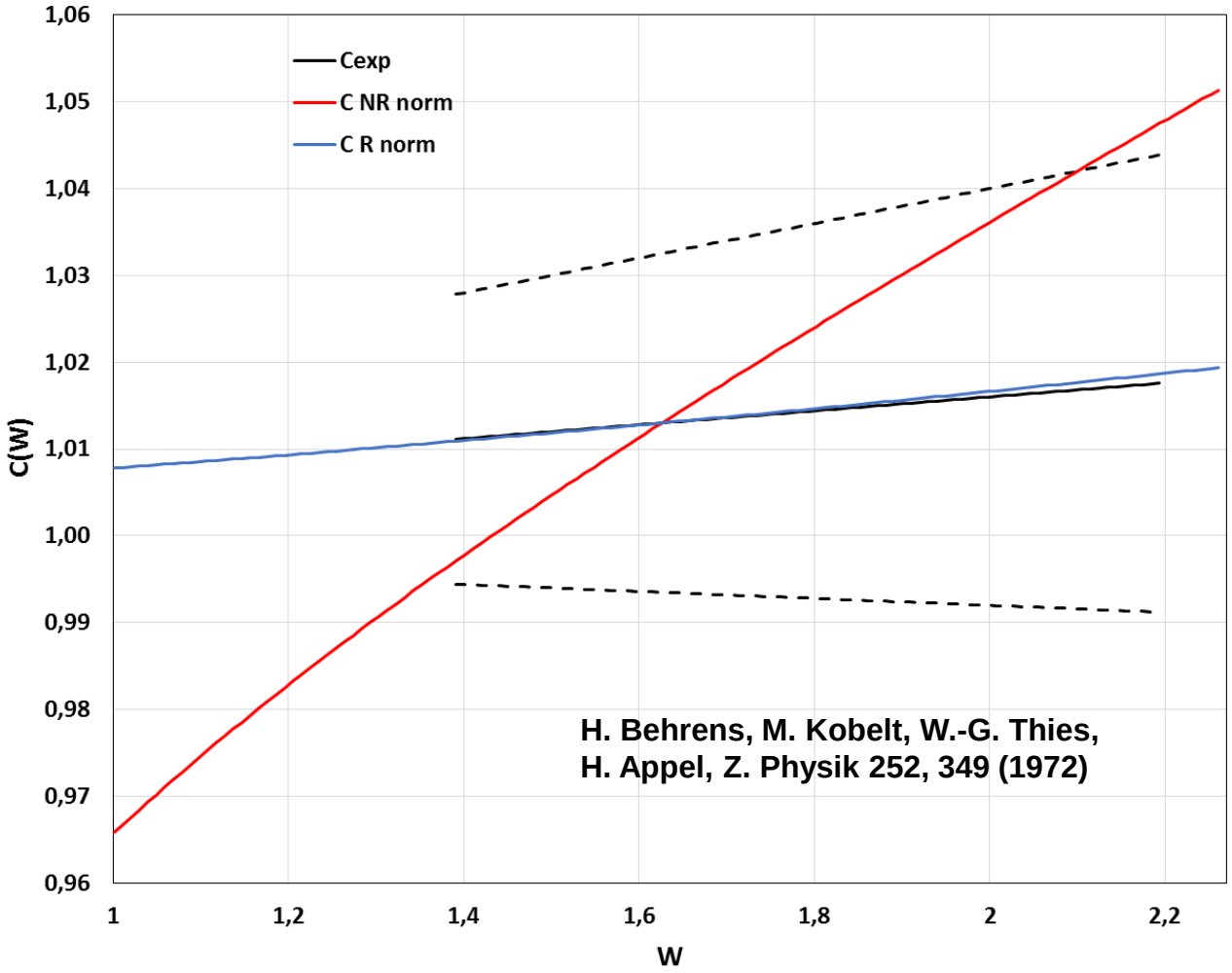
Theoretical shape factor: ^{207}Tl



First forbidden non-unique

Initial state	Final state
$\left\|\pi^{-1}, 3s_{1/2}\right\rangle$	$\left\|\nu^{-1}, 3p_{1/2}\right\rangle$

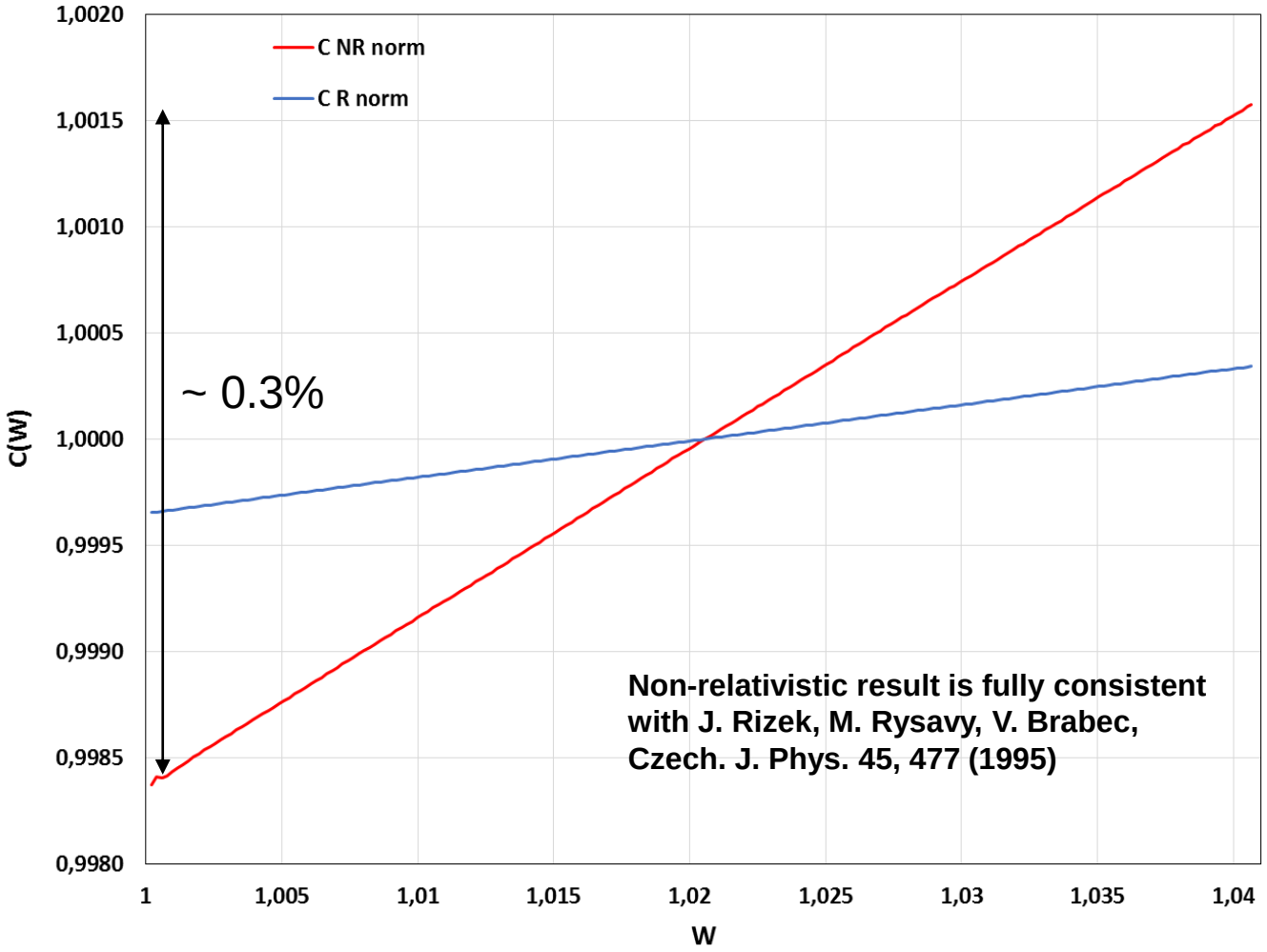
Theoretical shape factor: ^{209}Pb



First forbidden non-unique

Initial state	Final state
$\lvert\nu, 2g_{9/2}\rangle$	$\lvert\pi, 1h_{9/2}\rangle$

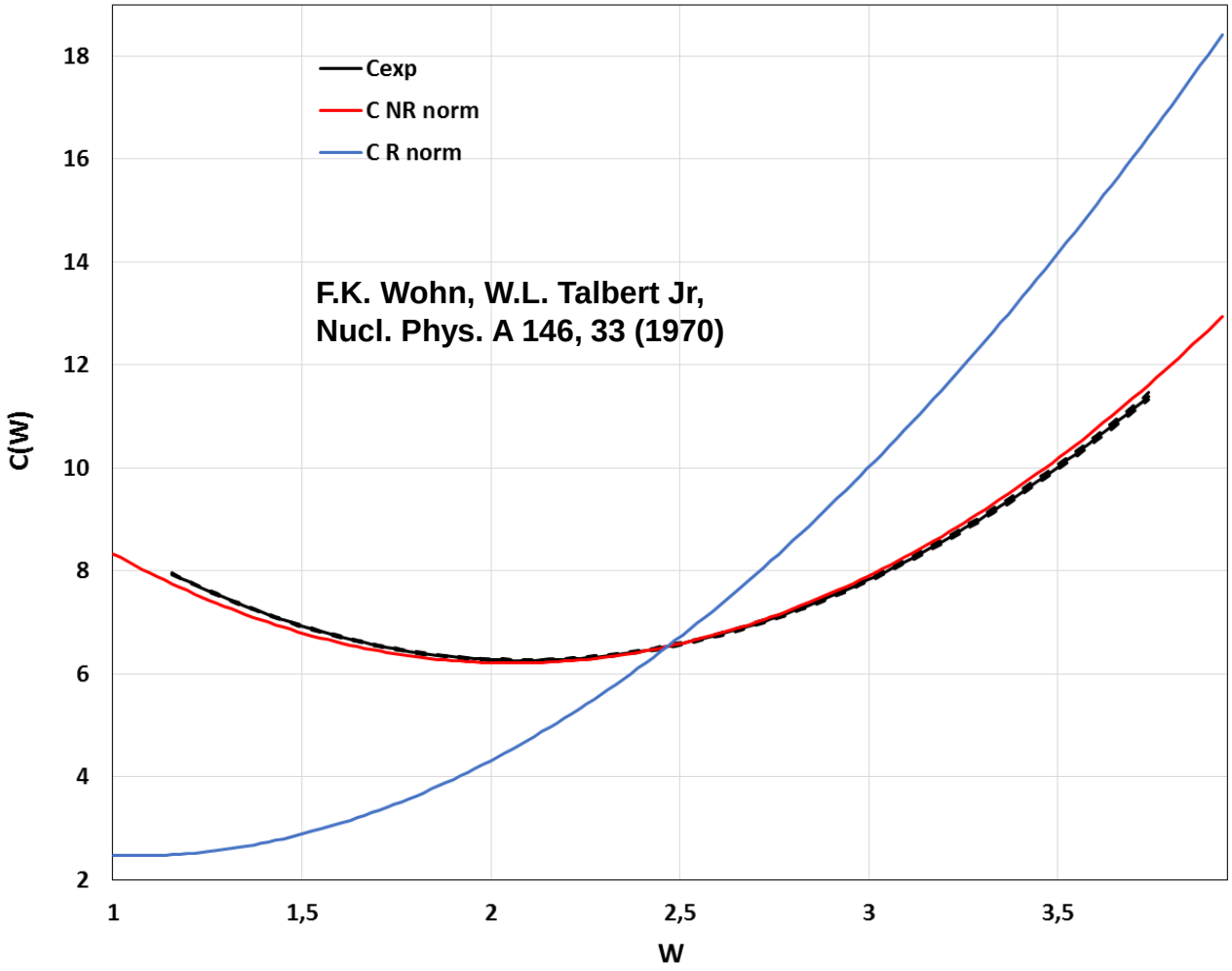
Theoretical shape factor: ^{241}Pu



First forbidden non-unique

Initial state	Final state
$\|\nu, 3d_{5/2}\rangle$	$\|\pi, 2f_{5/2}\rangle$

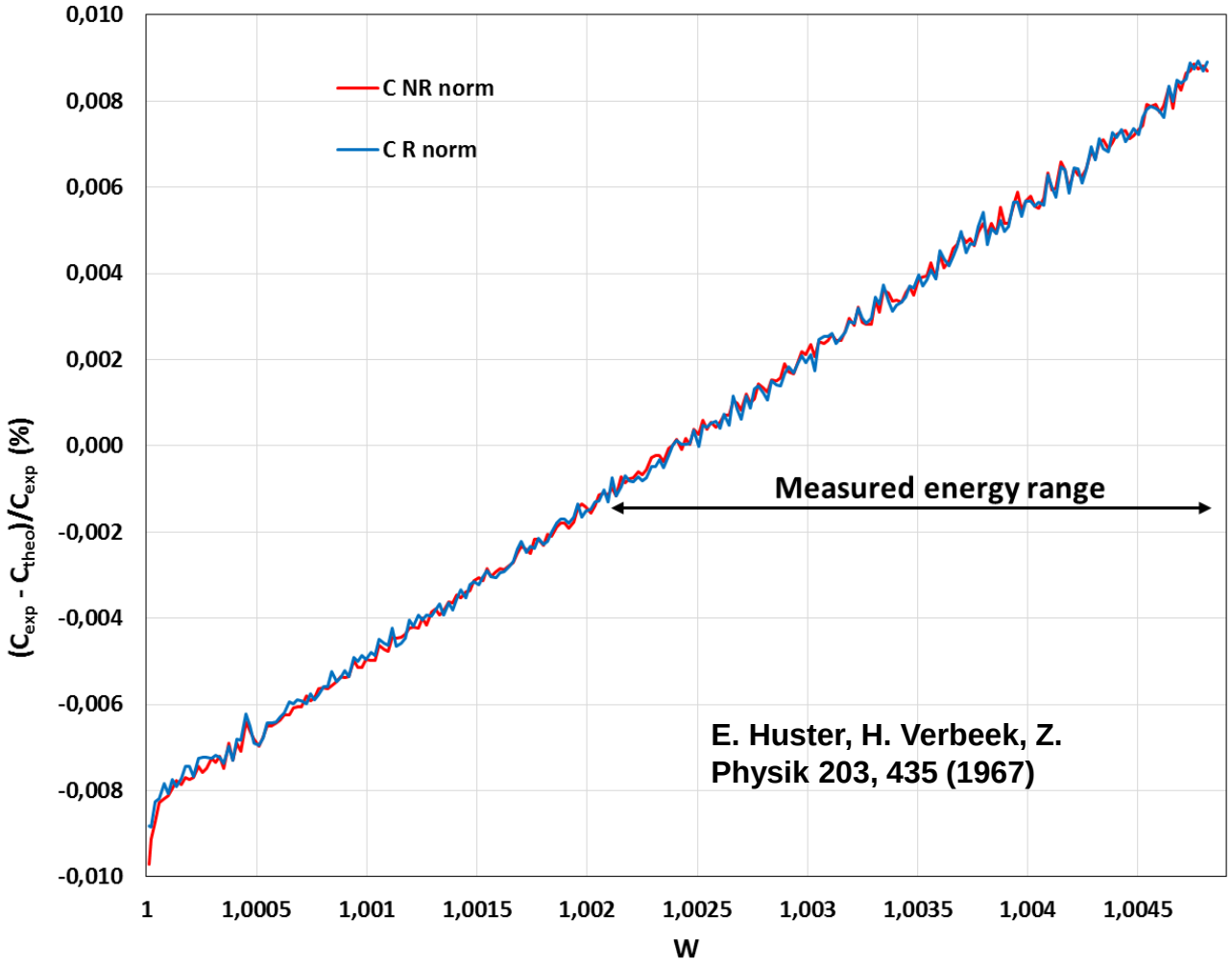
Theoretical shape factor: ^{89}Sr



First forbidden unique

Initial state	Final state
$\lvert\nu, 2d_{5/2}\rangle$	$\lvert\pi, 2p_{1/2}\rangle$

Theoretical shape factor: ^{187}Re



First forbidden unique

Initial state	Final state
$\|\nu, 3p_{1/2}\rangle$	$\|\pi, 2d_{5/2}\rangle$

Beta decay to and from an even-even ground state

Many particle matrix elements in the $j-j$ coupling scheme are "simply" related to single particle matrix elements by a coefficient which depends on K:

$$\mathcal{M}_{KLs}^{\text{many part.}}(q^2) = C(K) \times \mathcal{M}_{KLs}^{\text{sing. part.}}(q^2)$$

A sum has to be performed over different configurations, weighted by $C(K)$. This coefficient depends on fractional parentage coefficients, which are very difficult to calculate.

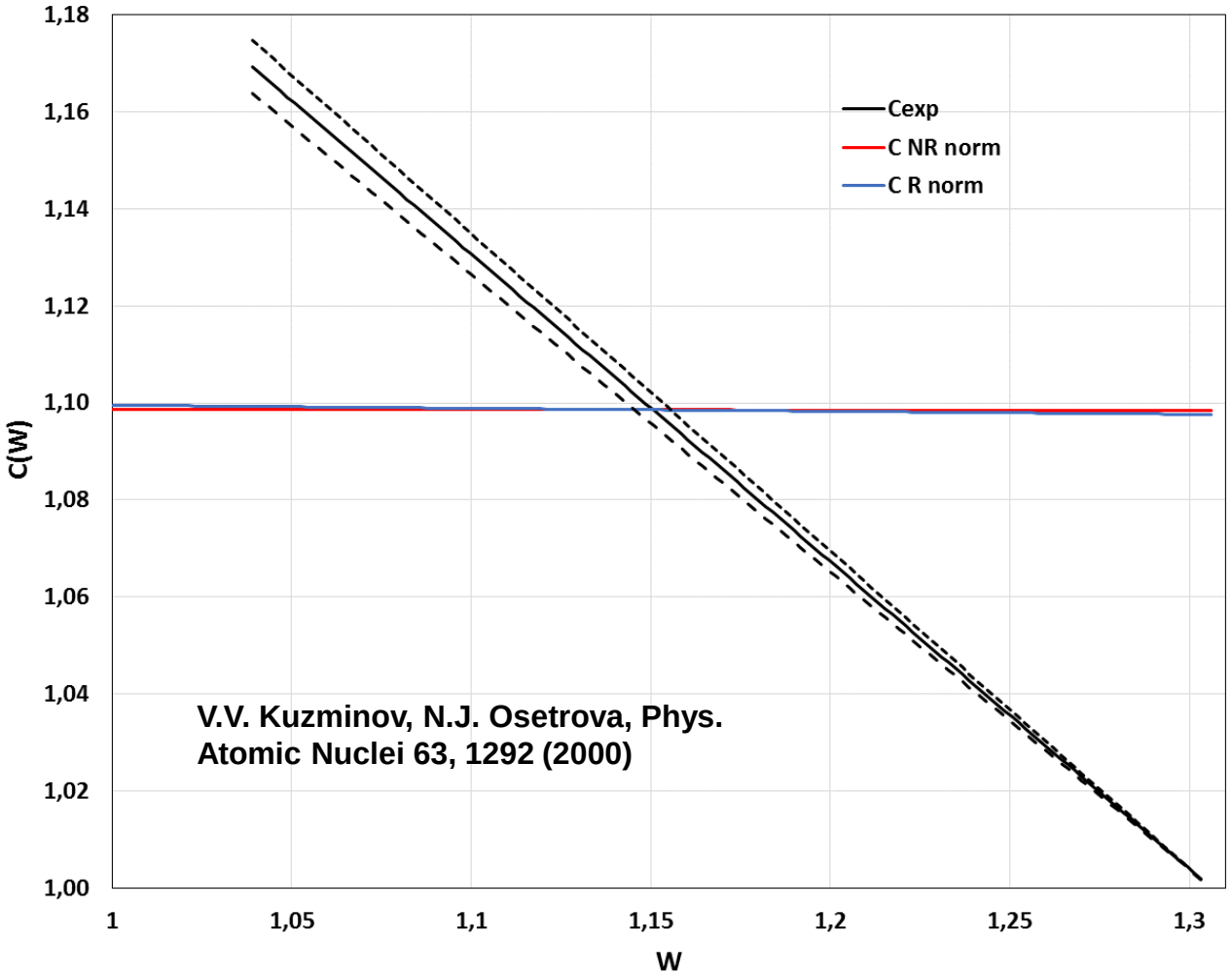
An even-even nucleus can be considered as the vacuum of particle-hole excitations used to describe adjacent nuclei.

The ground state of such reference nucleus is always 0^+. A transition to or from this state is therefore constrained to a single K value, the spectrum shape being only normalized by $C^2(K)$.

From: $C(K) = \sqrt{2K_{\min} + 1}$

To: $C(K) = (-1)^{j_{i,\text{part.}} - j_{i,\text{hole}} + K_{\min}} \sqrt{2K_{\min} + 1}$

Allowed transition of ^{14}C decay



$$^{14}_{6}C_8 \rightarrow ^{14}_{7}N_7$$

$$0^+ \rightarrow 1^+$$

$$\left|\pi, 1p_{1/2}; \nu^{-1}, 1p_{1/2}\right\rangle$$

$$C(1) = \sqrt{3}$$

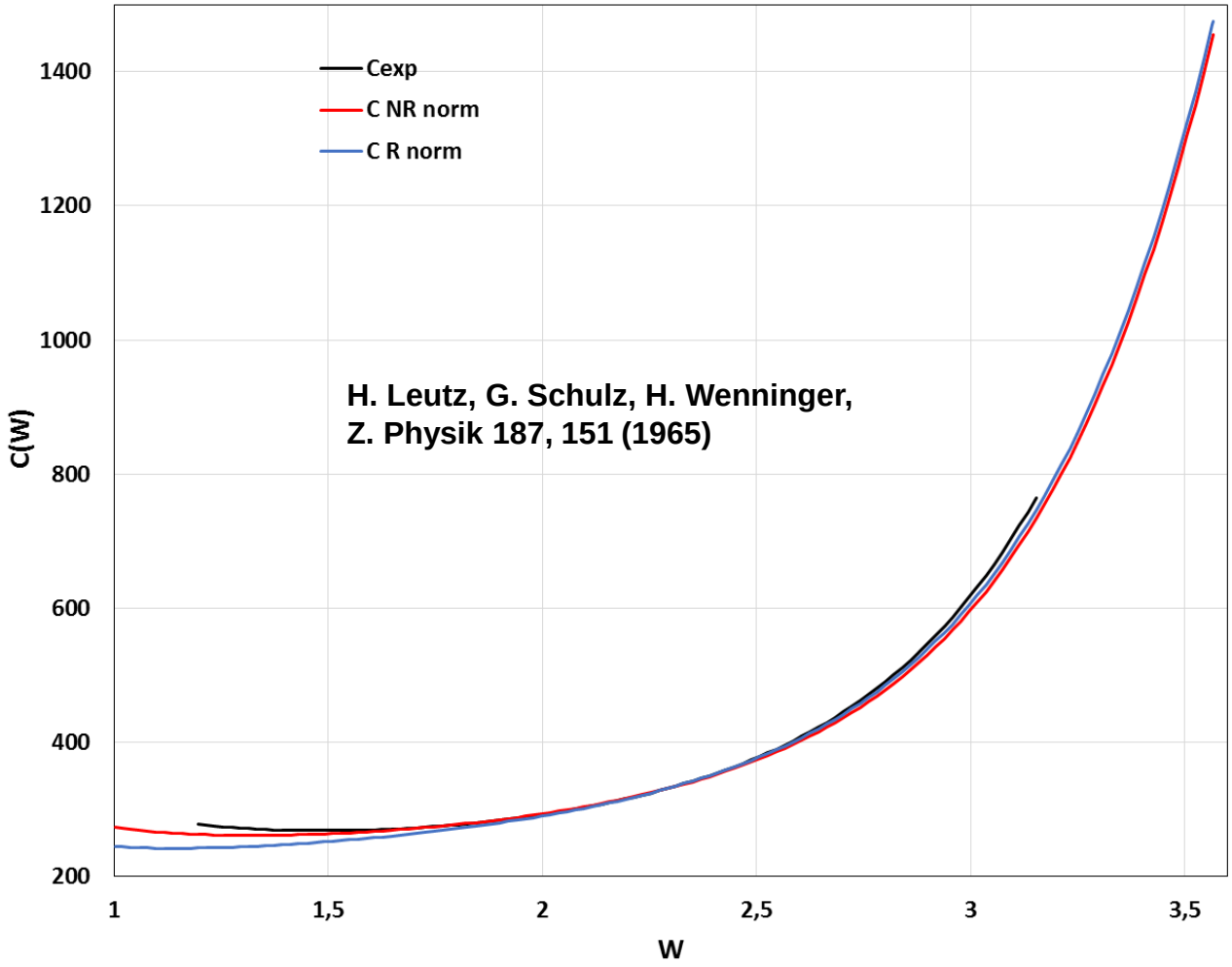
E_0 = 156,476(4) keV

$t_{1/2}$ exp. = 5700(30) a

$t_{1/2}$ NR = 0,009 a

$t_{1/2}$ R = 0,012 a

Third forbidden unique transition of ^{40}K decay



$^{40}_{19}\mathrm{K}_{21} \rightarrow ^{40}_{20}\mathrm{Ca}_{20}$

$4^- \rightarrow 0^+$

$\left|\nu, 1f_{7/2}; \pi^{-1}, 1d_{3/2}\right\rangle$

$C(4) = 3$

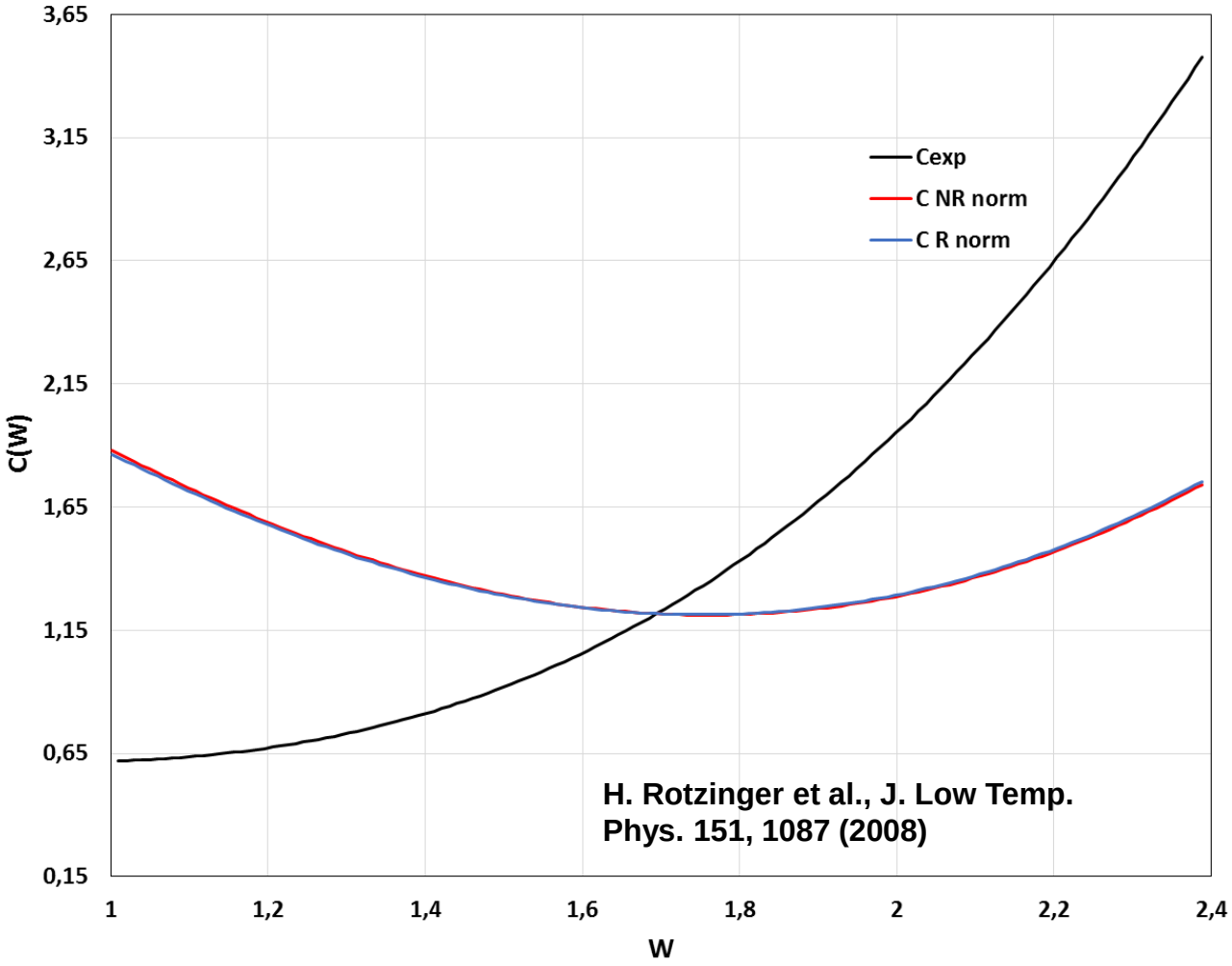
E_0 = 1310,89(6) keV

$t_{1/2}$ exp. = 1,4010(43)·10^9 a

$t_{1/2}$ NR = 5,491·10^8 a

$t_{1/2}$ R = 1,057·10^9 a

Second forbidden non-unique transition of ^{36}Cl decay



$$^{36}_{17}\mathrm{Cl}_{19} \rightarrow ^{36}_{18}\mathrm{Ar}_{18}$$

$$2^+ \rightarrow 0^+$$

$$\left|\nu^{-1}, 1d_{3/2}; \pi, 1d_{3/2}\right\rangle$$

$$C(2) = -0{,}73116$$

taken in R. Sadler, H. Behrens, Z. Phys. A 346, 25 (1993)

E_0 = 709,53(4) keV

$t_{1/2}$ exp. = 3,078(41)·10^5 a

$t_{1/2}$ NR = 1,634·10^4 a

$t_{1/2}$ R = 1,605·10^4 a

Summary

Conclusion

The precise knowledge of low-energy weak interaction decays is becoming an important limitation in many applicative and research fields. Both high-precision measurements and calculations are necessary to improve the situation.

We are urged to provide more information, better accuracy and better uncertainties than before. Evolution of the ENSDF format and supplementary databases are two possibilities which should be closely considered.

The BetaShape code is a first answer for beta decays. It has been designed to be fast and easy to use. This is a serious impediment for more precise, but more complicated, calculations.

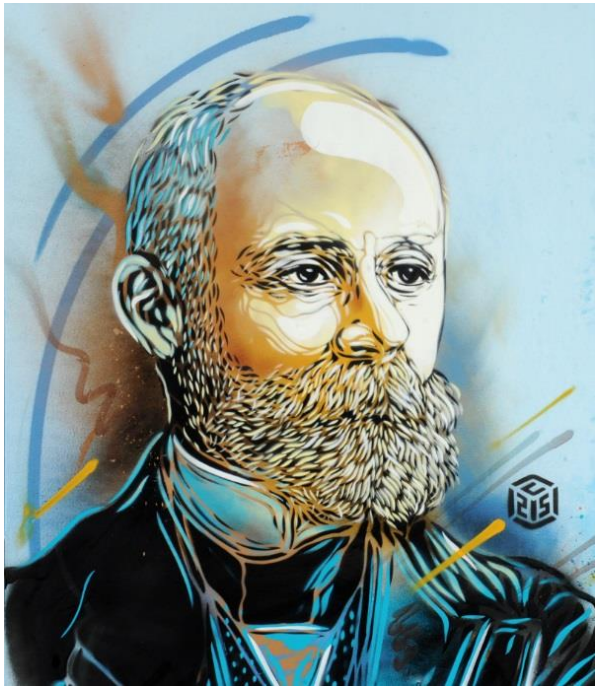
Ongoing developments

Ongoing

- European EMPIR project MetroBeta (2016-2019): improved beta decay calculations. Inclusion of more precise nucleon wave functions from a semi-phenomenological nuclear mean-field approach, still in spherical symmetry. Will be used afterwards for electron captures.
- European EMPIR project MetroMMC (2018-2021): improved electron capture calculations. Development of an atomic code for high precision wave functions. Will be used afterwards for atomic effects in beta decays.

Future (European EMPIR project RealBq submitted in October, review in progress)

- Nuclear component: introduction of nuclear deformation and pairing correlations, which is expected to inherently account for configuration mixing.
- Atomic component: extension of exchange effect to forbidden beta decays.
- Uncertainties: estimate of theoretical components and propagation via a Monte Carlo method.



Thank you for your attention

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