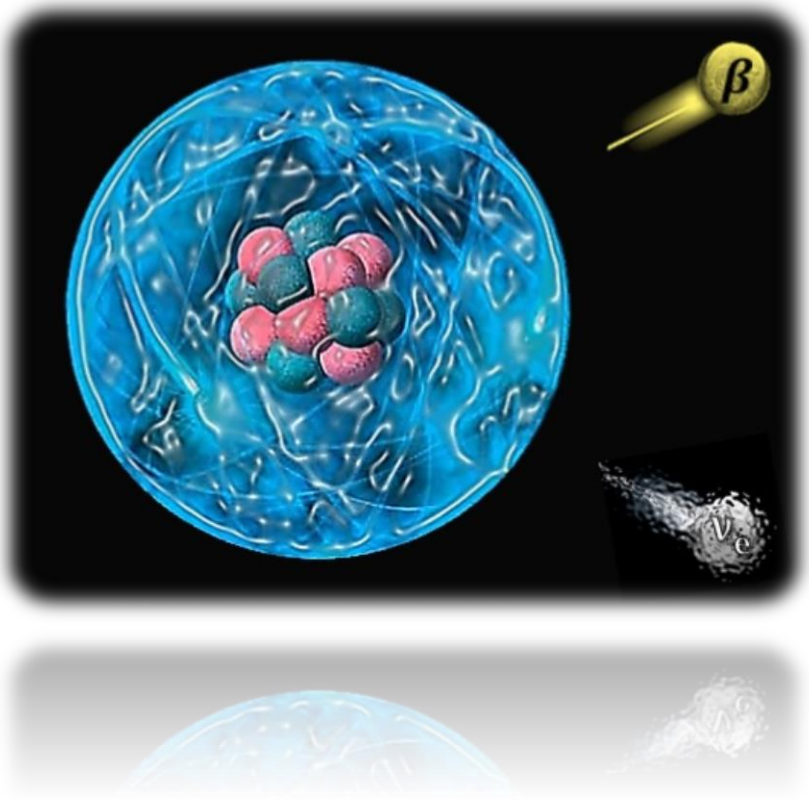


BetaShape

NSDD Technical Meeting 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

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
v1.0

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

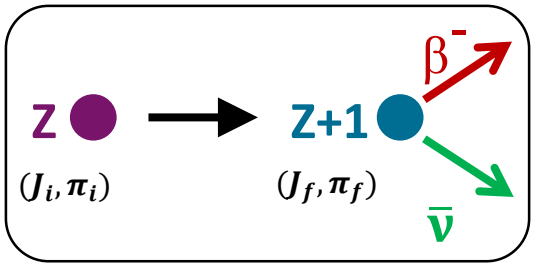
Physics modelling

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)

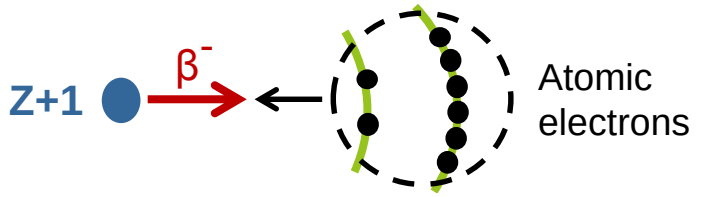
All quantities depend on the normalization of electron wave functions

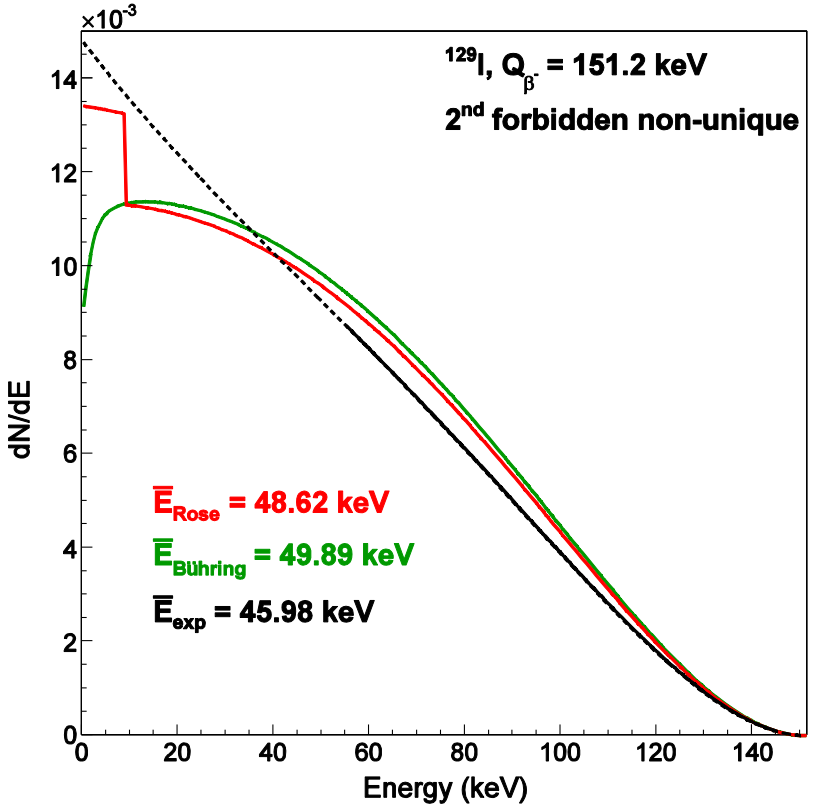
⇒ **Analytical solutions** and **leading order** at the nucleus + **asymptotic** solutions

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

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)

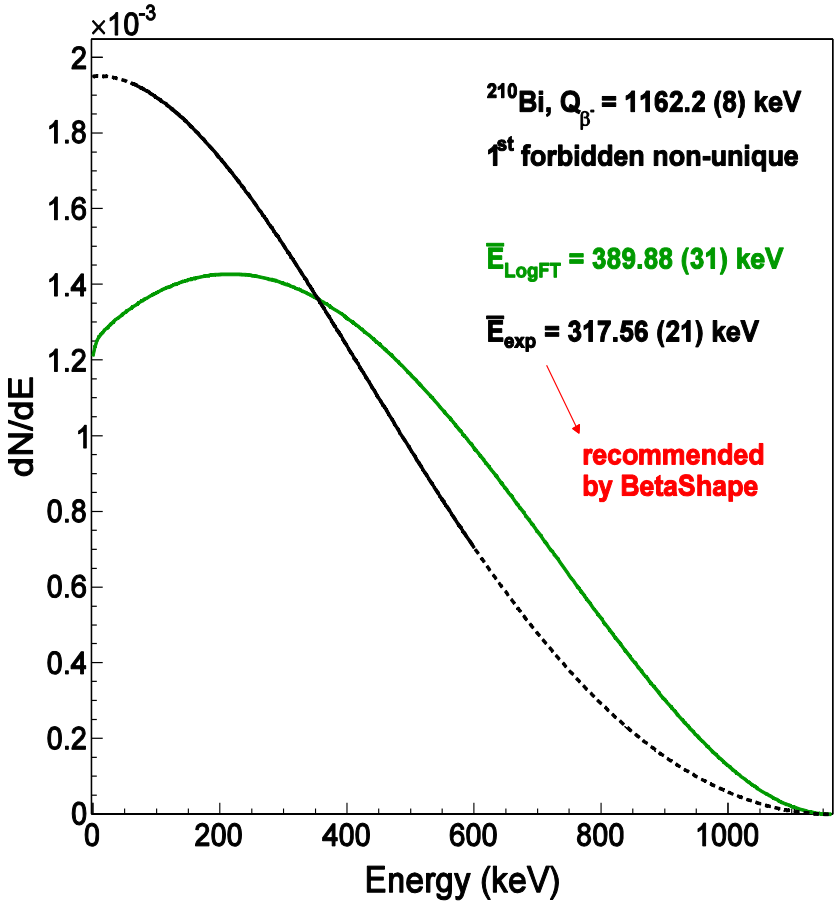
n_x: relative occupation number of the orbital, not accounted for in the LogFT program

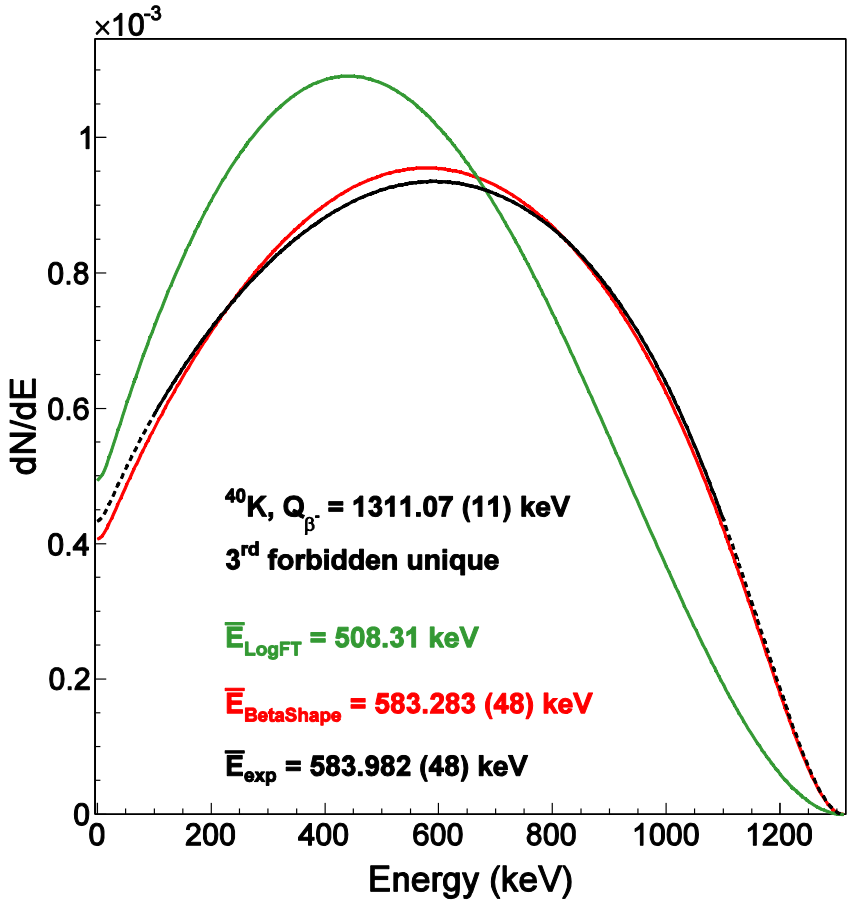
$$\rightarrow \log ft = \log\left(\frac{f_\varepsilon + f_{\beta^+}}{I_\varepsilon + I_{\beta^+}} T_{1/2}\right)$$

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

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

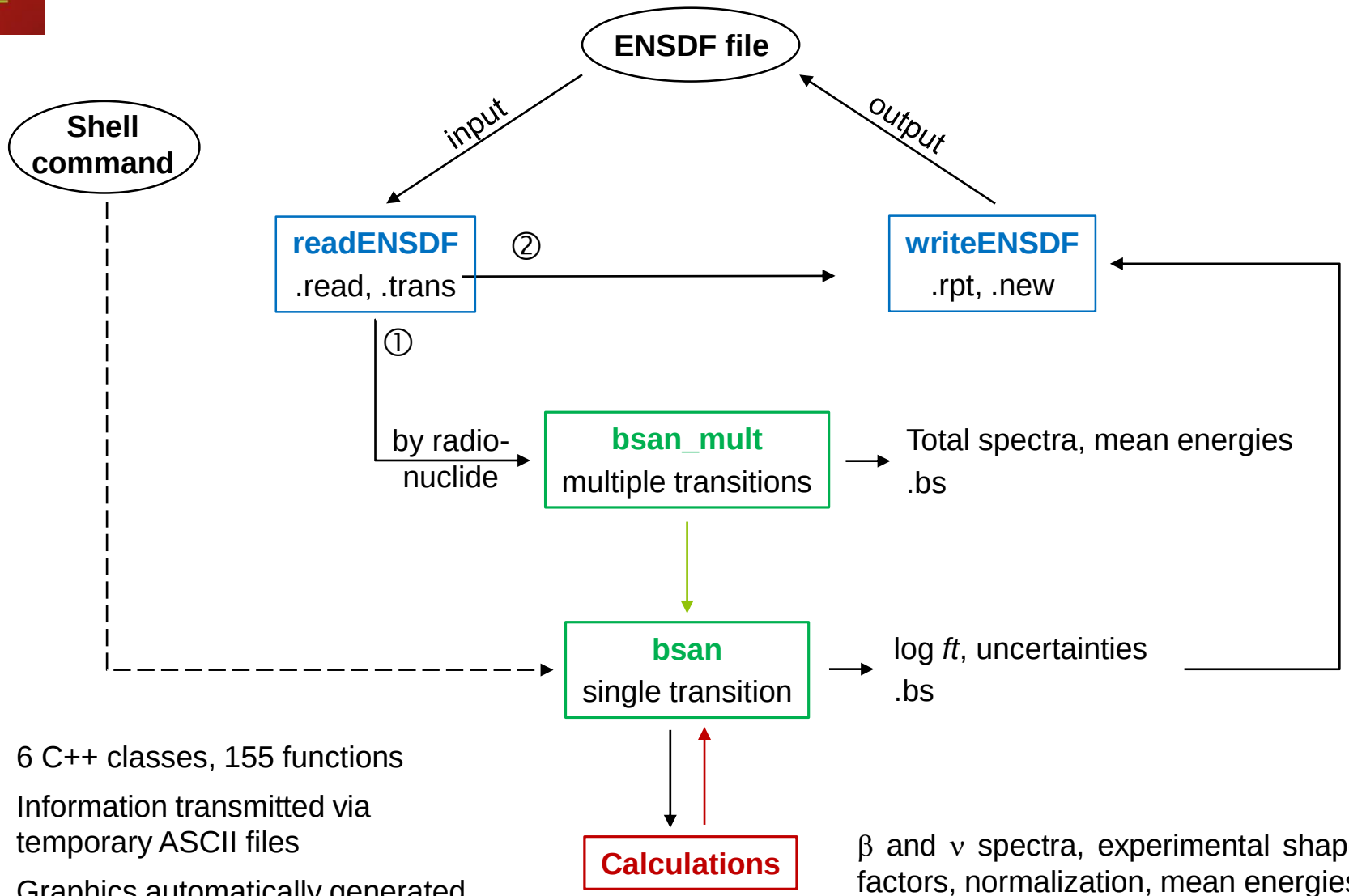
Examples of improved calculations





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*)

β and ν spectra, experimental shape factors, normalization, mean energies

BetaShape
v1.1

Executables soon available on LNHB website

Changes

- Input file should not given anymore via ‘inpf=‘
  → Drag and drop of ENSDF file on BetaShape executable now possible, with default options.
- Few number of display bugs in READ files.
- Uncertainties: if no uncertainty v1.0 estimates a ~60% uncertainty from flat distribution. Now, same as in LogFT, i.e. null uncertainty. Asymmetric uncertainties are still symmetrized (as in AME).
- Update of the database of experimental shape factors: new for ^{138}La and addition of ^{14}O. Currently, 131 shape factors for single beta transitions.
- Parameters of experimental shape factors are provided as a Beta Continuation Record.
- Implementation of SPE files: continuous spectra in ENSDF format. Unplaced transitions not included yet.
- New radiative corrections, from the 1970’s in v1.0.

Radiative corrections

Electrons – Old correction

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

Electrons – New correction

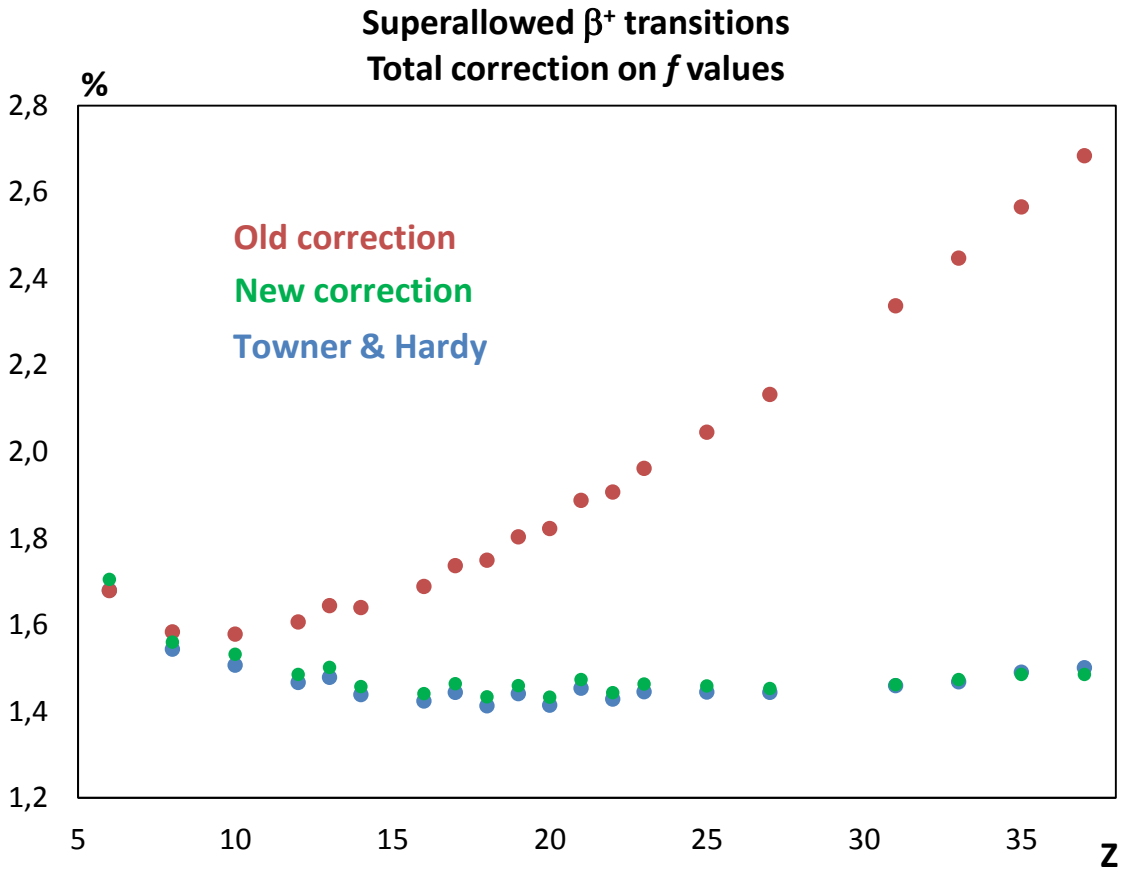
I.S. Towner, J.C. Hardy, PRC 77, 025501 (2008)
A. Czarnecki et al., PRD 70, 093006 (2004)

Neutrinos

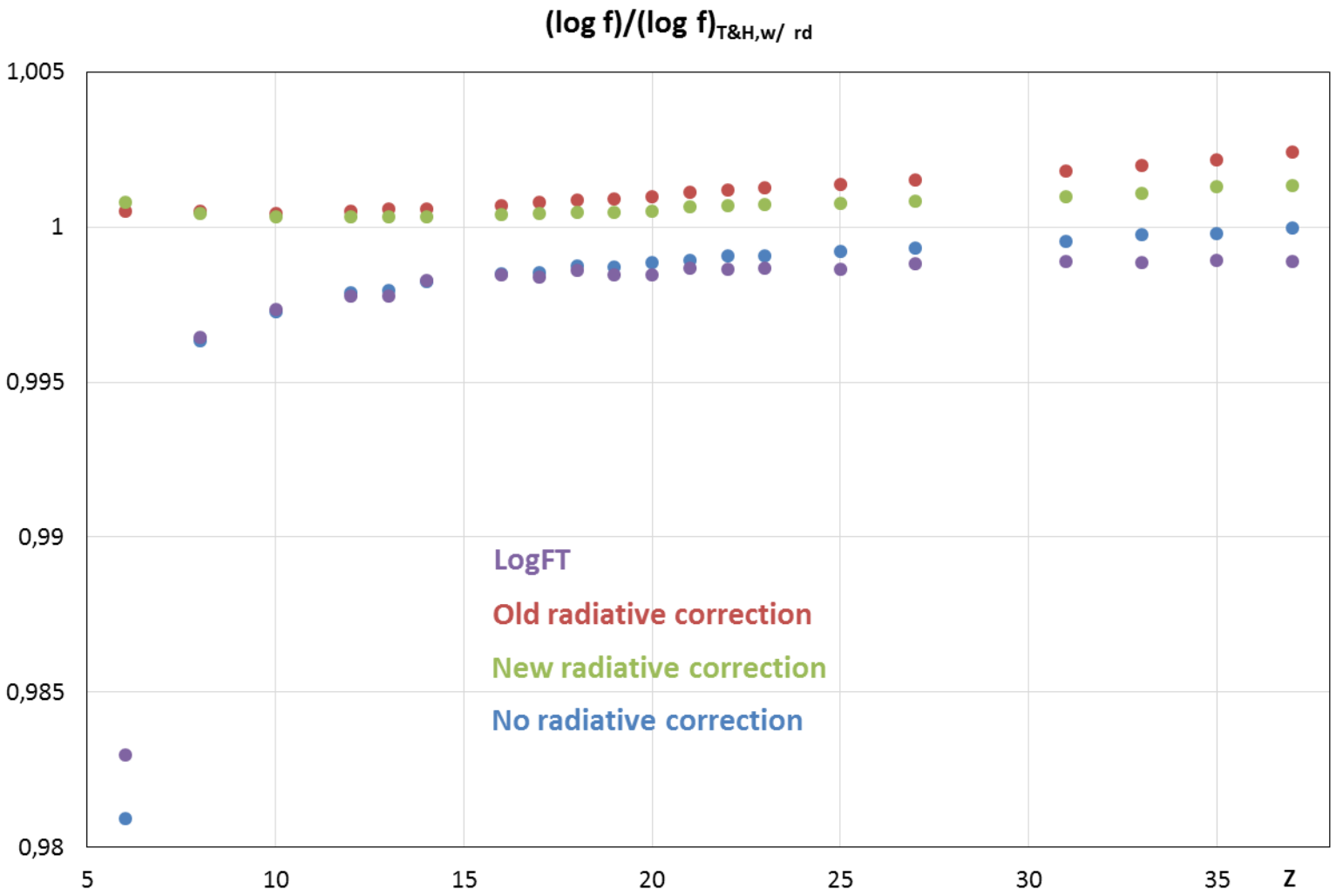
A. Sirlin, Phys. Rev. D 84, 014021 (2011)

First version of BetaShape

New version of BetaShape



Radiative corrections



Running BetaShape

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

- Mass chain or even more can treated at once

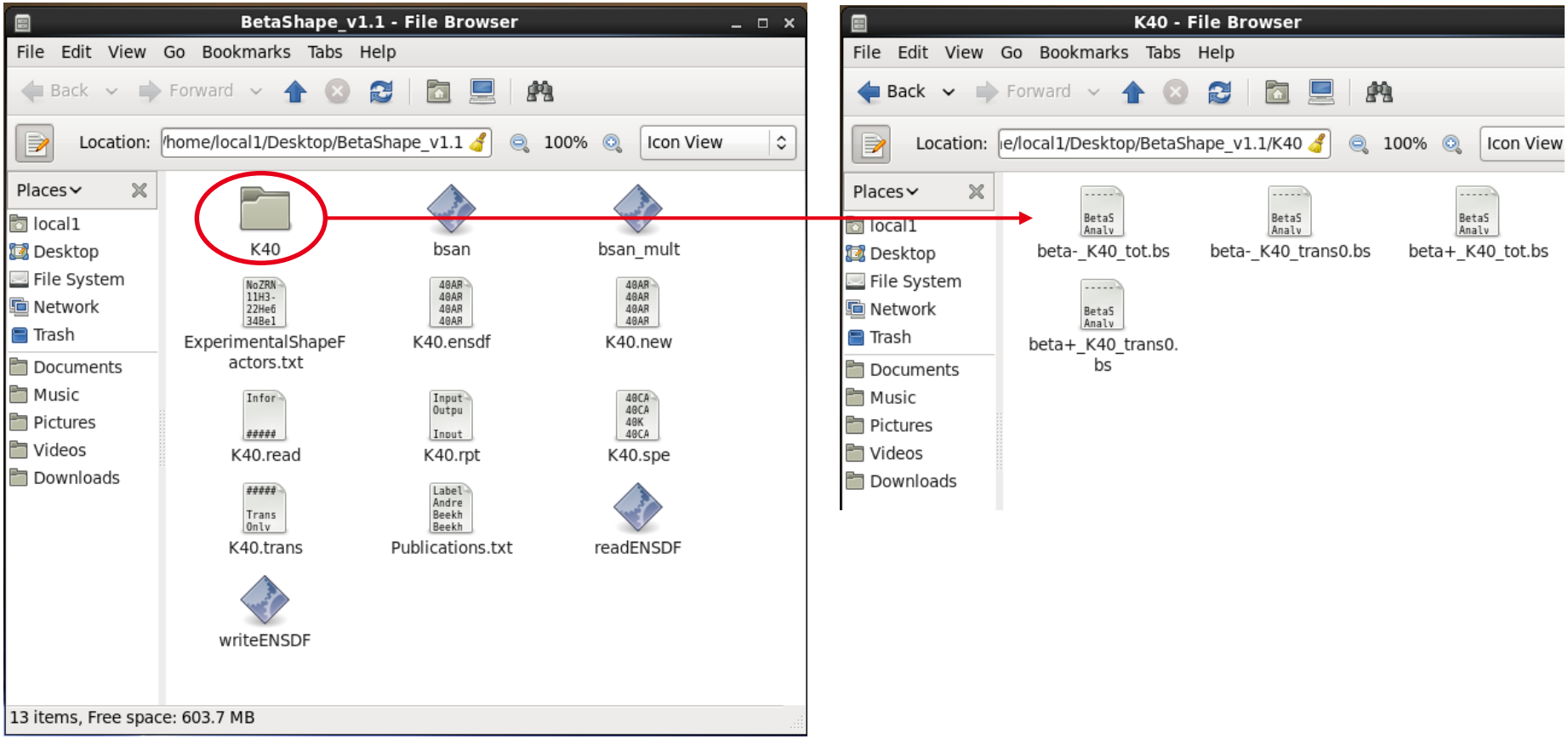
- Example:

  # readENSDF K40.ensdf

  Output files

  - K40.read: information read in K40.ensdf
  - K40.trans: transition to be calculated
  - K40.rpt: report file
  - K40.new: updated ENSDF file (log*ft* values, mean energies, experimental shape factors)
  - BS files: single and total beta spectra with many details, in ./K40/ directory
  - K40.spe: single and total beta spectra in ENSDF format

Output files



Single transition file

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 (24/06/2016)
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: 19-K-40 [4-] g.s.  -->  Daughter nucleus: 20-Ca-40 [0+] g.s.
Calculation of the 3rd forbidden unique transition from the beta - decay of K-40

Bühring's screening correction is considered.

End-point energy: 1311.07 (11) keV     Energy step: 4 keV     Intensity: 0.8921 (17)

An experimental shape factor has been found: 1.05*q^6 + 6.3*q^4*p^2 + 6.25*q^2*p^4 + 0.95*p^6
Energy range of the measurement: 100 - 1100 keV      In database, transition #21
From [1965LE15] H. Leutz, G. Schulz, H. Wenninger, Z. Physik 187, 151 (1965)

Input mean energy: 583.982 (48) keV
Mean energy from the calculated spectrum: 583.639 (48) keV
Mean energy from the experimental shape factor: 583.982 (48) keV

Input log ft value: 20.58
Log ft value from the calculated spectrum: log ft 20.5938 (13)   with components: log f 3.94802 (33) and log partial T1/2 16.6457 (13)
Log ft value from the experimental shape factor: log ft 20.5793 (13)   with component: log f 3.93358 (33)

Agreement of the experimental and calculated spectra in [100,1100] keV: 98.77 %
Corresponding disagreement: 1.23 %
Variation of the mean energies: -5.88e-02 %

E(keV)      dN/dE calc.      unc.             dN/dE exp.       unc.
     0      4.02693e-04      3.54693e-08      4.33819e-04      3.72568e-08
     4      4.04766e-04      3.59052e-08      4.35849e-04      3.75815e-08
     8      4.08385e-04      3.64707e-08      4.39534e-04      3.80543e-08
    12      4.13549e-04      3.71660e-08      4.44873e-04      3.86750e-08
    16      4.19883e-04      3.79692e-08      4.51190e-04      3.93863e-08
    20      4.26884e-04      3.88382e-08      4.58040e-04      4.01500e-08
    24      4.34246e-04      3.97463e-08      4.65166e-04      4.09440e-08
    28      4.41790e-04      4.06777e-08      4.72418e-04      4.17552e-08
     ⋮            ⋮                                ⋮
```

Single transition file

Transition parameters and options for calculation

```
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```

Single transition file

Experimental shape factor

```
An experimental shape factor has been found: 1.05*q^6 + 6.3*q^4*p^2 + 6.25*q^2*p^4 + 0.95*p^6
Energy range of the measurement: 100 - 1100 keV      In database, transition #21
From [1965LE15] H. Leutz, G. Schulz, H. Wenninger, Z. Physik 187, 151 (1965)
```

Single transition file

Mean energies, log *ft* values, analysis parameters

```
Input mean energy: 583.982 (48) keV
Mean energy from the calculated spectrum: 583.639 (48) keV
Mean energy from the experimental shape factor: 583.982 (48) keV

Input log ft value: 20.58
Log ft value from the calculated spectrum: log ft 20.5938 (13)   with components: log f 3.94802 (33) and log partial T1/2 16.6457 (13)
Log ft value from the experimental shape factor: log ft 20.5793 (13)   with component: log f 3.93358 (33)

Agreement of the experimental and calculated spectra in [100,1100] keV: 98.77 %
Corresponding disagreement: 1.23 %
Variation of the mean energies: -5.88e-02 %
```

Single transition file

β and ν spectra

E (keV)	dN/dE calc.	unc.	dN/dE exp.	unc.
0	4.02693e-04	3.54693e-08	4.33819e-04	3.72568e-08
4	4.04766e-04	3.59052e-08	4.35849e-04	3.75815e-08
8	4.08385e-04	3.64707e-08	4.39534e-04	3.80543e-08
12	4.13549e-04	3.71660e-08	4.44873e-04	3.86750e-08
16	4.19883e-04	3.79692e-08	4.51190e-04	3.93863e-08
20	4.26884e-04	3.88382e-08	4.58040e-04	4.01500e-08
24	4.34246e-04	3.97463e-08	4.65166e-04	4.09440e-08
28	4.41790e-04	4.06777e-08	4.72418e-04	4.17552e-08
32	4.49411e-04	4.16228e-08	4.79707e-04	4.25756e-08
36	4.57047e-04	4.25754e-08	4.86979e-04	4.34003e-08
40	4.64658e-04	4.35318e-08	4.94200e-04	4.42261e-08
44	4.72220e-04	4.44892e-08	5.01351e-04	4.50511e-08
48	4.79720e-04	4.54460e-08	5.08419e-04	4.58738e-08
52	4.87147e-04	4.64009e-08	5.15396e-04	4.66934e-08
56	4.94498e-04	4.73529e-08	5.22280e-04	4.75092e-08
60	5.01768e-04	4.83014e-08	5.29069e-04	4.83207e-08

⋮ ⋮ ⋮

Additional beta continuation record

```
63CU    63NI B- DECAY (98.7 Y)
63CU  H TYP=FUL$AUT=K.B.LEE$CUT=28-SEP-2009$
63CU C  References:1950Wi**, 1951Br**, 1956Mc**, 1957Pr**, 1962Ho**, 1966Hs01,
63CU2C  1971Ba89, 1987He14, 1992Ka29, 1993Oh02, 1996Co25, 1996Sc33, 1999Ho09,
63CU3C  2003Au03
63NI   P 0.0          1/2-              98.7 Y    24              66.980    15
63CU   N 1.0          1.0       1         1.0
63CU   L 0            3/2-              STABLE
63CU   B 66.980    15100                 6.932   11
63CUS  B EAV=17.1872 41
63CUX  B C1=1213.5 $C2=-232.01 $C3=-1517.2 $C4=532.69
63CU  CB C(W) = 1 + 1213.49*W - 232.009/W - 1517.16*W^2 + 532.69*W^3
```

'X' for experimental

Parameters (with uncertainties)

Comment for the correct use

SPE file in ENSDF format

Total beta spectrum and mean energy

Beta spectrum and mean energy for each transition

```
1   210PB    210TL B- DECAY (1.30 M)
2   210PB  H TYP=FUL$AUT=V.CHISTE$CUT=31-AUG-2007$
3   210TL CB Total beta - spectrum      $BIN=358
4   210TL CB EAV=1.17E3 36
5   210TL CB E(keV)       dNtot/dE b-      unc.
6   210TL TB       0      3.35959e-04      1.87719e-05
7   210TL TB       4      3.43013e-04      1.91778e-05
8   210TL TB       8      3.49082e-04      1.95320e-05
9   210TL TB      12      3.54169e-04      1.98346e-05
10  210TL TB      16      3.58383e-04      2.00853e-05
11  210TL TB      20      3.62045e-04      2.03004e-05
                  ⋮              ⋮
362 210TL TB    4374      3.03406e-09      1.19774e-09
363 210TL TB    4386      0.00000e+00      0.00000e+00
364 210TL  P 0.0          (5)+              1.30 M    3              5482      12
365 210PB  N 1.0          1.0       1         1.0
366 210PB  L 0            0+                22.23 Y   12
367 210PB  L 799.6     3  2+                17 PS     5
368 210PB  L 1096      3  4+                0.6 NS    1
369 210PB  B 4386      1213                   7.429    11
370 210PBS B EAV=1771 5
371 210PB CB From theory (2015MO10) $BIN=315 $NORM=0.13
372 210PB CB E(keV)       dN/dE calc.      unc.
373 210PB TB       0      1.28258e-05      7.33575e-08
374 210PB TB      14      1.35042e-05      7.70220e-08
375 210PB TB      28      1.41187e-05      8.03015e-08
376 210PB TB      42      1.46692e-05      8.31960e-08
377 210PB TB      56      1.51975e-05      8.59443e-08
378 210PB TB      70      1.57149e-05      8.86109e-08
```

Number of bins

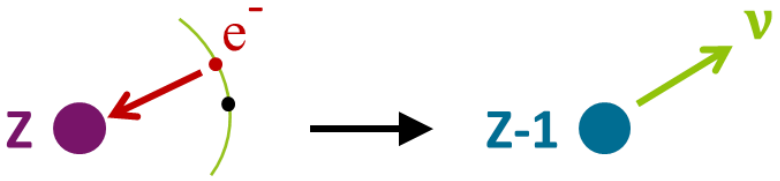
Total mean energy

Mean energy

Number of bins and normalization

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

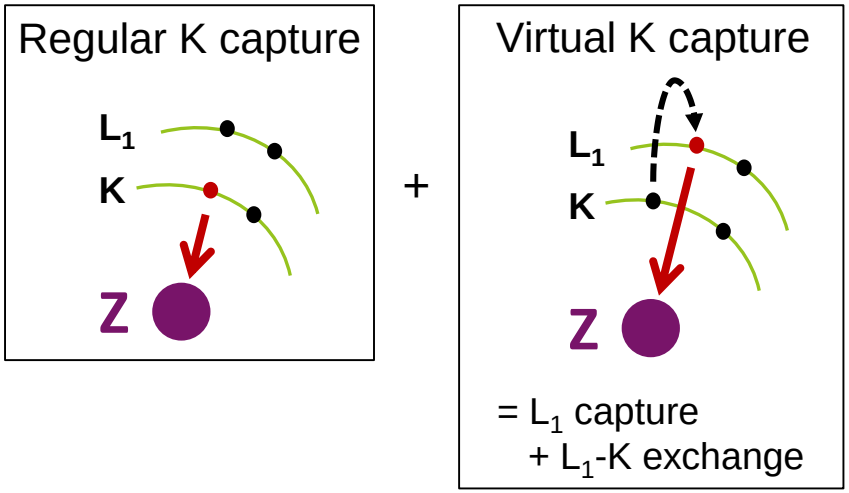
Overlap effect

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**

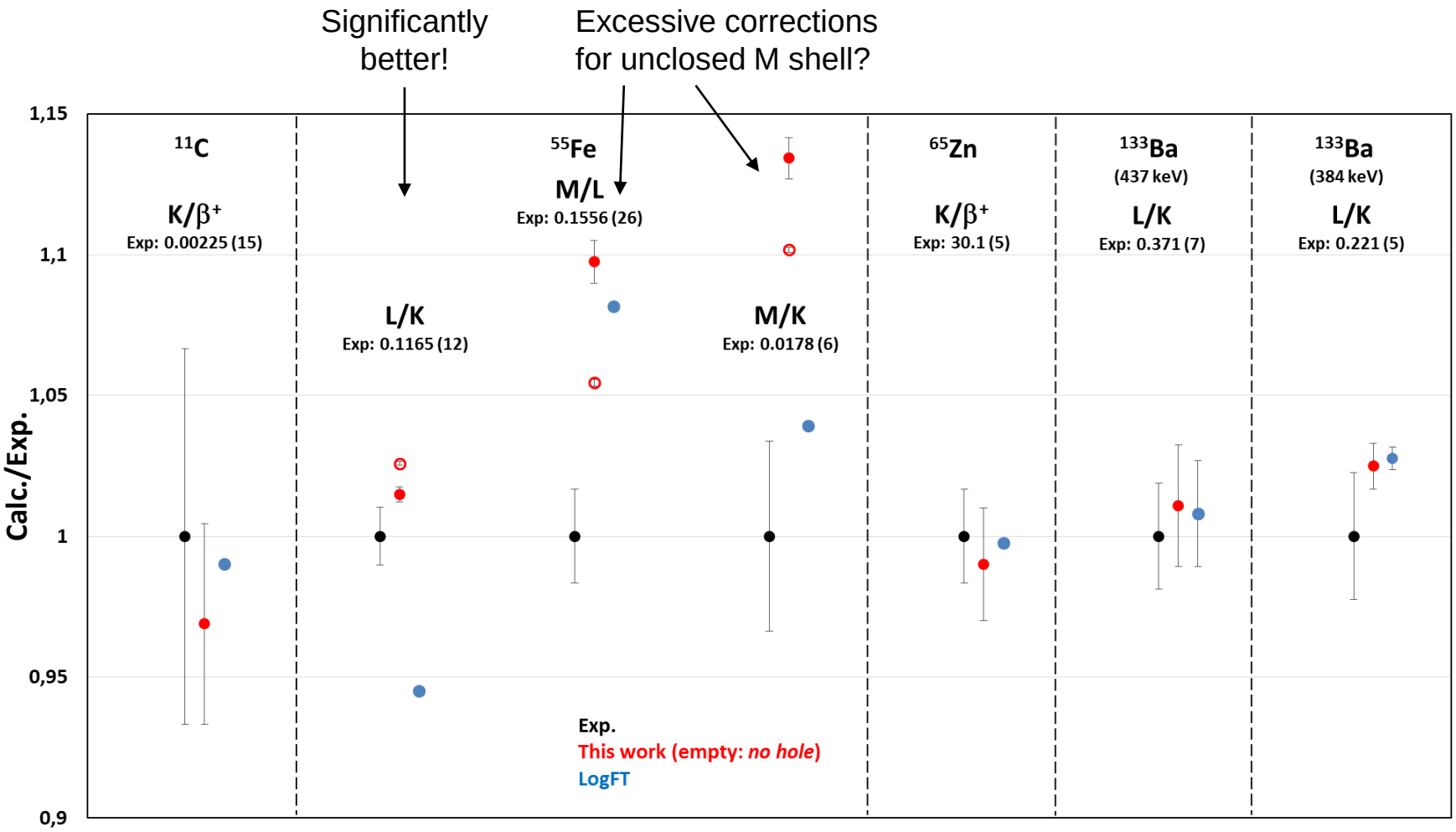
$$\langle(j,\kappa)'|(i,\kappa)\rangle = \frac{\langle(j,\kappa)|\mathcal{H}'|(i,\kappa)\rangle}{W_j - W_i}$$

with

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

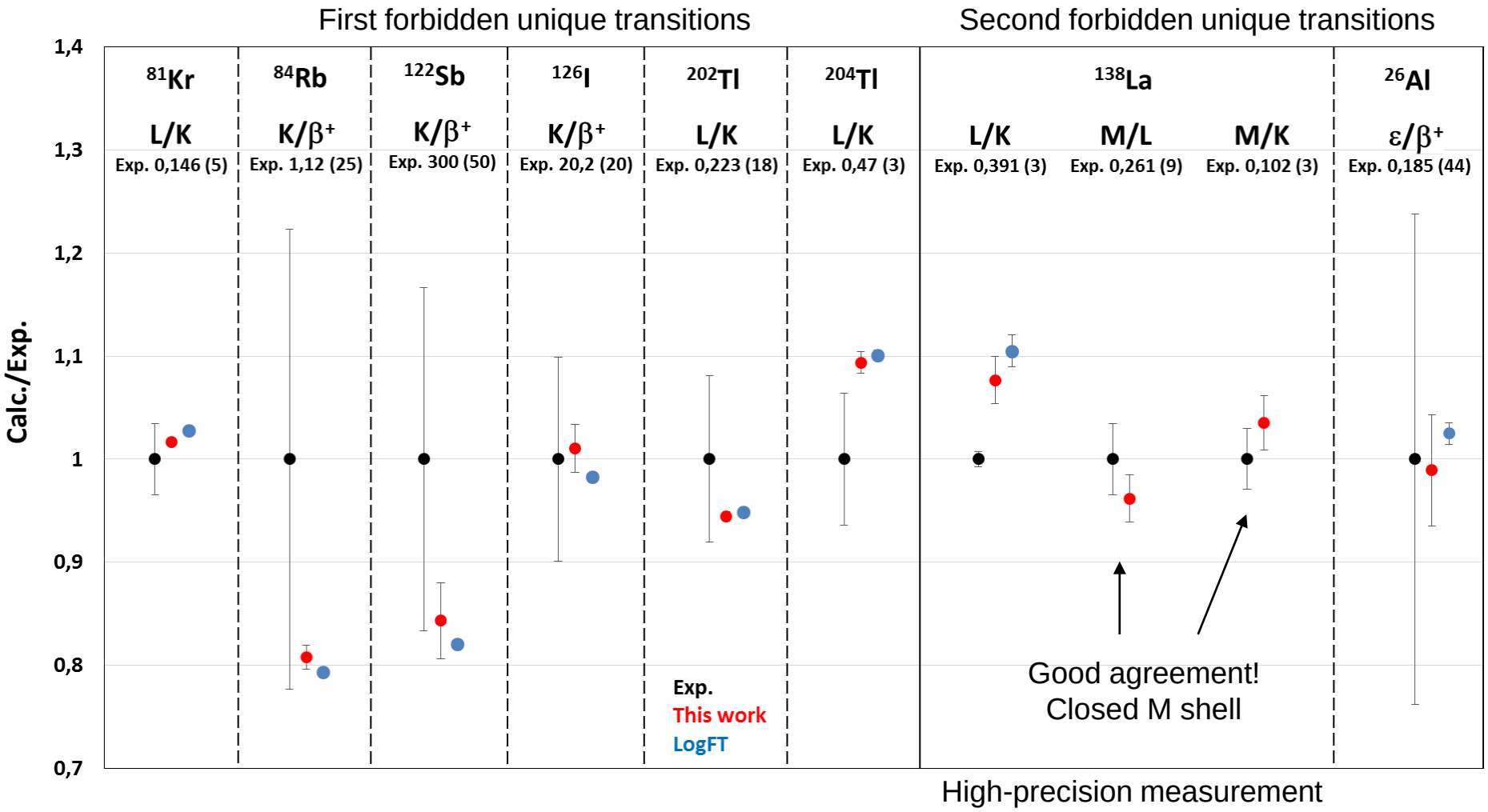
$$\left\{1 - \int_0^r x^2[g_{n\kappa}^2(x) + f_{n\kappa}^2(x)]\mathrm{d}x - r\int_r^\infty x[g_{n\kappa}^2(x) + f_{n\kappa}^2(x)]\,\mathrm{d}x\right\}\mathrm{d}r$$

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.

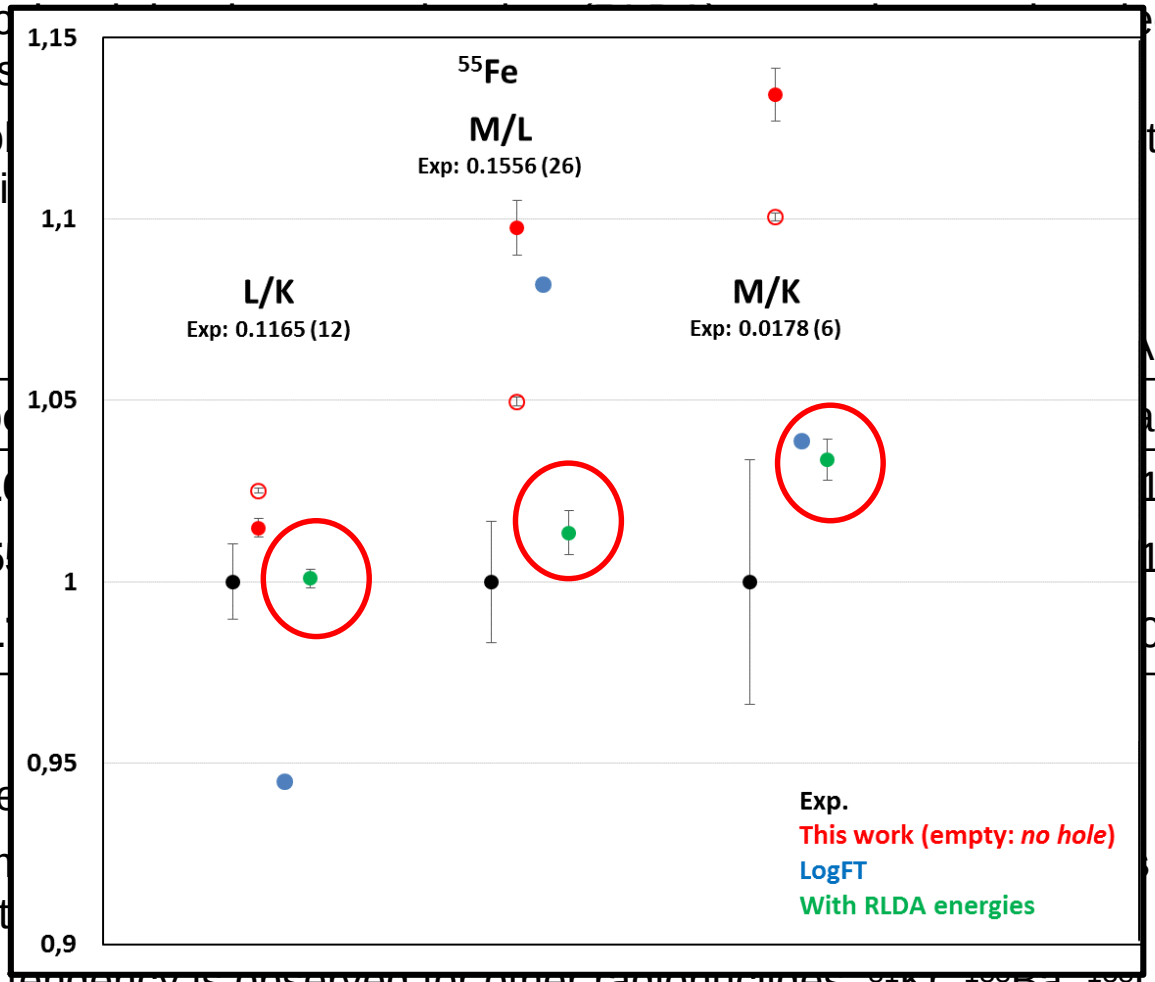
→ It seems also possible to see the better predictive power of Vatai's approach, as expected from a pure theoretical point of view.

→ 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.

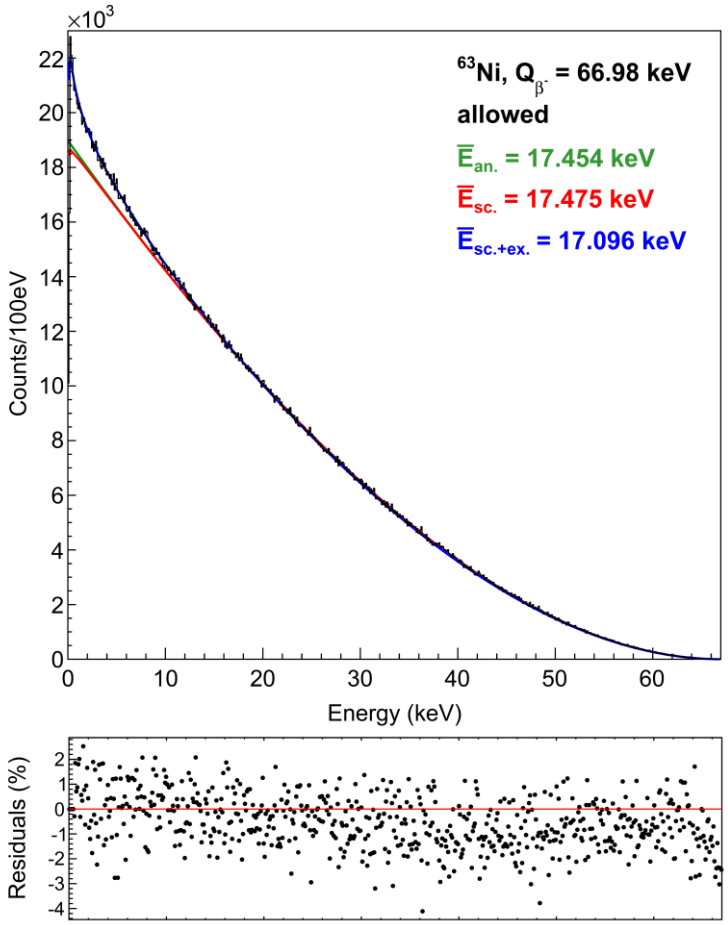
→ Still difficult to distinguish between Bahcall's and Vatai's approaches.

→ 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.

Atomic effects in beta decays

Atomic effects: ^{63}Ni



Atomic effects in allowed beta decays have been studied with high precision. Formalism of the **atomic exchange effect** has been revised to include **both $s_{1/2}$ and $p_{1/2}$ orbitals**.

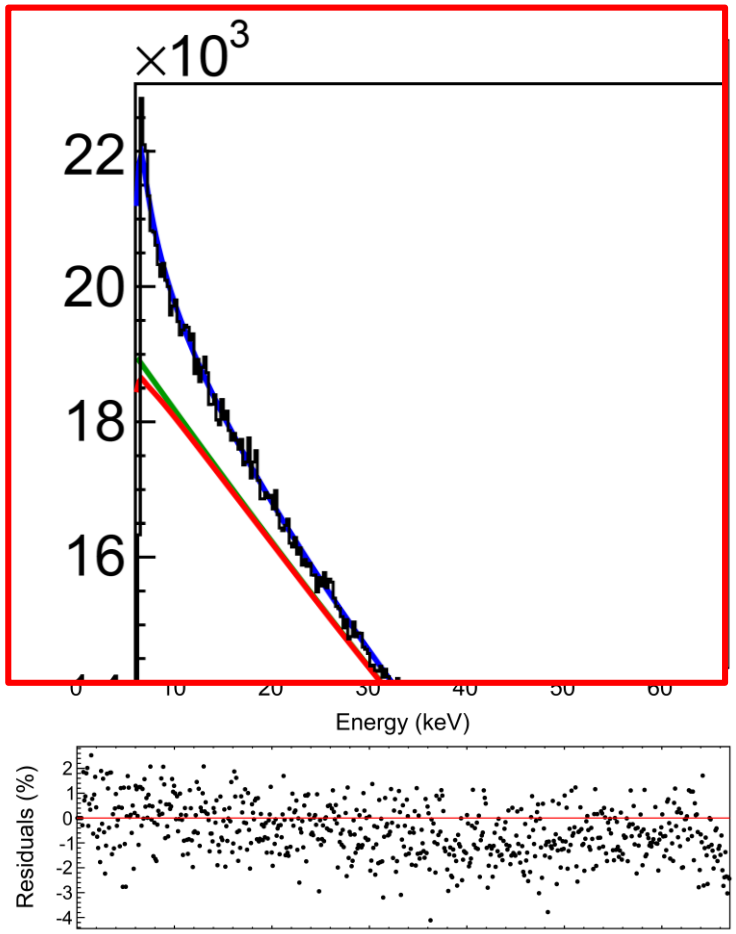
In addition, **new radiative correction** and **new orbital energies** have been considered.

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.

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

Influence of orbital energies: ^{63}Ni



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

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.

Relativistic electron wave functions

Dirac equation is solved numerically using local power series expansions following:

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

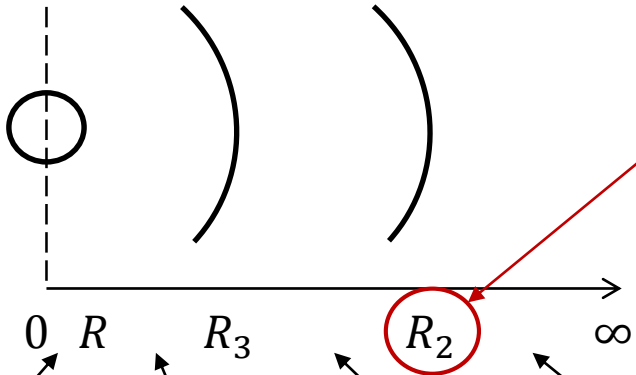
Wave functions are then split in large (*H*,*D*) and small (*h*,*d*) components

$$g_{-k_e}(r) = \alpha_{-k_e} \frac{(p_e r)^{k_e - 1}}{(2k_e - 1)!!} \{H_{k_e}(r) - h_{k_e}(r)\}$$

$$f_{-k_e}(r) = -\alpha_{-k_e} \frac{(p_e r)^{k_e - 1}}{(2k_e - 1)!!} \frac{r}{R} \{D_{k_e}(r) - d_{k_e}(r)\}$$

Coulomb potential: uniformly charged sphere with screening

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



Important parameter which determines the length of the *r*-grid

Finite nuclear size, quadratic behavior

Total potential

2nd order polynomial for reconnection

Asymptotic solutions

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 ($\omega/\hbar$)

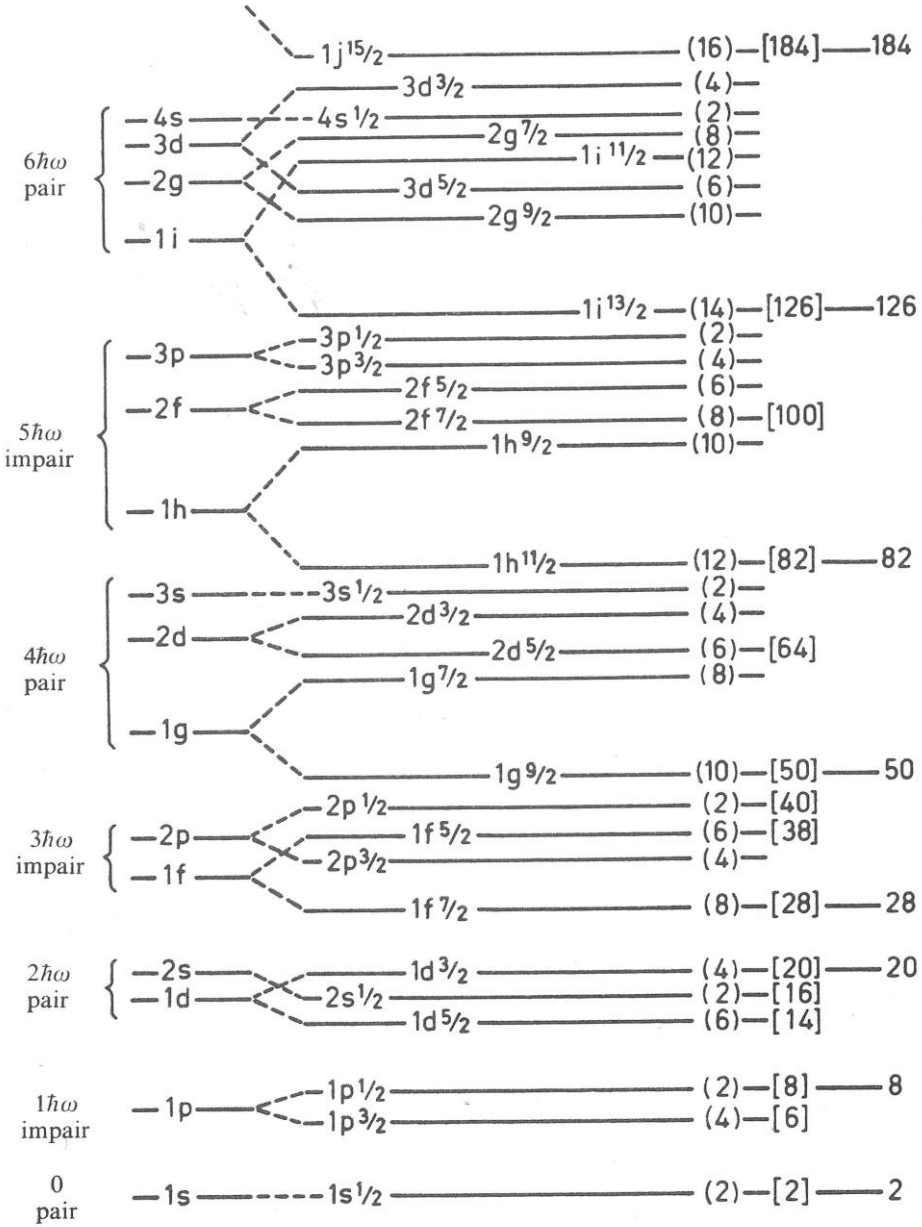
Protons ≠ neutrons: introduction of a quadratic Coulomb potential

→ 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)



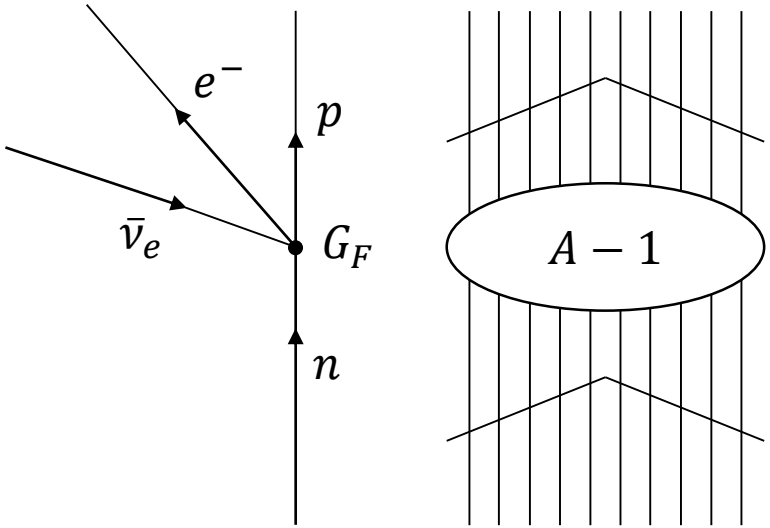
Description of the weak decay process

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.



Optimization

In principle, the multipole expansion is unlimited. However, the lowest orders should contribute more.

Recommendation from Behrens and Bühring is to consider only the terms with $K = K_{\min}$, $K_{\min} + 1$ and $(k_e + k_v) = K,\ K + 1$. This recommendation is relevant for a precision at nearly the percent level but additional terms can be necessary.

A specific algorithm has thus been developed in order to control the precision of the calculation. A pre-analysis is performed at $W_0/2$ and many possibilities are tested into nested loops:

- Loop on k_e from 1 to $K_{\min} + 4$.
- Loop on all possible values of K.
- Loop on all possible values of k_v for definite values of k_e and K.
- Loop on all possible values of L and s for definite values of K.

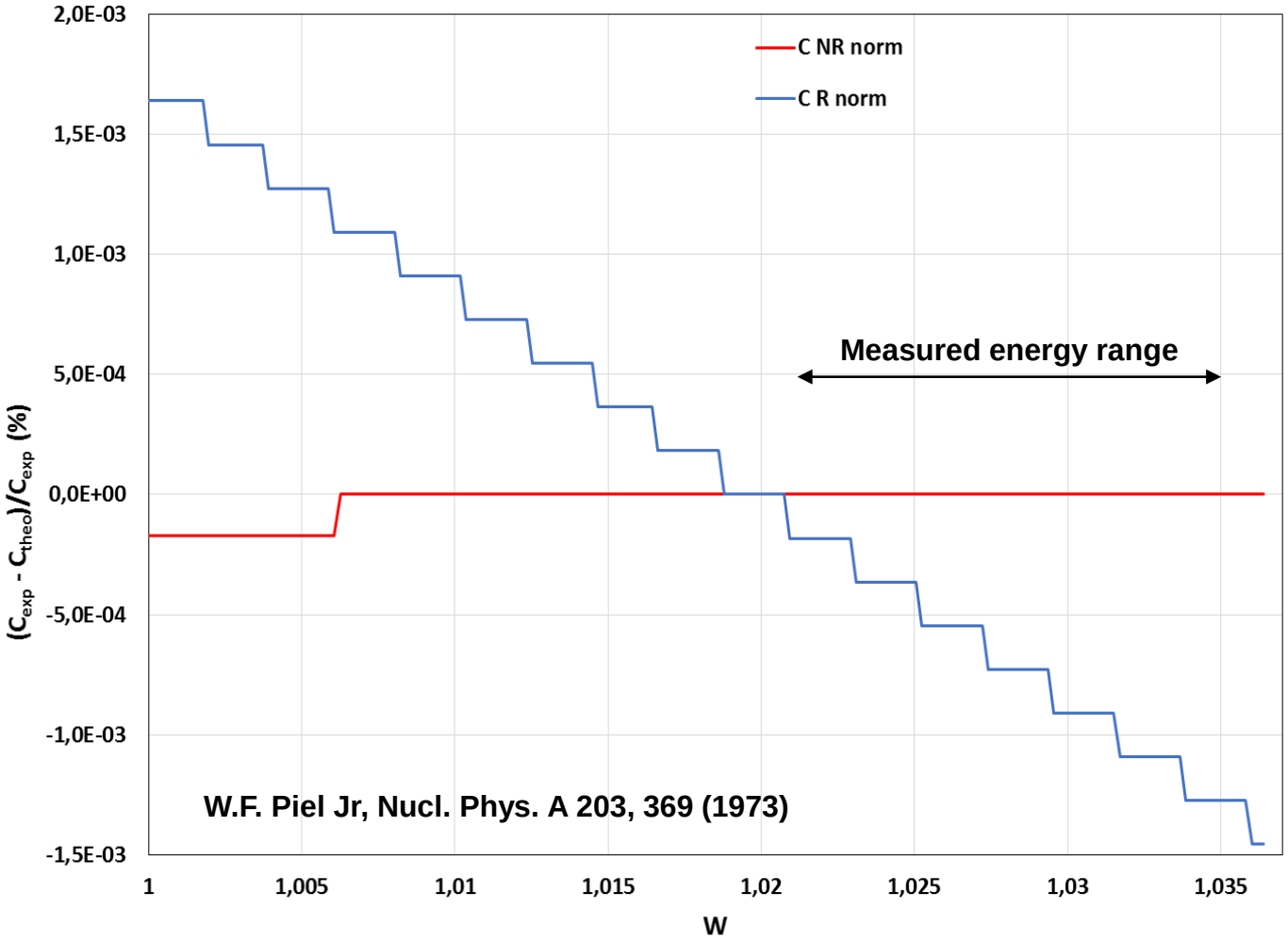
Then, each $C(W_0/2\,; k_e, K, k_v)$ which contributes to the total shape factor $C(W_0/2)$ more than a fixed precision limit – 10^{-5}% in present work – is selected.

Only these relevant (k_e, K, k_v) combinations are calculated for the requested energies over the entire spectrum.

Inclusion of nuclear structure

Allowed transitions

Theoretical shape factor: ^{3}H



Allowed

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

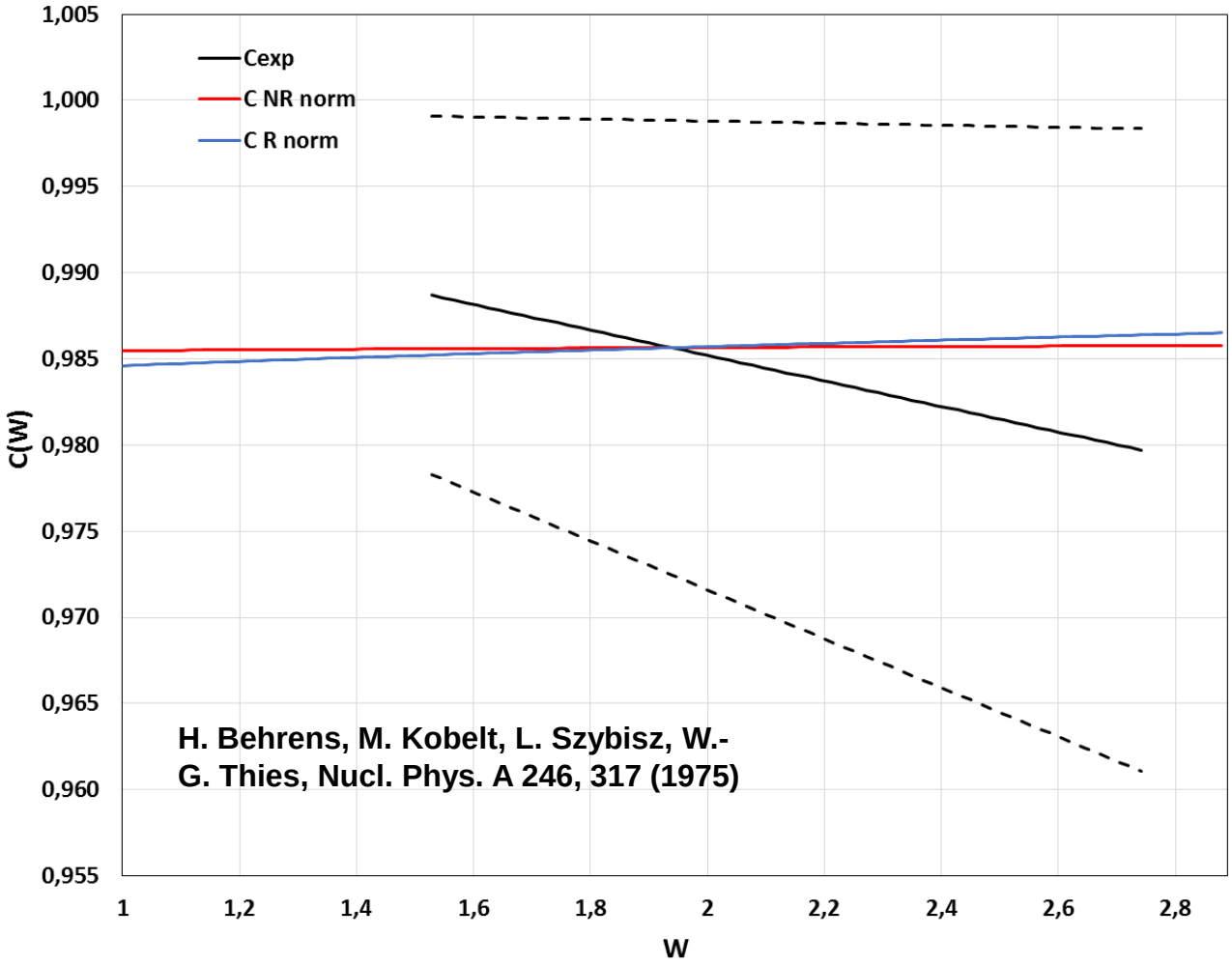
E_0 = 18,592(1) keV

$t_{1/2}$ exp. = 12,32(2) a

$t_{1/2}$ NR = 10,51 a

$t_{1/2}$ R = 11,25 a

Theoretical shape factor: ^{11}C



Allowed

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

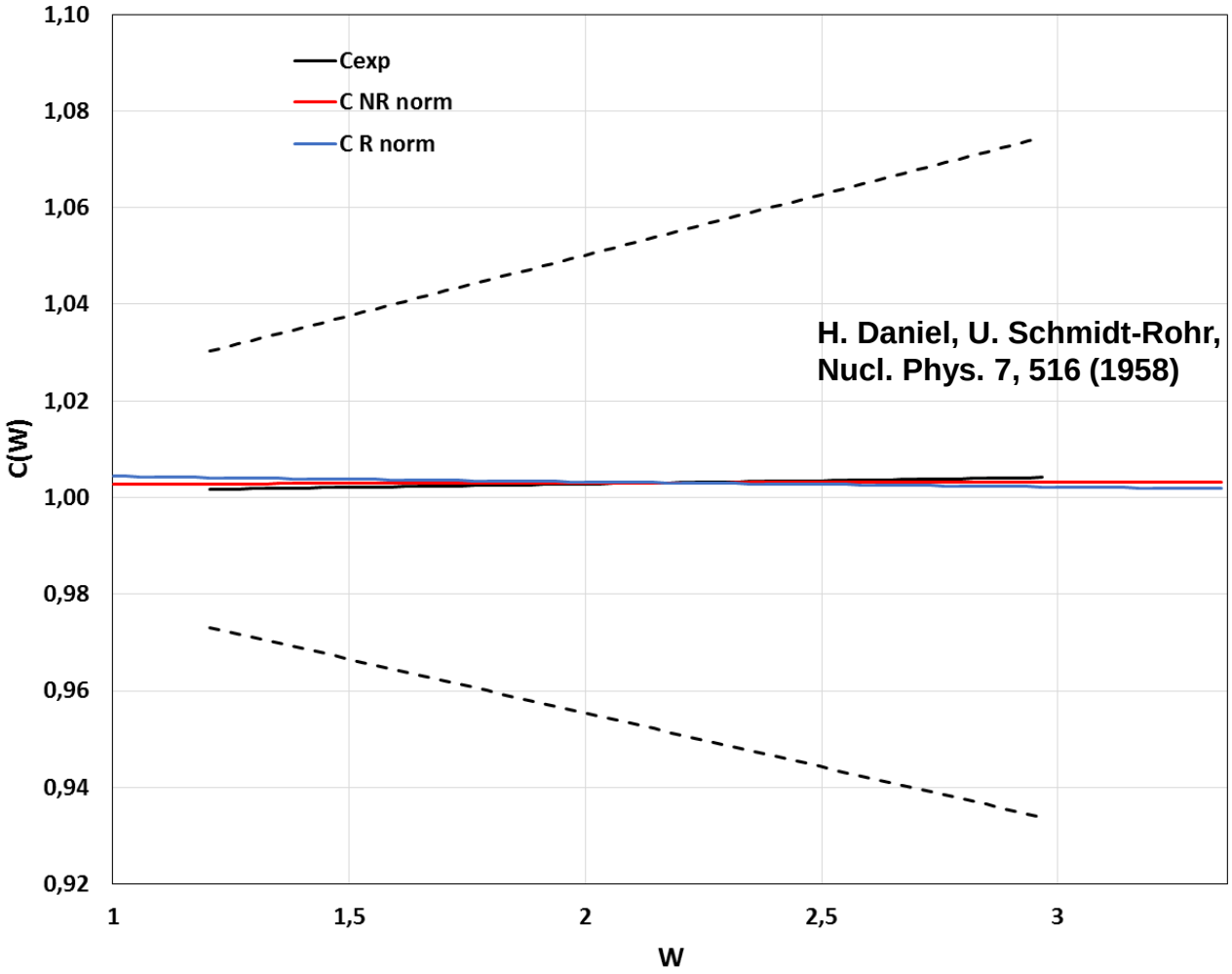
E_0 = 959,69(6) keV

$t_{1/2}$ exp. = 1224,7(8) s

$t_{1/2}$ NR = 473,6 s

$t_{1/2}$ R = 497,6 s

Theoretical shape factor: ^{13}N



Allowed

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

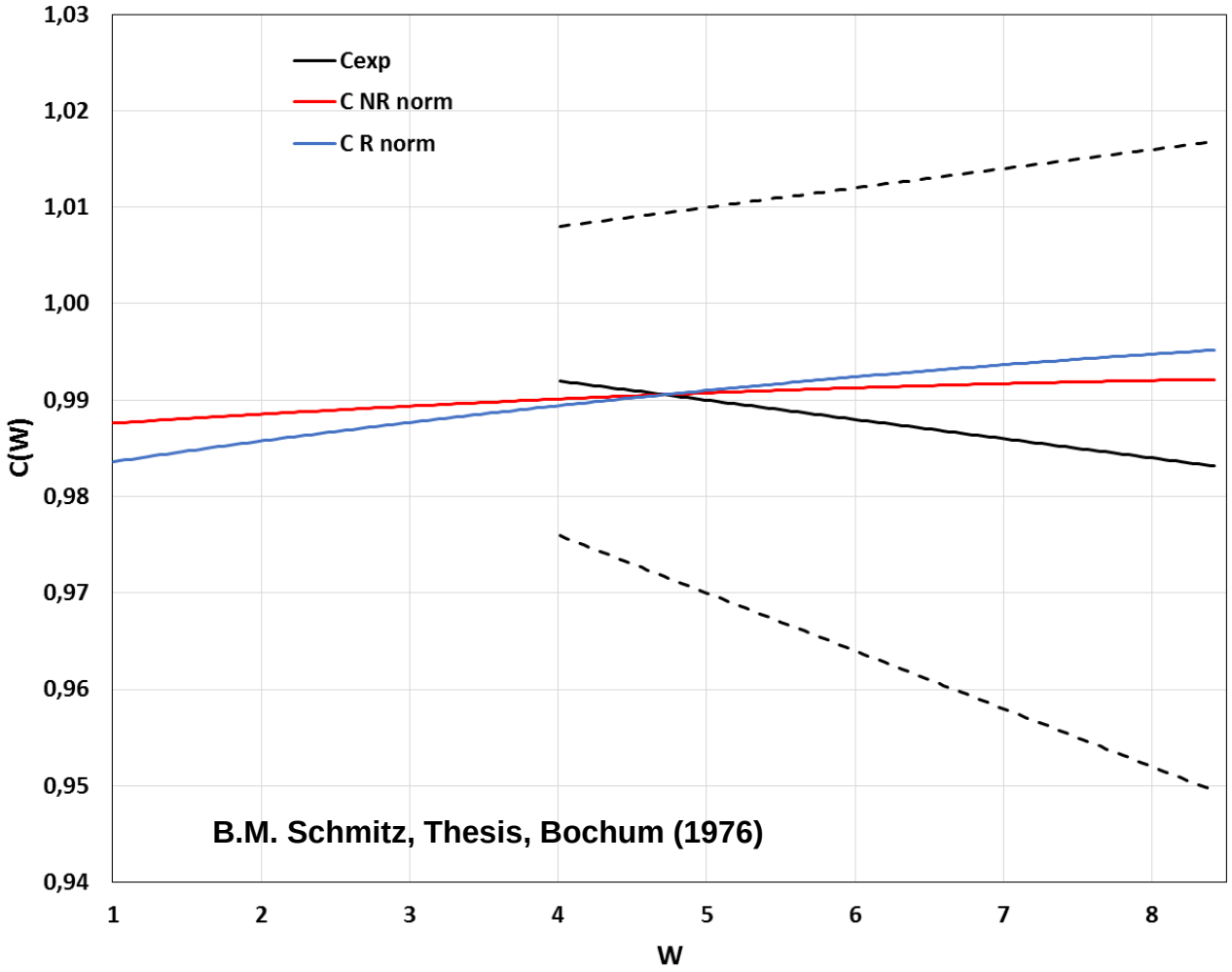
E_0 = 1198,47(27) keV

$t_{1/2}$ exp. = 9,9846(40) min

$t_{1/2}$ NR = 7,84 min

$t_{1/2}$ R = 8,42 min

Theoretical shape factor: ^{27}Si



Allowed

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

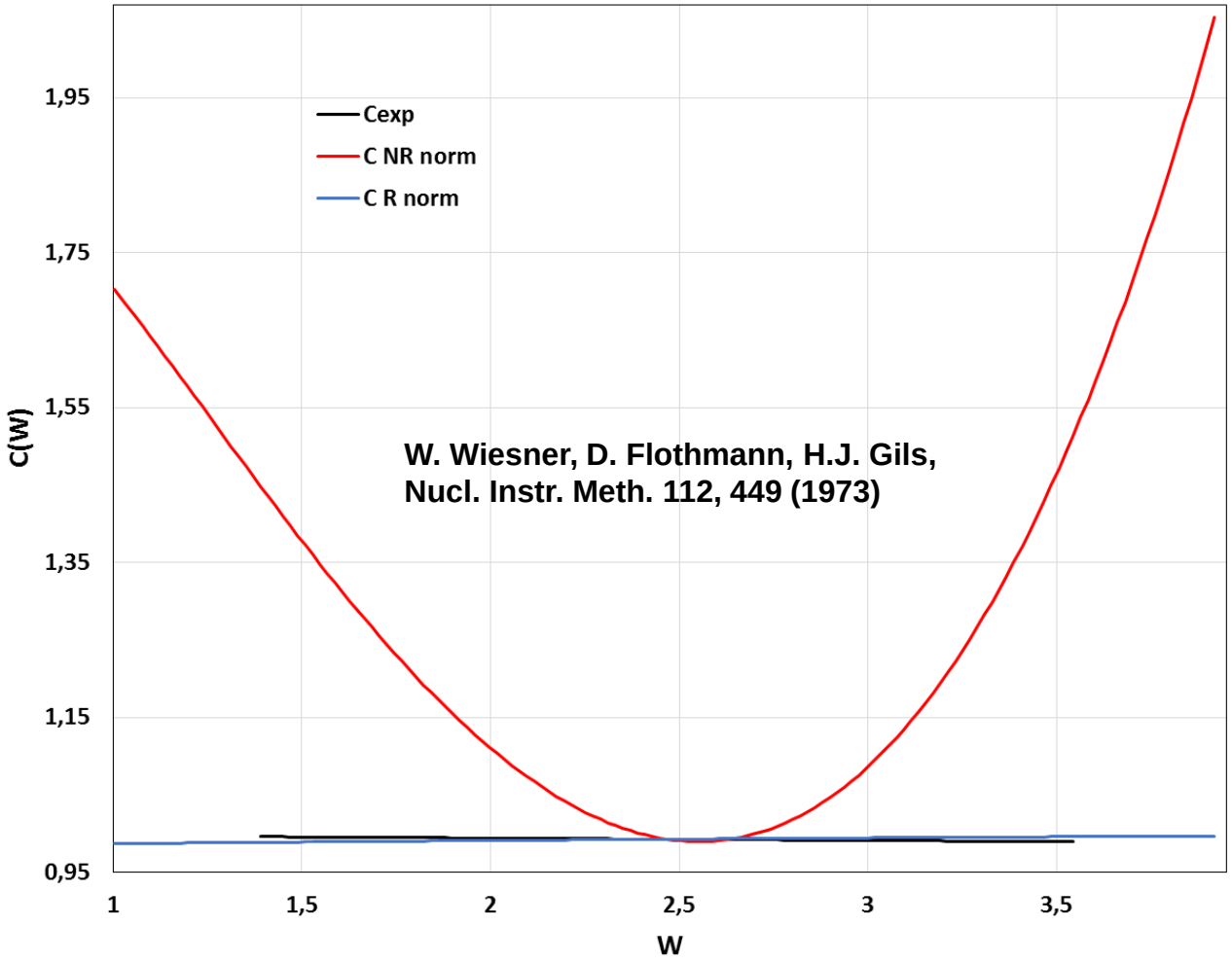
E_0 = 3790,36(10) keV

$t_{1/2}$ exp. = 4,162(40) s

$t_{1/2}$ NR = 1,723 s

$t_{1/2}$ R = 1,793 s

Theoretical shape factor: ^{31}Si



Allowed

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

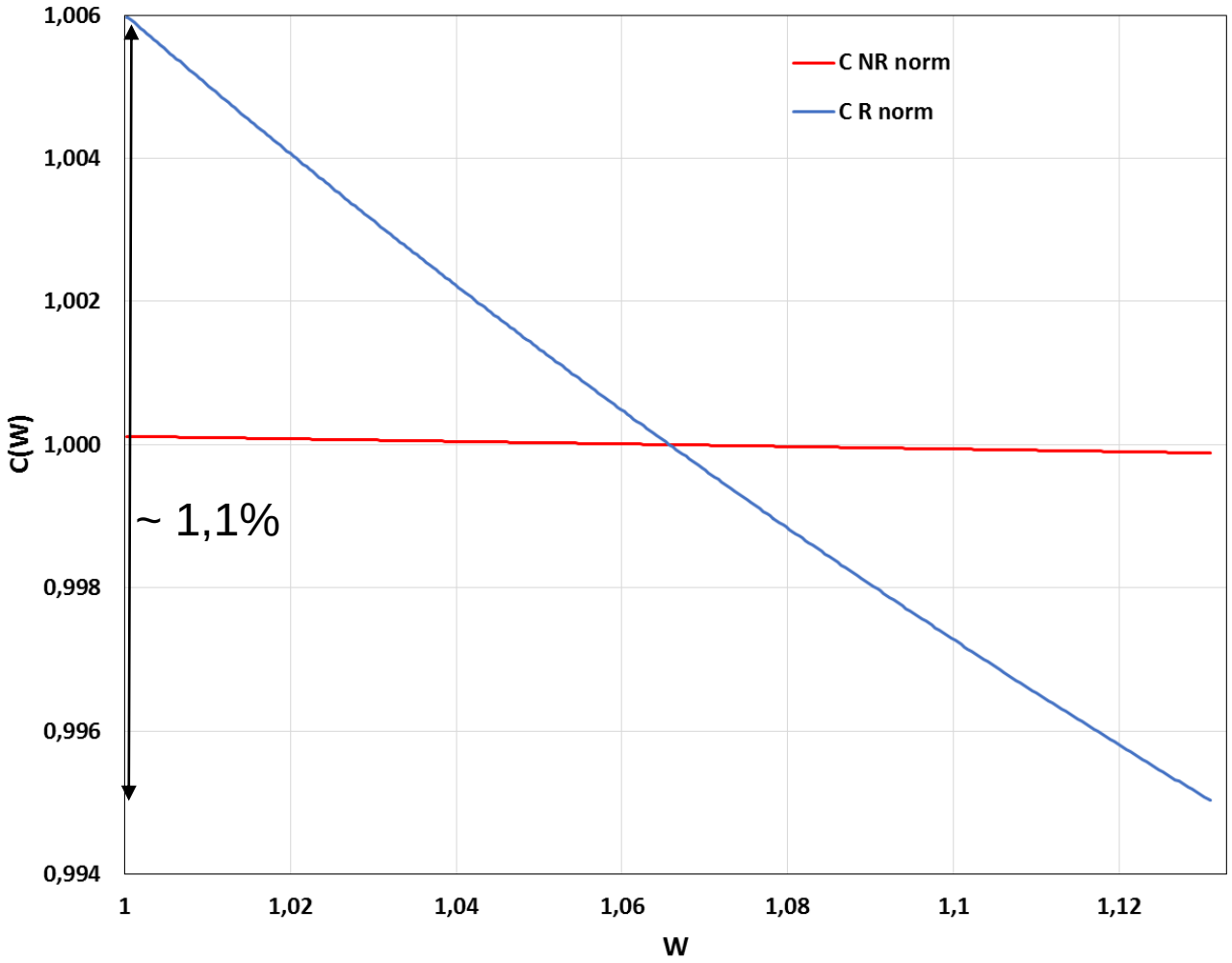
E_0 = 1491,50(4) keV

$t_{1/2}$ exp. = 157,45(26) min

$t_{1/2}$ NR = 2,2·10^7 min

$t_{1/2}$ R = 2,5·10^6 min

Theoretical shape factor: ^{63}Ni



Allowed

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

E_0 = 66,977(15) keV

$t_{1/2}$ exp. = 101,2(15) a

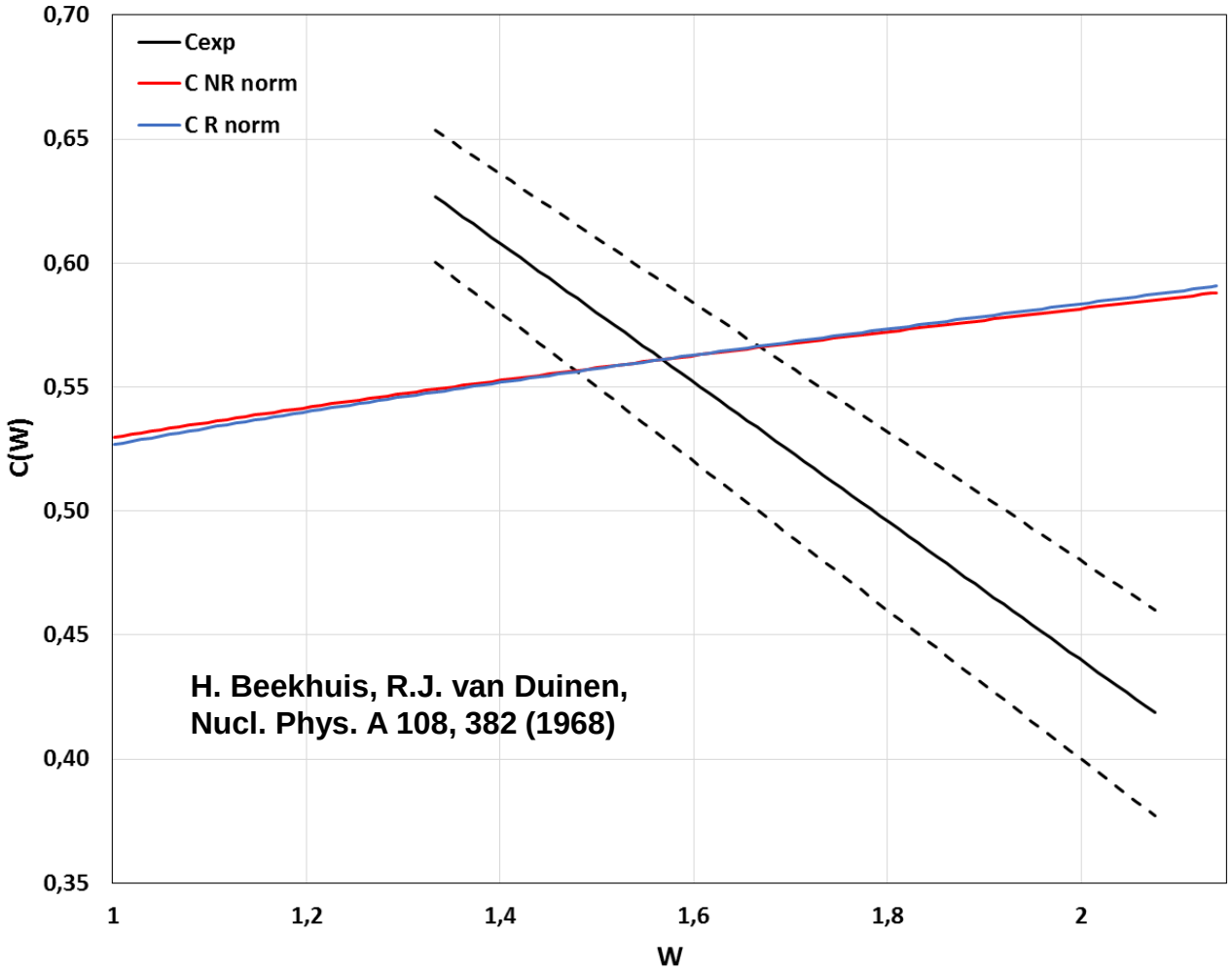
$t_{1/2}$ NR = 0,029 a

$t_{1/2}$ R = 694,5 a

Inclusion of nuclear structure

Forbidden transitions

Theoretical shape factor: ^{141}Ce



First forbidden non-unique

Initial state	Final state
$\|\nu, 2f_{7/2}\rangle$	$\|\pi, 2d_{5/2}\rangle$

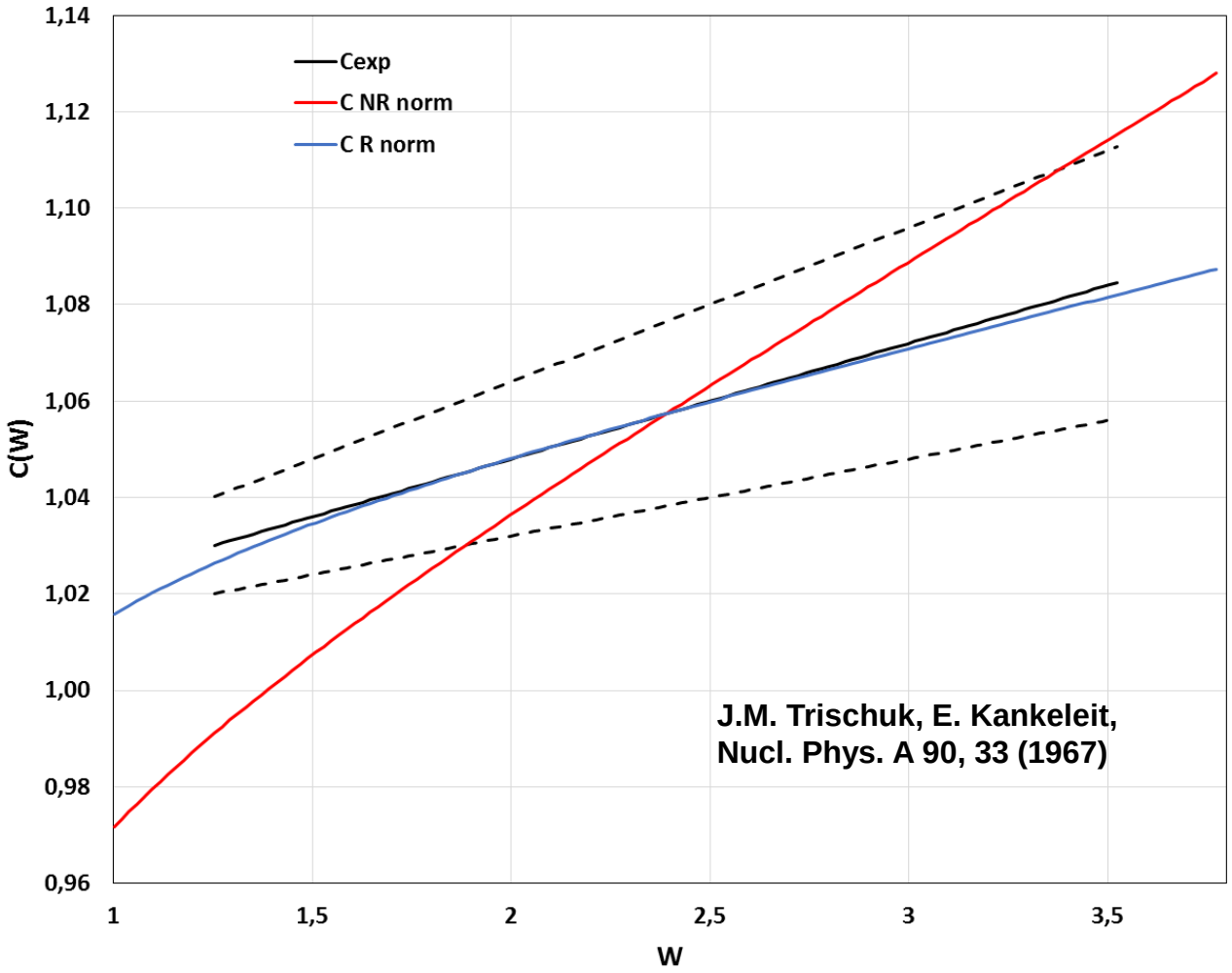
E_0 = 582,7(12) keV

$t_{1/2}$ exp. = 107,3(14) d

$t_{1/2}$ NR = 0,254 d

$t_{1/2}$ R = 0,250 d

Theoretical shape factor: ^{207}Tl



First forbidden non-unique

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

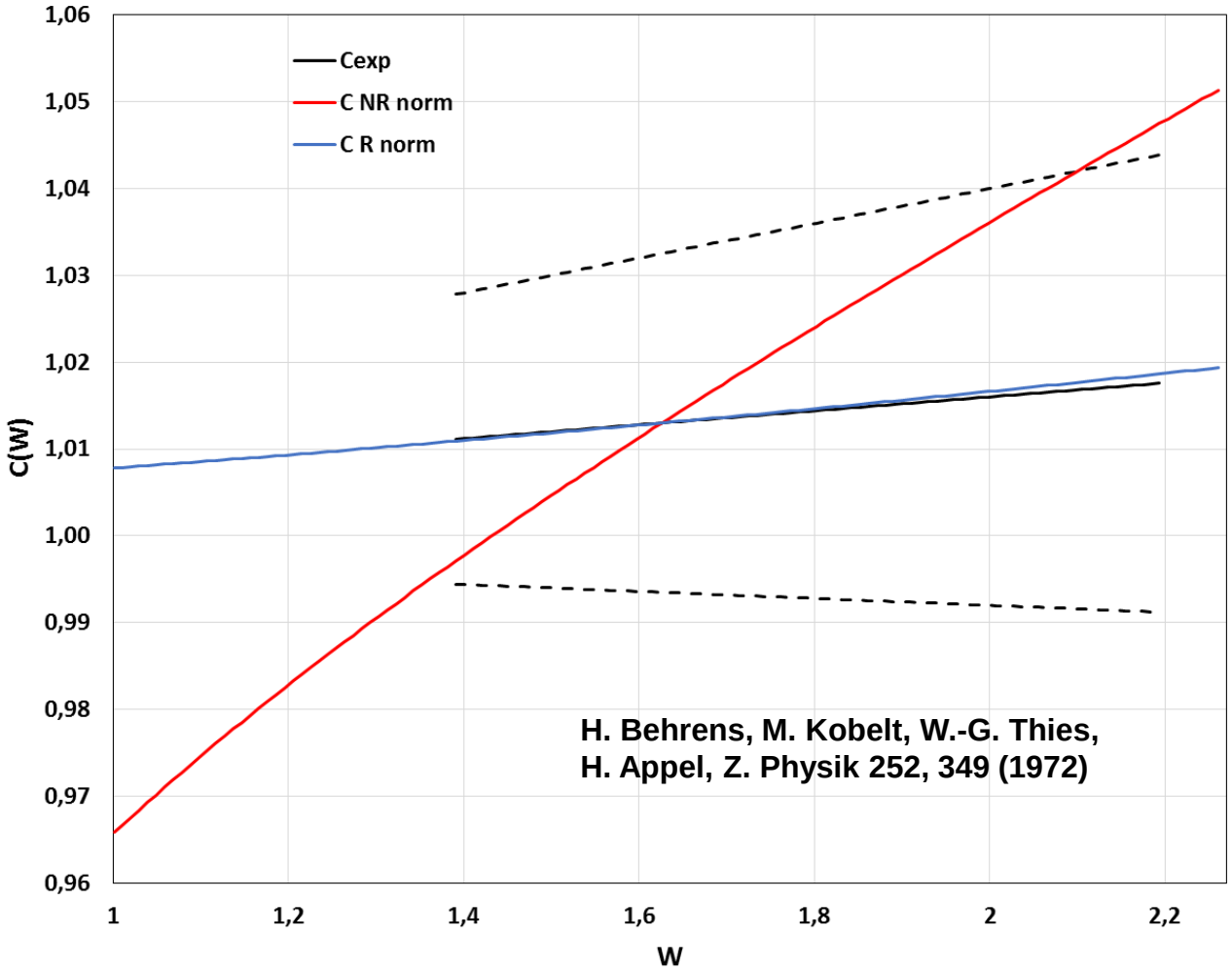
E_0 = 1418(5) keV

$t_{1/2}$ exp. = 4,787(12) min

$t_{1/2}$ NR = 1,32 min

$t_{1/2}$ R = 1,40 min

Theoretical shape factor: ^{209}Pb



First forbidden non-unique

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

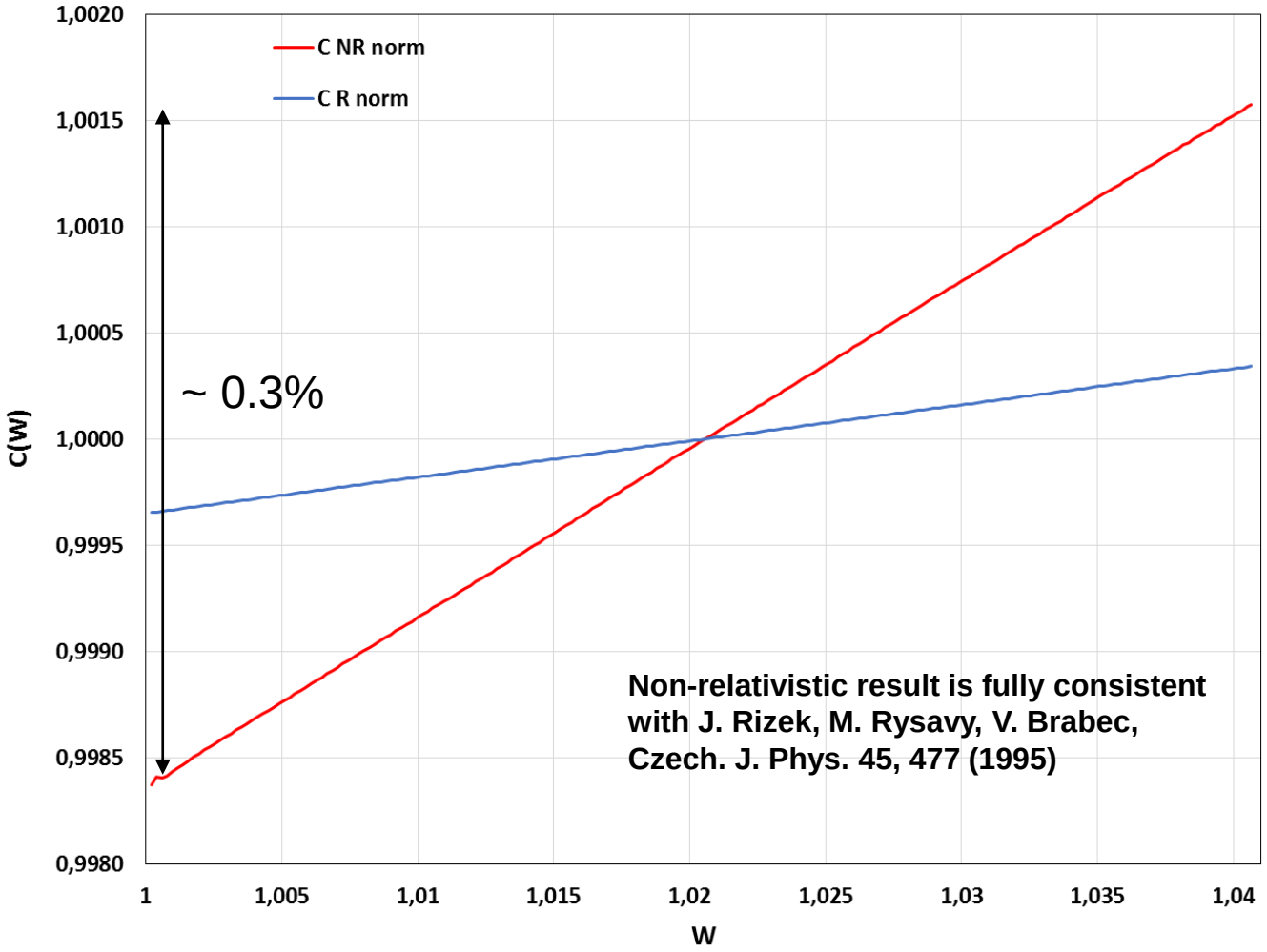
E_0 = 644,0(11) keV

$t_{1/2}$ exp. = 3,234(7) h

$t_{1/2}$ NR = 2,862 h

$t_{1/2}$ R = 252,2 h

Theoretical shape factor: ^{241}Pu



First forbidden non-unique

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

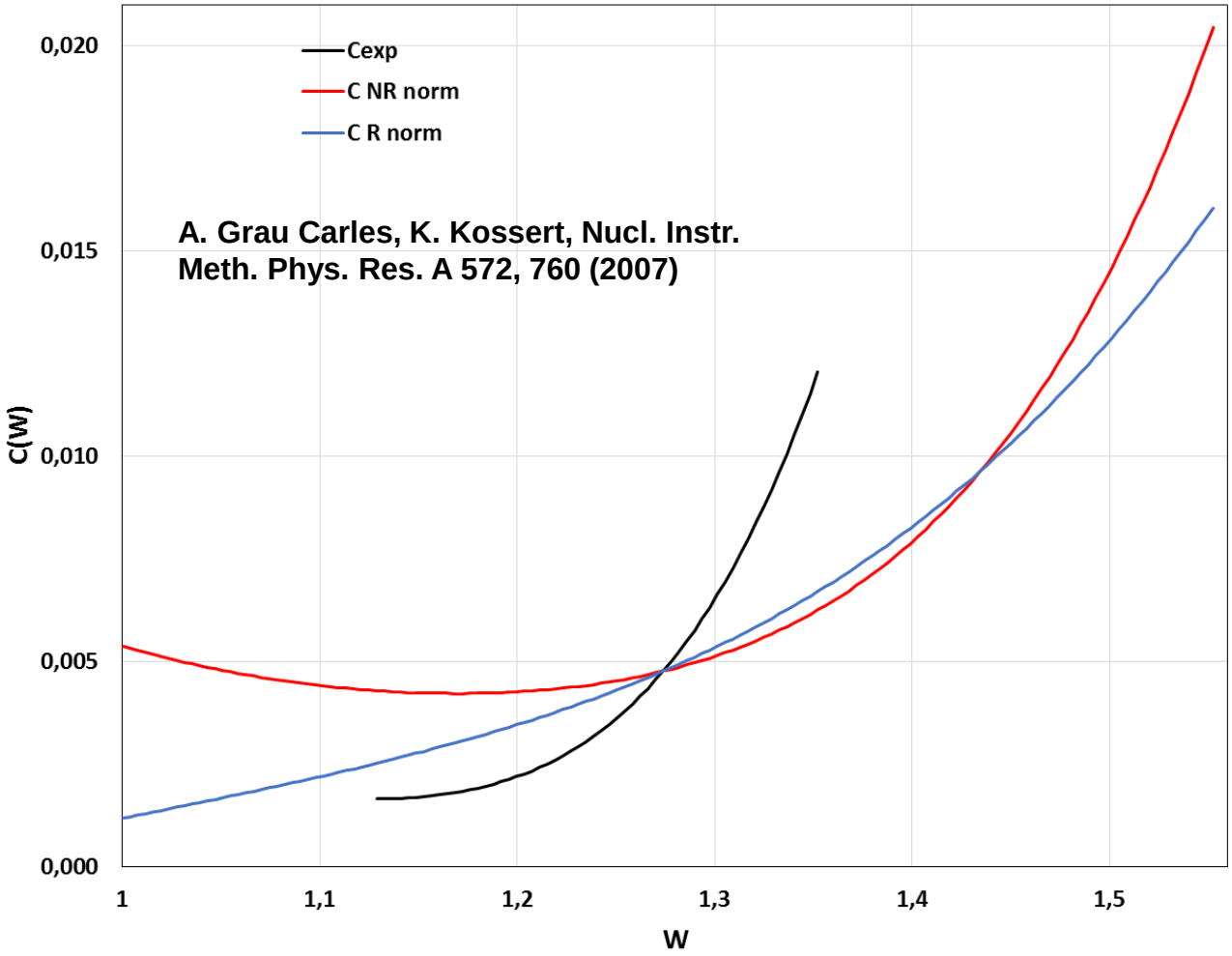
E_0 = 20,78(17) keV

$t_{1/2}$ exp. = 14,329(29) a

$t_{1/2}$ NR = 2,503 a

$t_{1/2}$ R = 173,4 a

Theoretical shape factor: ^{87}Rb



Third forbidden non-unique

Initial state	Final state
$\left\|\pi^{-1}, 2p_{3/2}\right\rangle$	$\left\|\nu^{-1}, 1g_{9/2}\right\rangle$

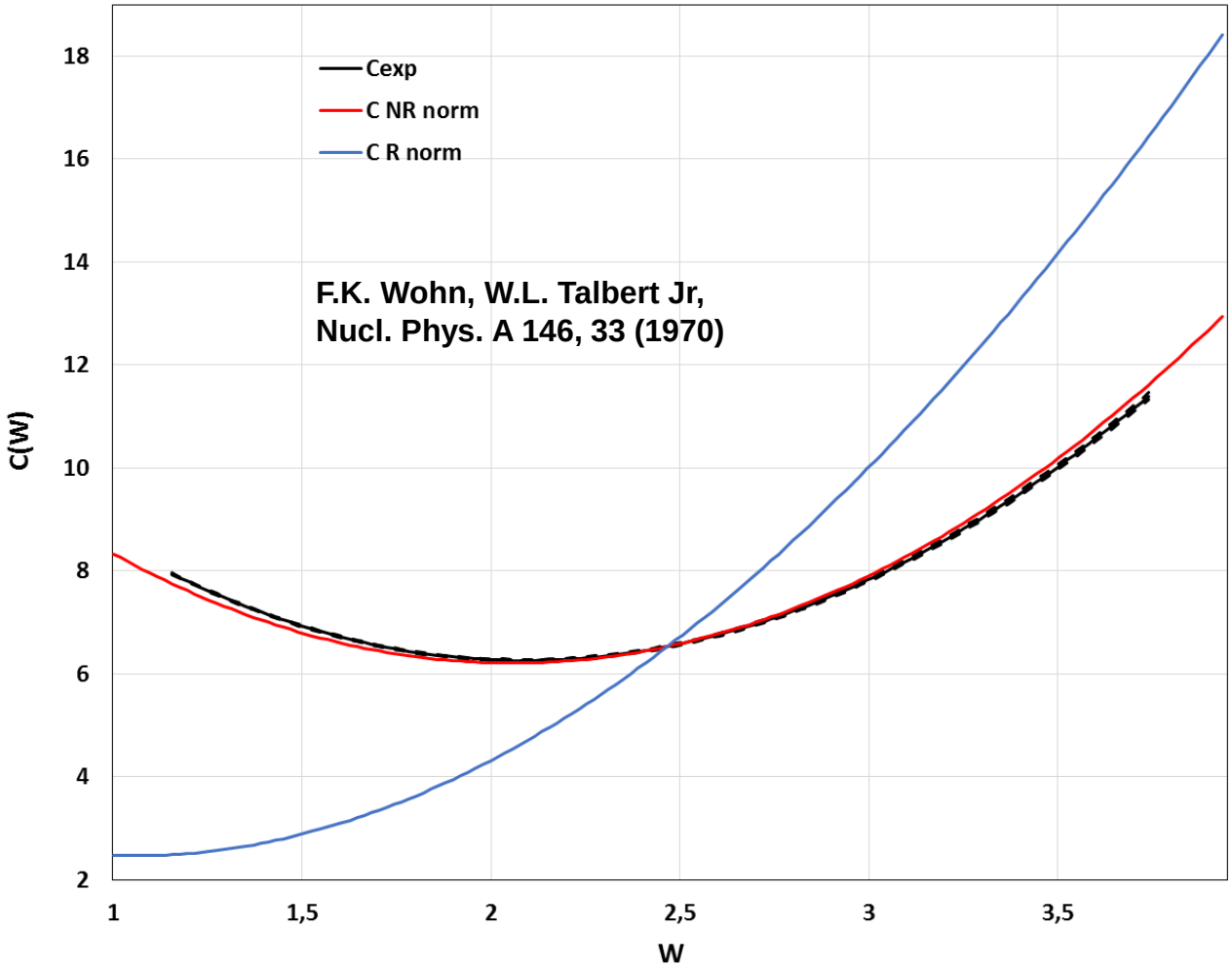
E_0 = 282,275(6) keV

$t_{1/2}$ exp. = 4,97(3)·10^{10} a

$t_{1/2}$ NR = 1,13·10^{11} a

$t_{1/2}$ R = 2,46·10^{8} a

Theoretical shape factor: ^{89}Sr



First forbidden unique

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

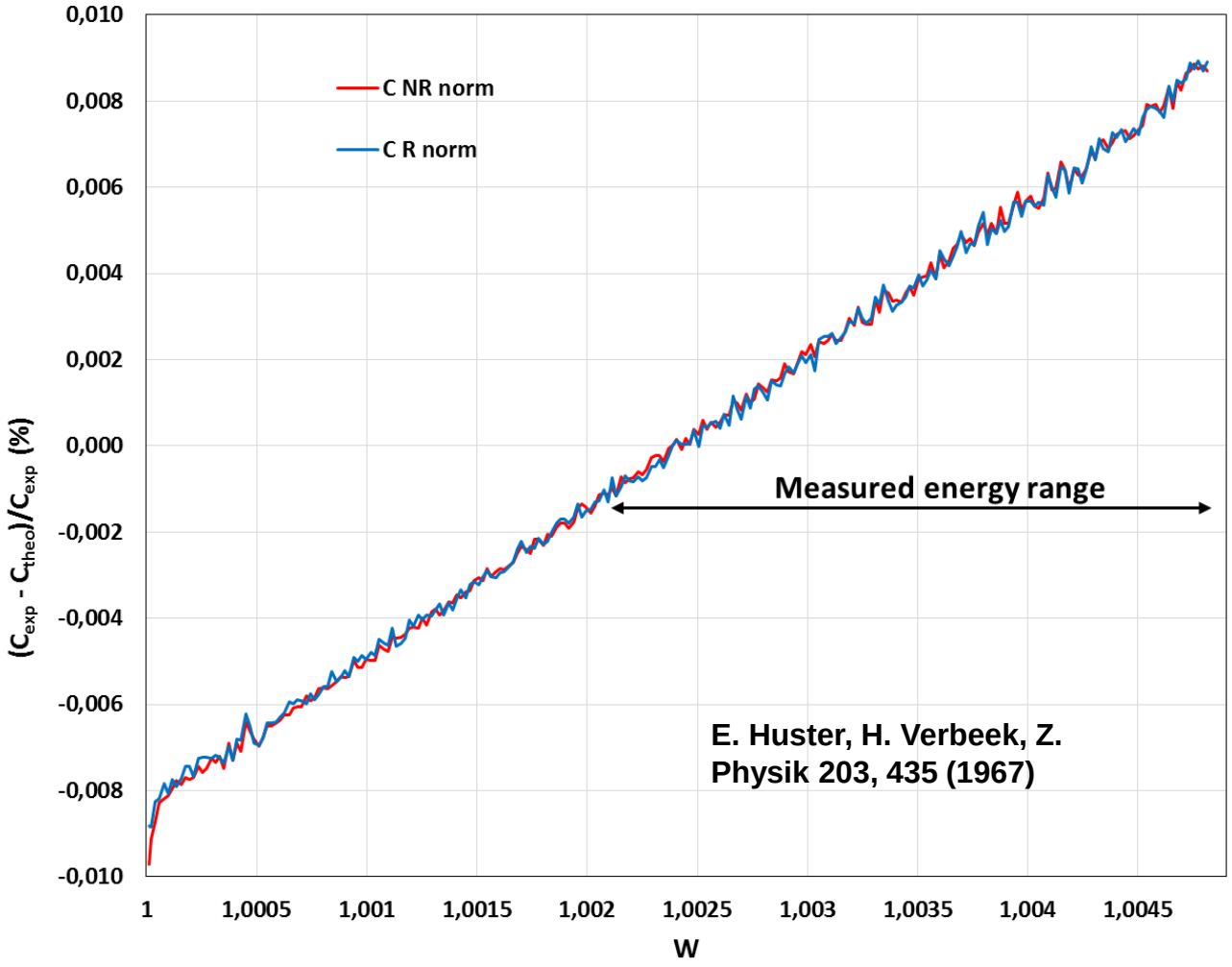
E_0 = 1499,3(16) keV

$t_{1/2}$ exp. = 50,568(25) d

$t_{1/2}$ NR = 3,531 d

$t_{1/2}$ R = 162 887 d

Theoretical shape factor: ^{187}Re



First forbidden unique

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

E_0 = 2,467(2) keV

$t_{1/2}$ exp. = 4,33(7)·10^{10} a

$t_{1/2}$ NR = 9,99·10^{7} a

$t_{1/2}$ R = 4,54·10^{7} a

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.

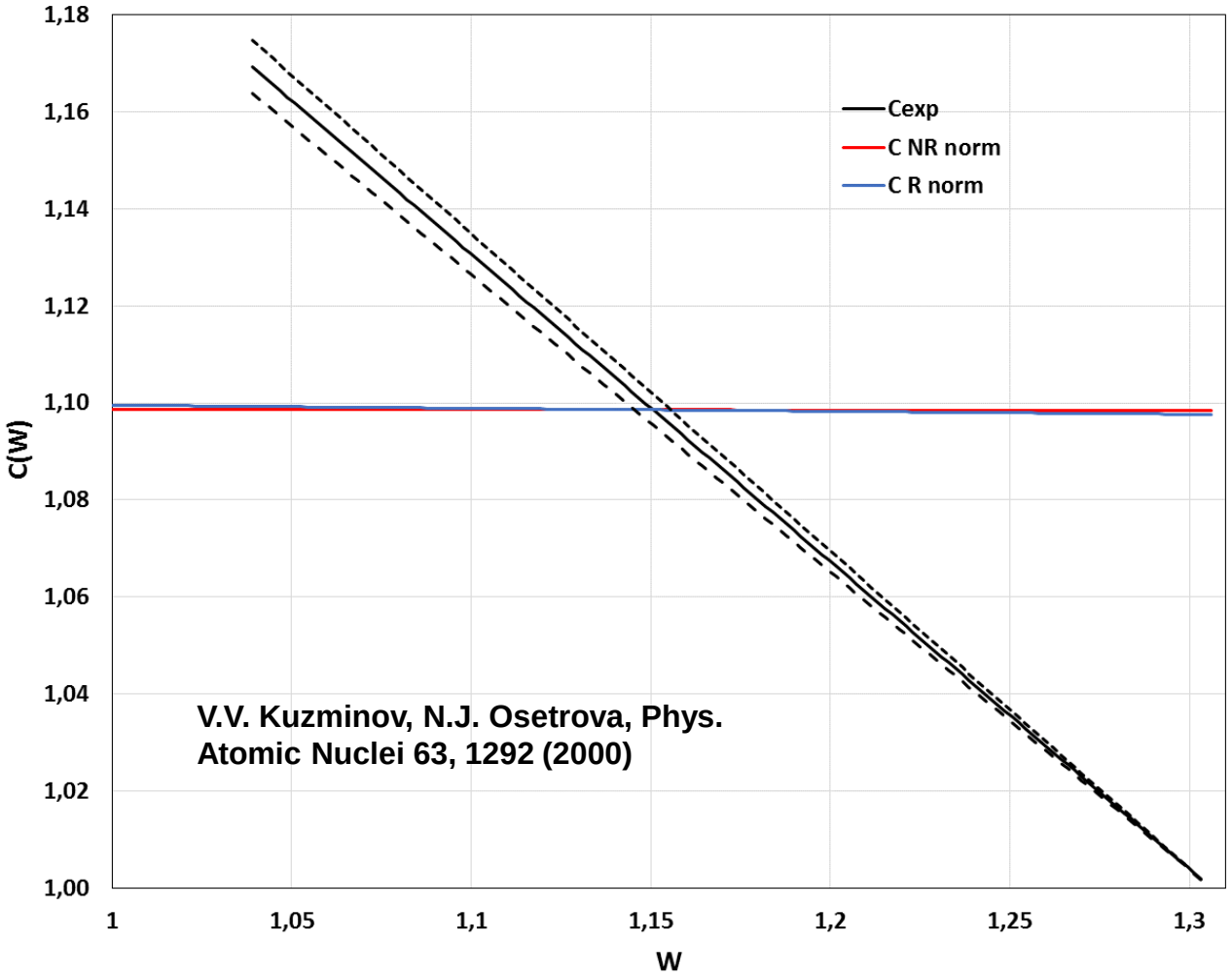
An even-even nucleus can be considered as the vacuum of particle-hole excitations used to describe adjacent nuclei.

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



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

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

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

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

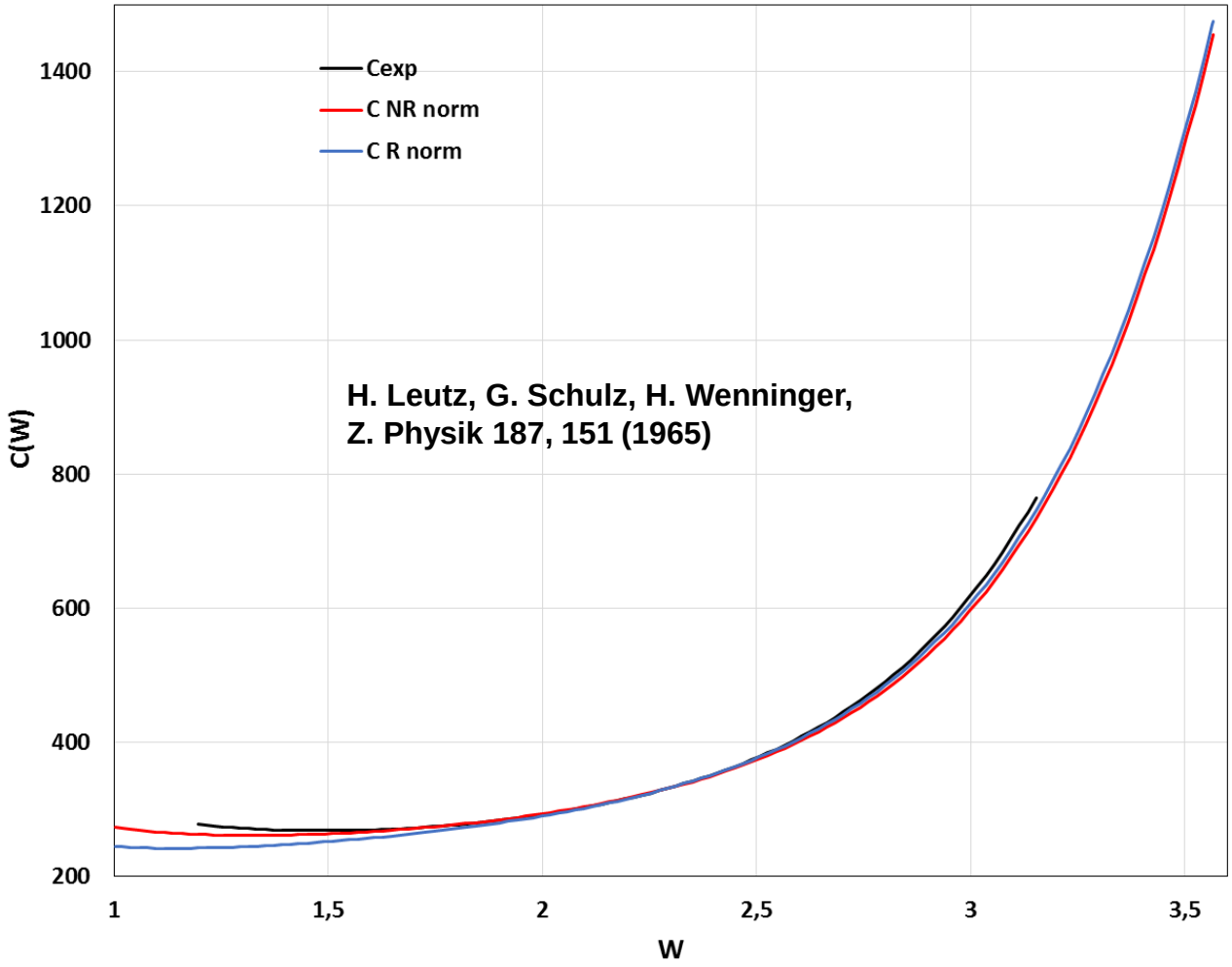
E_0 = 156,476(4) keV

$t_{1/2}$ 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



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

$$4^- \rightarrow 0^+$$

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

$$C(4) = 3$$

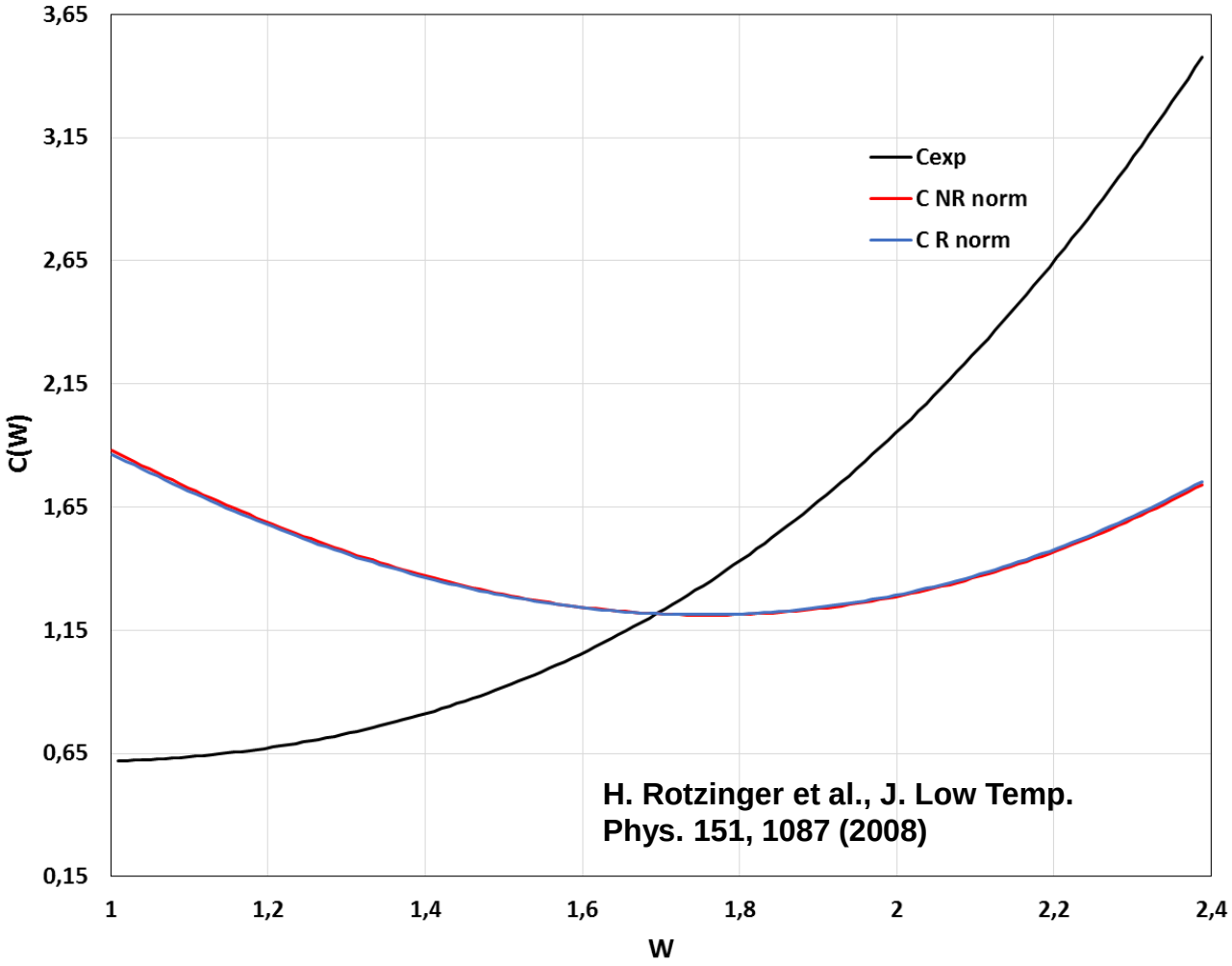
E_0 = 1310,89(6) keV

$t_{1/2}$ 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

European projects

Theoretical shape factors

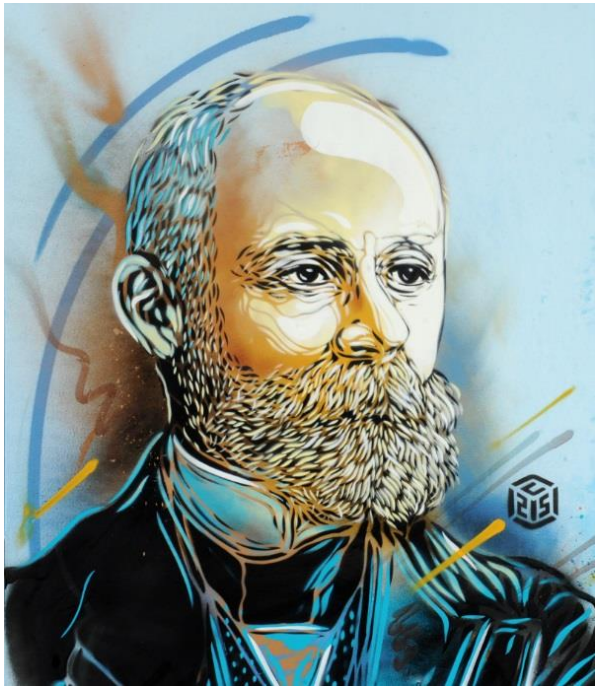
European EMPIR project MetroBeta (2016-2019): improved beta decay calculations. Inclusion of more precise nucleon wave functions from a semi-phenomenological nuclear mean-field approach, still in spherical symmetry. Will be used afterwards for electron captures.

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

- 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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