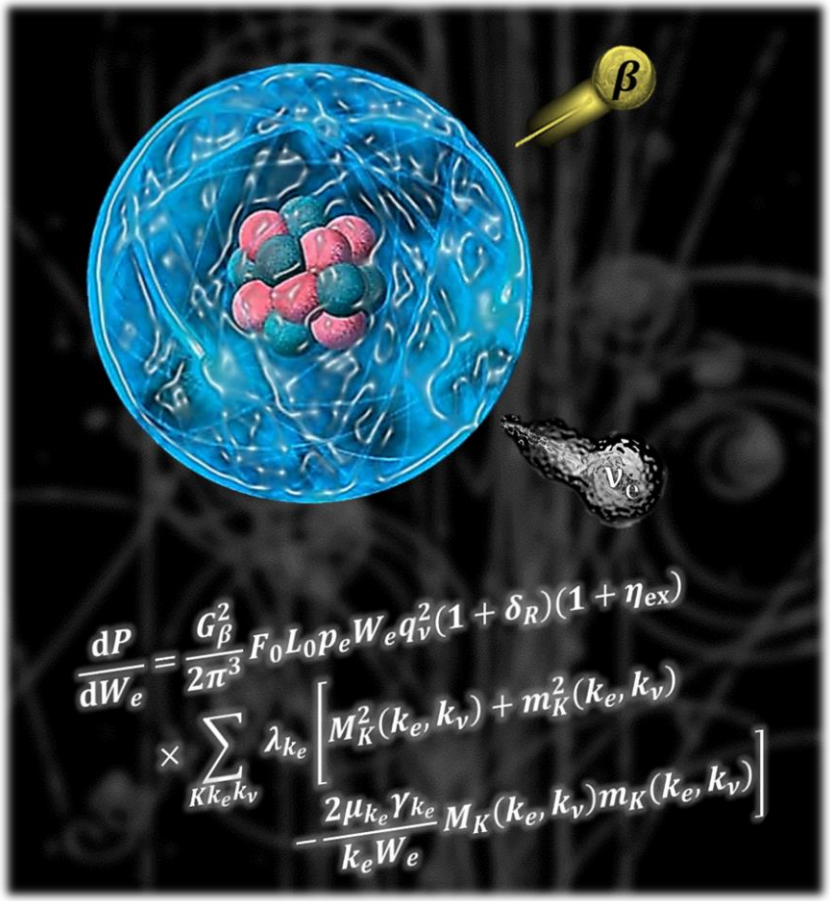


BetaShape

v2

list
cea tech

LNHB
Laboratoire National Henri Becquerel

LABORATOIRE NATIONAL DE MÉTROLOGIE ET D'ESSAIS
LNE

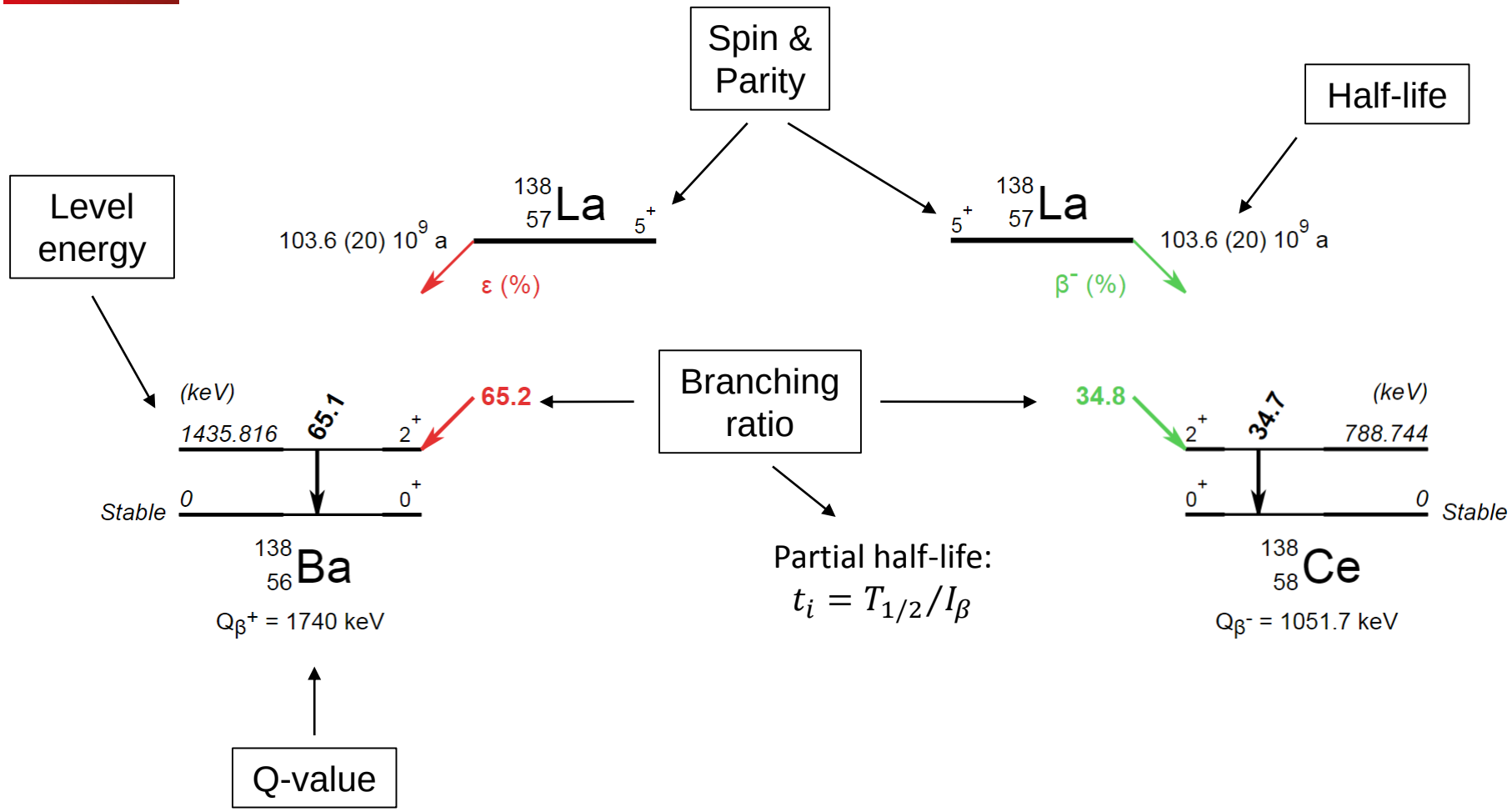
université PARIS-SACLAY

EURAMET

Outline

- **Short review of LogFT modelling**
- **The BetaShape code (v2)**
  - Beta decays, experimental shape factors
  - Electron captures, comparison with precise measurements
  - Output files
- **Application to radionuclide metrology**
- **Ongoing developments and perspectives**

Weak interaction decays in nuclear data



- **Beta transition**: energy spectra, mean energies, ft-values
- **Electron capture**: capture probabilities, ft-values

LogFT

General features

Input data form ENSDF file

- Propagates uncertainties from input parameters
- Unc. <0.1% not given, i.e. null unc. in output results

Output results

- Beta decays: mean energies, log *ft* values
- Electron captures: log *ft* values, (K, L, M+) capture probabilities, (P_{L_2}/P_{L_1}, P_{L_3}/P_{L_1}, $P_\varepsilon/P_{\beta^+}$ and P_K/P_{β^+}) probability ratios
- Report file, updated ENSDF file

Code

- 3 036 lines in total
- One data file, 98 lines

Beta decay modelling

Theoretical model is very simple:

- Analytical Fermi function (point nucleus)
- Analytical wave functions for electrons, only at nuclear surface
- Power series approximation for low-energy beta minus particles
- Analytical correction for finite nuclear size effect
- Rose's screening (1936!) with Thomas-Fermi potential, for both beta minus and beta plus decays
- Treatment of allowed, first forbidden unique and second forbidden unique transitions

Electron capture modelling

Theoretical model relies on atomic wave function parameters:

- Relativistic Hartree-Fock-Slater self-consistent approach
- Realistic Fermi-Dirac distribution for the nuclear charge density
- Neutral atoms, closed shells, no electron correlation
- Overlap and exchange effects for K, L_1, $L_{2,3}$ and M_1 shells
- Tabulated parameters, impossible to consistently improve the modelling
- Arbitrary 1% unc. added to ε/β^+ ratio in addition to unc. propagation from input parameters

BetaShape (v2)

Executables of the BetaShape program for Windows, Linux and OS X are available at
http://www.lnhb.fr/rd-activities/spectrum-processing-software/

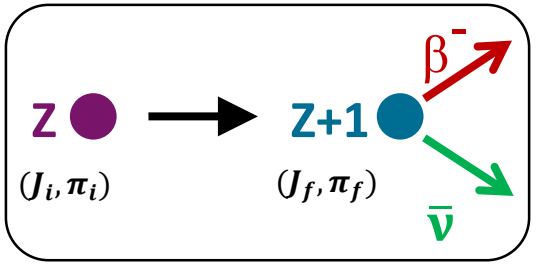
Beta decay modelling

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

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

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

→ Numerical solving of Dirac equation for the leptons

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 (Rose, Bühring)
- Radiative corrections from superallowed decays

Propagation of uncertainties

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

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)

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)

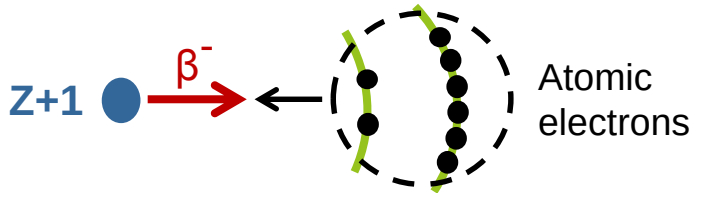
All quantities depend on the normalization of electron wave functions

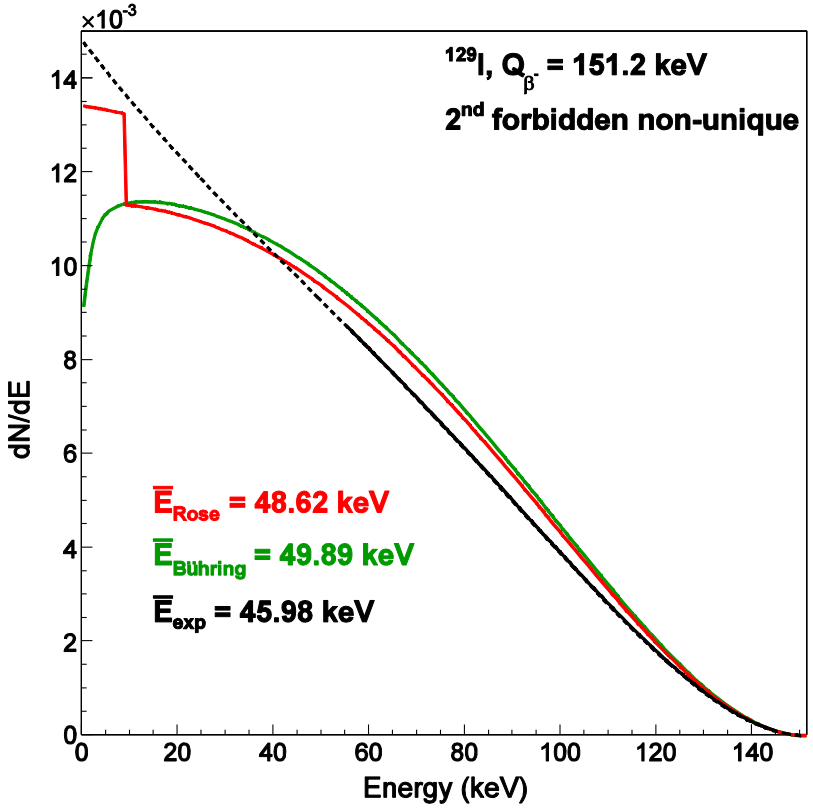
⇒ **Analytical solutions** and **leading order** at the nucleus + **asymptotic** solutions

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

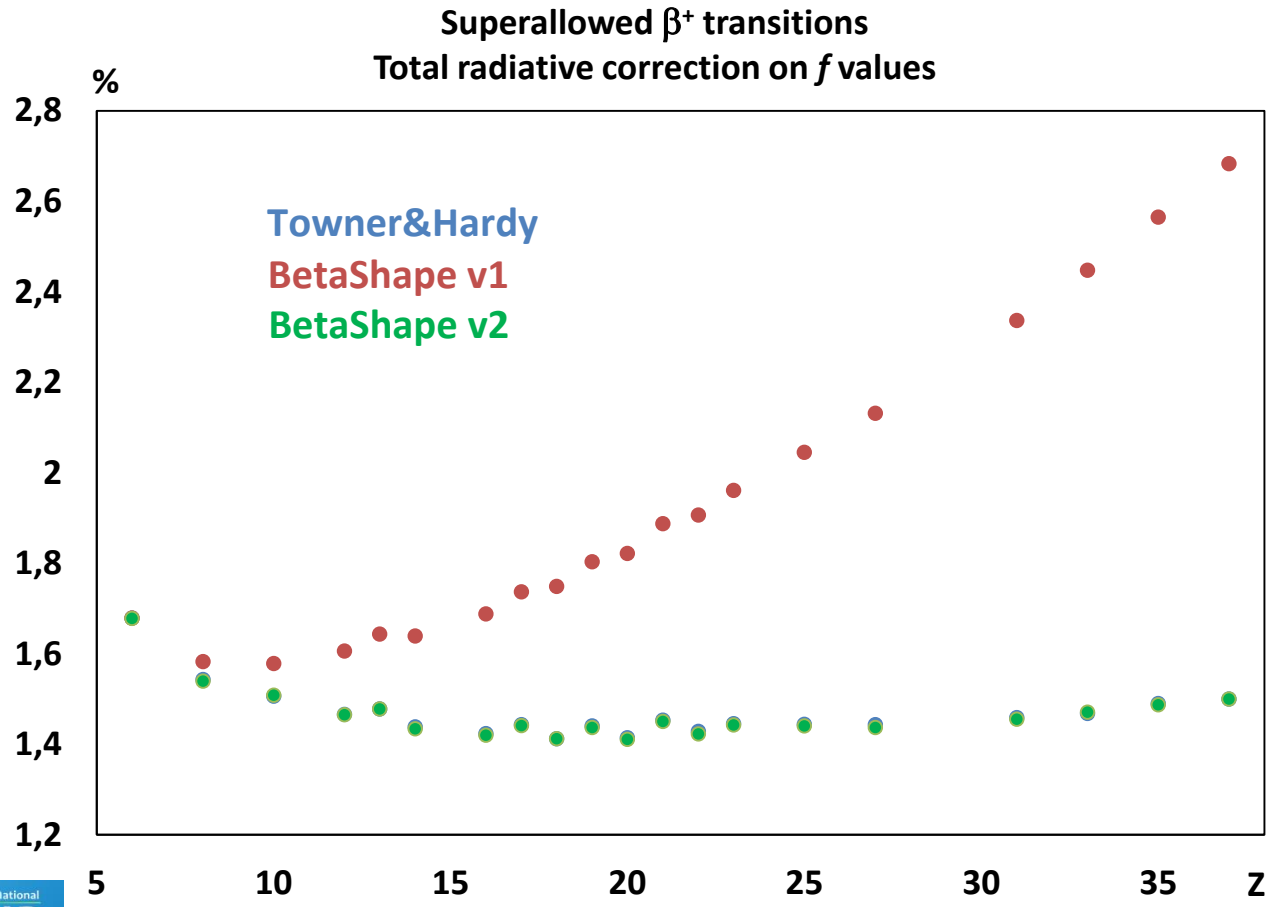
Radiative corrections

Electrons – Old correction

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

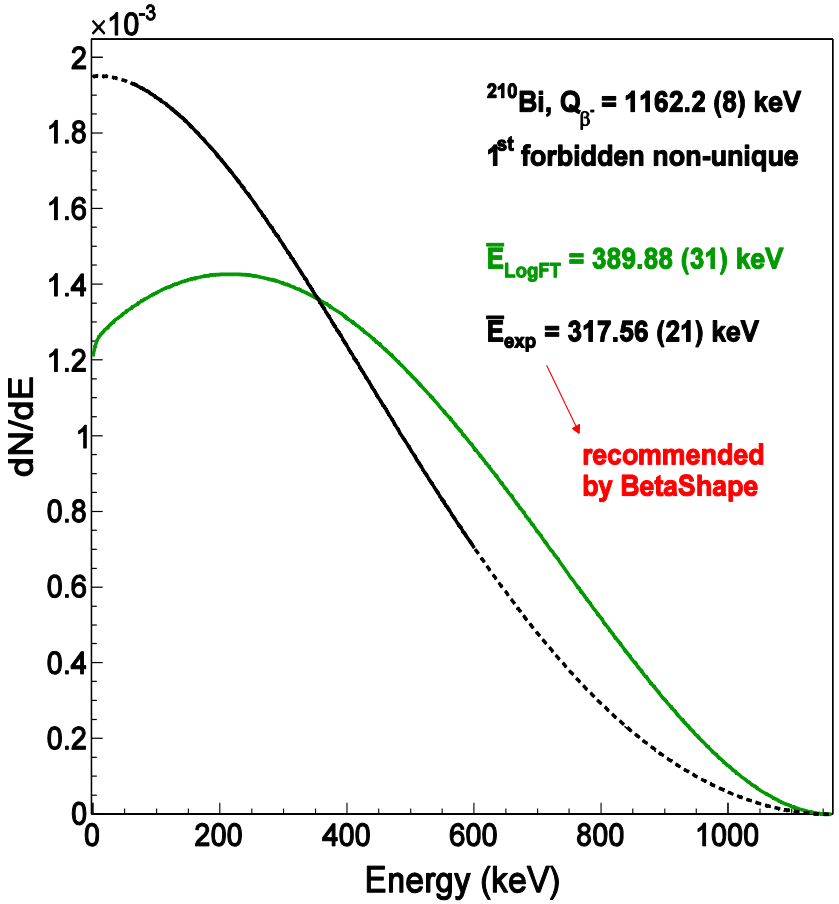
Electrons – New correction

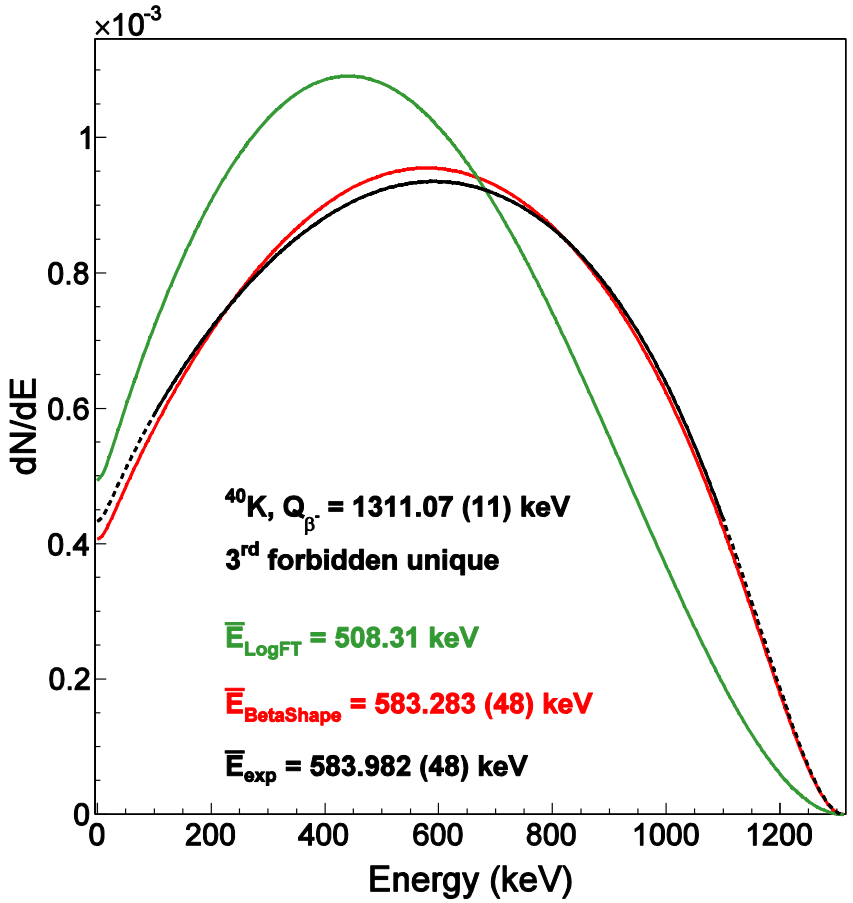
I.S. Towner, J.C. Hardy, PRC 77, 025501 (2008)
A. Czarnecki et al., PRD 70, 093006 (2004)



Nucleus	T&H (%)	New (%)
^{10}C	1,679	1,678
^{14}O	1,543	1,539
^{18}Ne	1,506	1,508
^{22}Mg	1,466	1,465
^{26}Si	1,438	1,434
^{30}S	1,423	1,420
^{34}Ar	1,412	1,412
^{38}Ca	1,414	1,410
^{42}Ti	1,428	1,423
^{26m}Al	1,478	1,478
^{34}Cl	1,443	1,441
^{38m}K	1,440	1,437
^{42}Sc	1,453	1,450
^{46}V	1,445	1,442
^{50}Mn	1,444	1,440
^{54}Co	1,443	1,437
^{62}Ga	1,459	1,455
^{66}As	1,468	1,471
^{70}Br	1,49	1,487
^{74}Rb	1,50	1,499

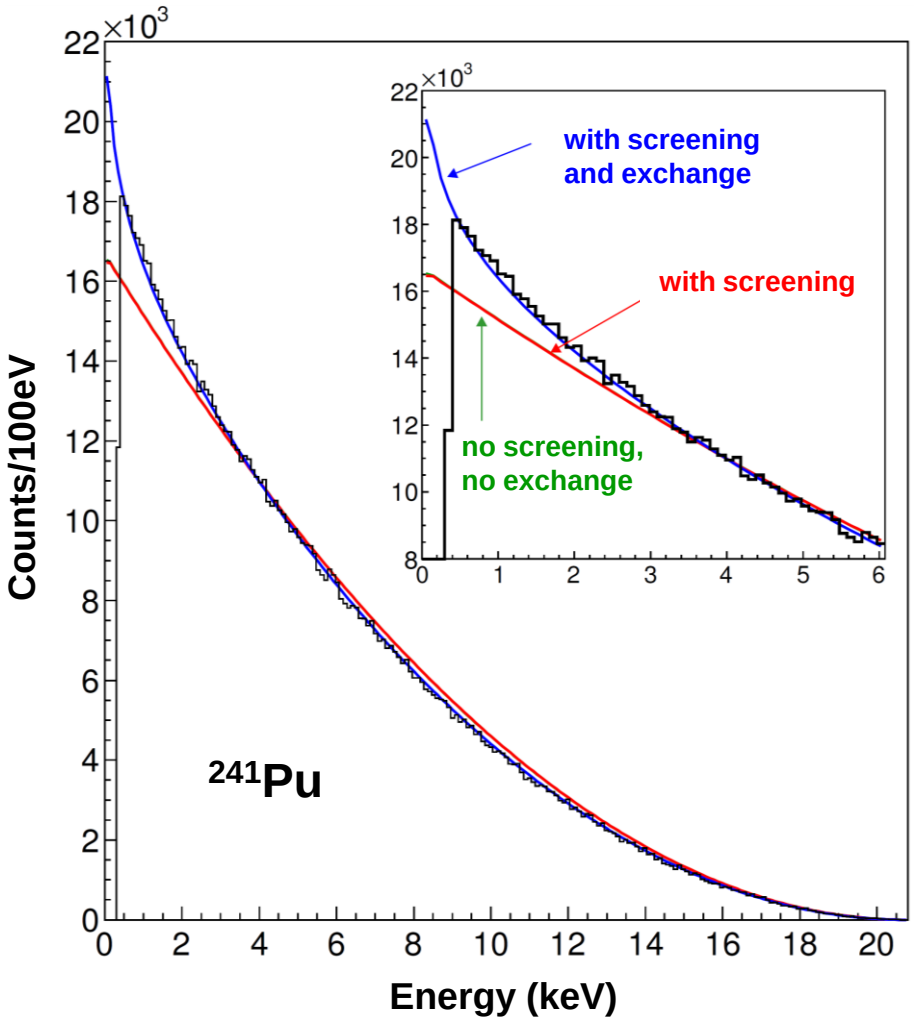
Examples of improved calculations





These two transitions are calculated as allowed by the LogFT program, which does not provide any beta spectrum.

^{241}Pu



LogFT
log ft = 5.8

BetaShape v1
log ft = 5.925 (8) from calculation

log ft = 3.284 (8) from exp. shape factor:

$$1 - 1.9582W + 0.96078W^2$$

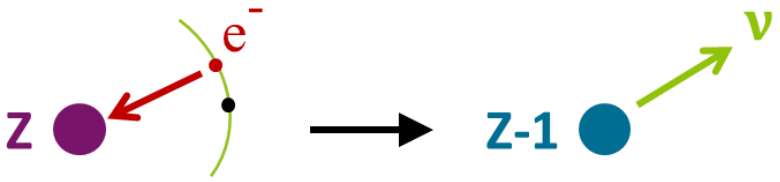
from 2011KO21. Recommended result.

Balraj Singh: **IT'S NOT POSSIBLE!**

Full calculation with precise atomic effects (not yet included in BetaShape v2)
log ft = 5.969 (8)

→ Problem comes from exp. shape factor, because normalization was free in the extraction. A constant factor of 420 takes up a part of the strength of nuclear matrix elements.

Electron capture modelling



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
- $P_{m\kappa}$: shaking effects

X. Mougeot, Appl. Radiat. Isot. 134, 225 (2018)

Relativistic atomic wave functions

Dirac equation is solved numerically

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

- 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)

Reference orbital energies

S. Kotochigova *et al.*, Phys. Rev. A 55, 191 (1997)

Iterative procedure to reach atomic energies from relativistic DFT approach with electron correlations.

→ More precise, realistic orbital energies from H to U. Extrapolation from U to $Z = 120$.

→ Fixed mass number A for each proton number Z along the stability line. Tabulation of parameters for each wave function from $Z = 1$ to $Z = 120$.

Corrections on capture probabilities

B_{κ_x}

J.N. Bahcall, Phys. Rev. 129, 2683 (1963)

E. Vatai, Nucl. Phys. A 156, 541 (1970)

Overlap: spectator electrons contribute to the total decay rate.

Exchange: indistinguishability of the electrons.

→ Single correction, either from Bahcall or Vatai. Generalized to every subshell. From theory point of view, Vatai's should be better.

Hole: the sudden disappearance of the captured electron modifies the atomic wave functions.

→ Corrected for by means of first order perturbation theory.

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

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

Shake-up: excitation to an unoccupied bound state.

Shake-off: ionization to a continuum state.

→ Single correction, following Crasemann et al. Probability to create a secondary vacancy for every subshell.

Radiative corrections: fully relativistic theory with Coulomb effects exists, but only for allowed transitions and K, L captures.

→ For consistency of the whole modelling, Coulomb-free theory is considered for *n*s orbitals, and a mean value for others.

Overlap and exchange corrections

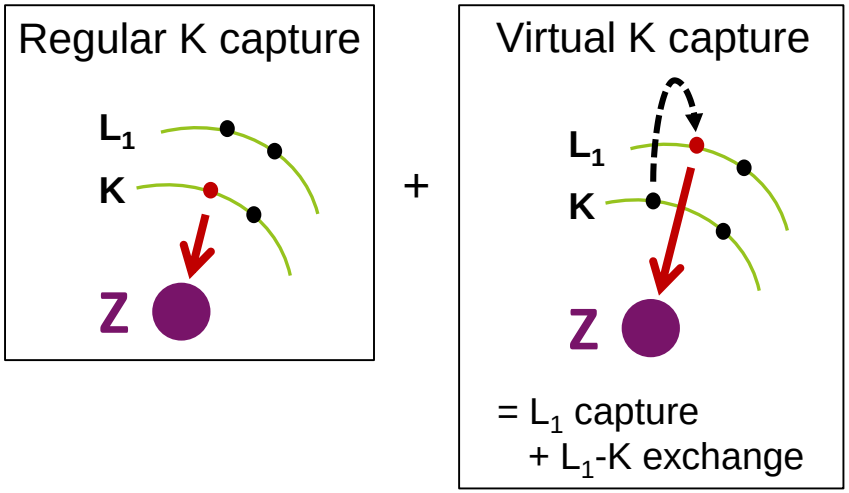
Overlap effect

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

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

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

Radiative correction

For transition energies $< 2m_e$, internal Bremsstrahlung process can occur.

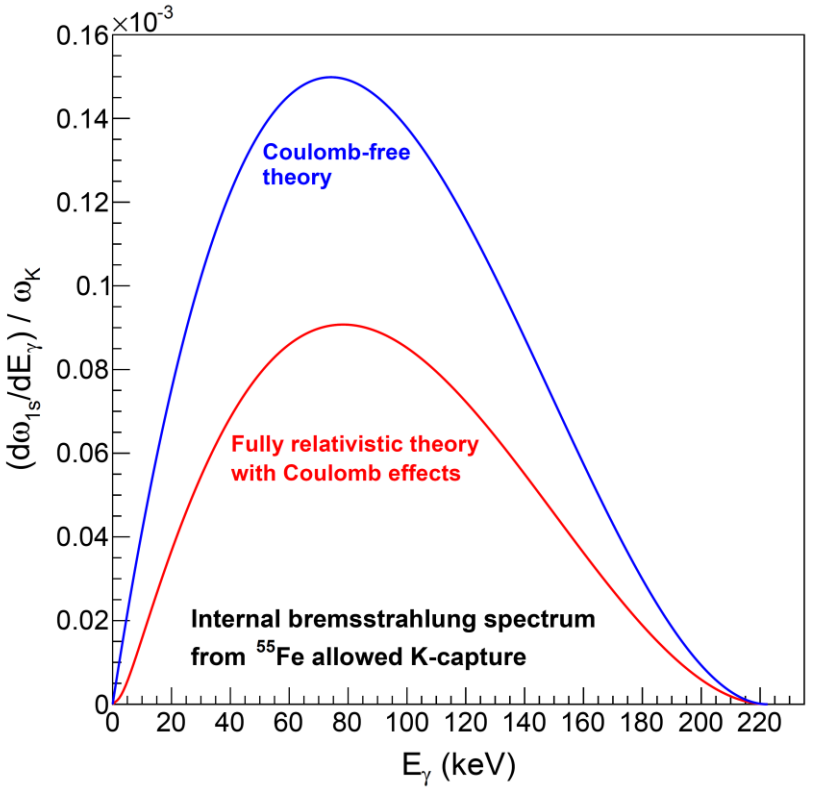
→ Neutrino energy shared with the emitted photon.

→ Total emission probability of ~ 10^{-5} but probability ratios are considered.

For transition energies $> 2m_e$, radiative corrections for β^+ transition must also be taken into account.

→ Correction of ~ 1%.

- Coulomb-free theory is very simple but not very accurate.
- Fully relativistic theory with Coulomb effects exists for allowed transitions and K, L captures.

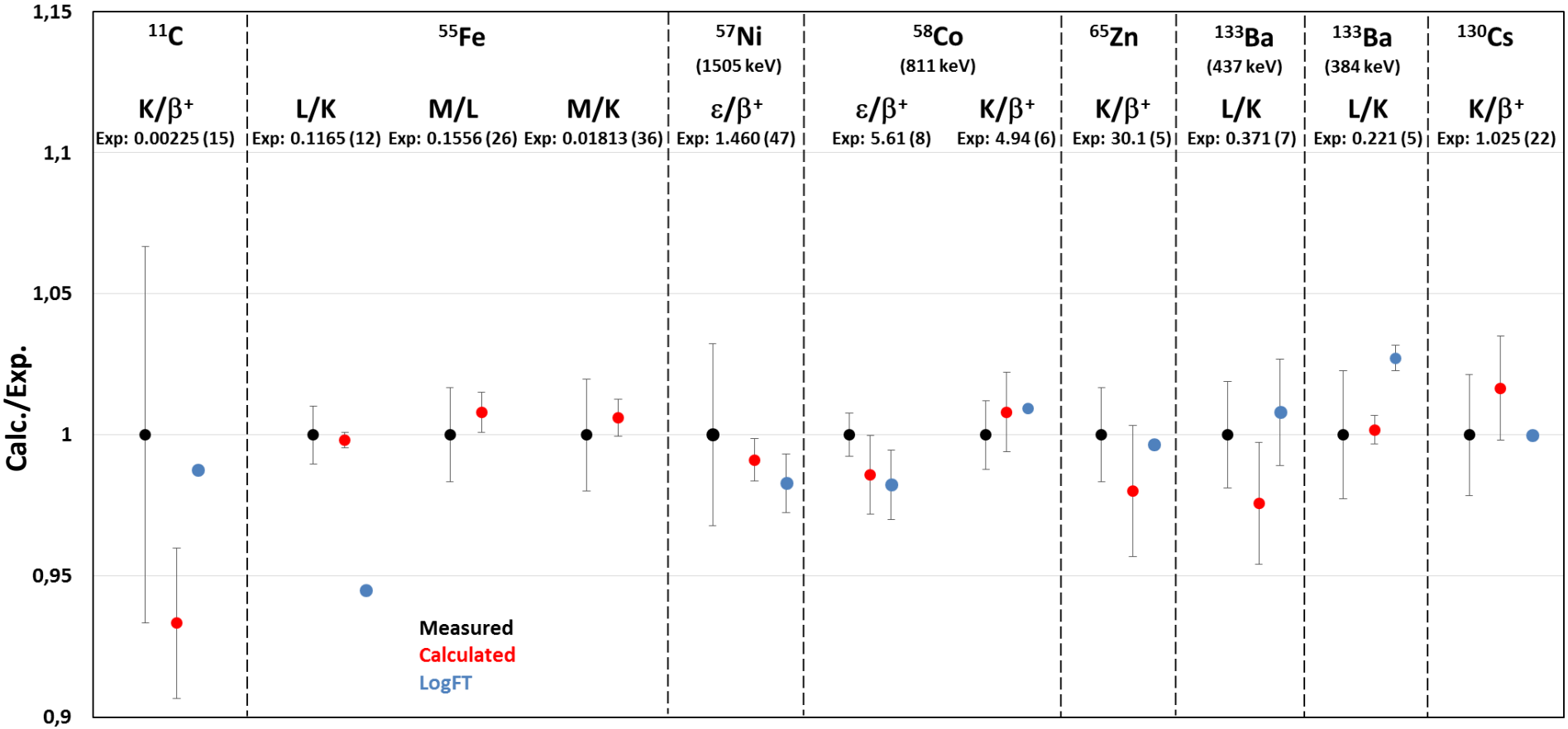


For consistency of the whole modelling, Coulomb-free theory is considered.

Allowed transitions

X. Mougeot, Appl. Radiat. Isot. 154, 108884 (2019)

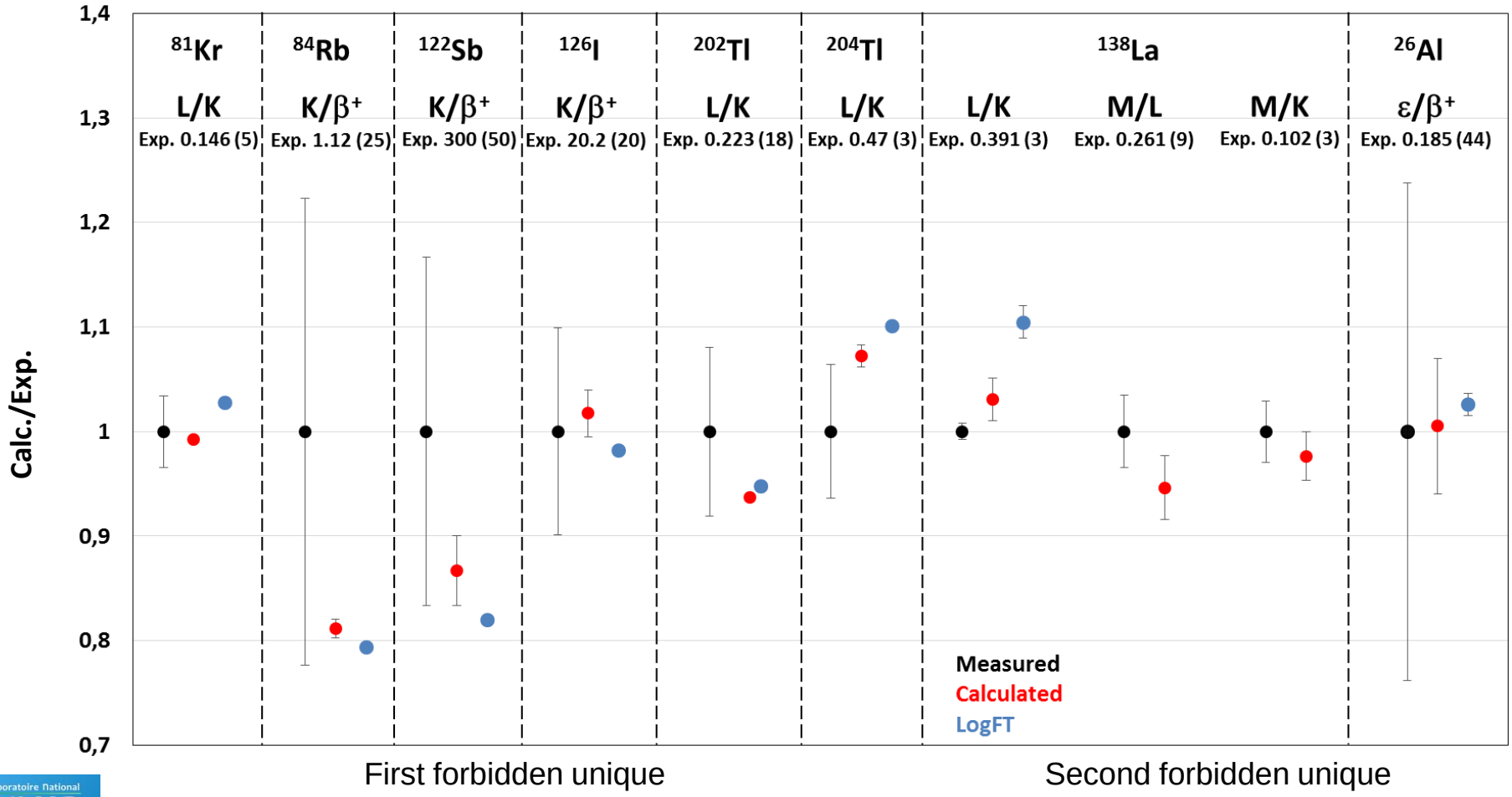
- ✓ Vatai's approach leads to more accurate results than Bahcall's approach, as expected from a theory point of view.
- ✓ All predictions are consistent with selected measurements.



Forbidden unique transitions

X. Mougeot, Appl. Radiat. Isot. 154, 108884 (2019)

- ✓ Vatai's approach leads to more accurate results than Bahcall's approach, as expected from a theory point of view.
- ✓ All predictions are consistent with selected measurements.



Forbidden unique transitions

X. Mougeot, Appl. Radiat. Isot. 154, 108884 (2019)

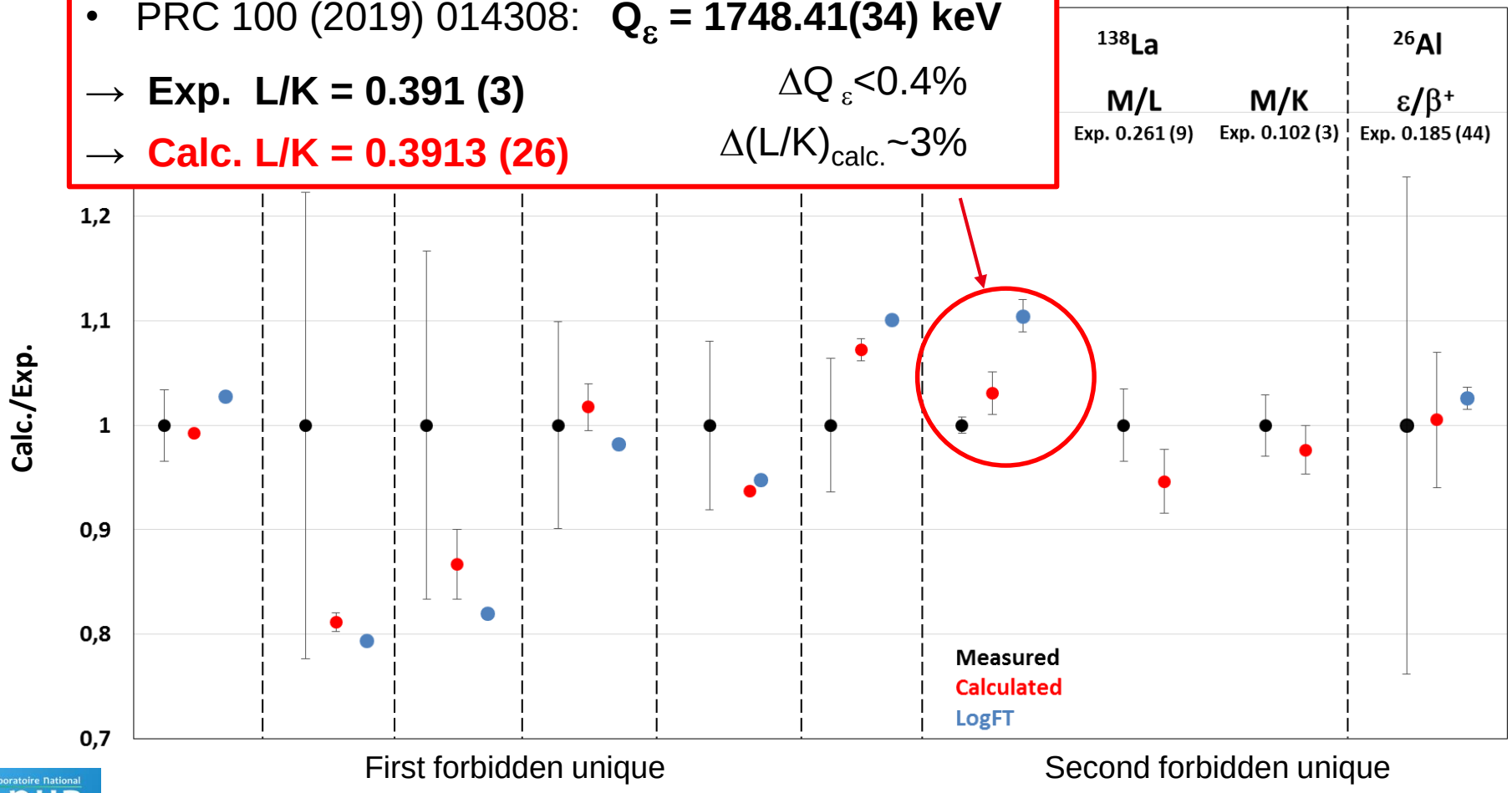
New high-precision measurement of ^{138}La Q-values

- AME2016: Q_ε = 1742(3) keV
- PRC 100 (2019) 014308: **Q_ε = 1748.41(34) keV**

→ **Exp. L/K = 0.391 (3)** ΔQ_ε<0.4%

→ **Calc. L/K = 0.3913 (26)** $\Delta(L/K)_{calc.}$~3%

predictions are consistent measurements.



General features

Code

- 7 programs, 9 C++ classes, 26 955 lines in total
- 6 external files, 6 300 lines in total

Beta decays

- Single and total β^+/β^- spectra
- Corresponding $\nu_e/\bar{\nu}_e$ spectra
- Mean energies, log *ft* values
- Experimental shape factor, if any in the database (131 transitions present)

Electron captures

- Capture probabilities and their ratios, with uncertainties, for all subshells
- Account of energetically hindered captures (e.g. K capture in ^{205}Pb)
- Splitting of the branch between capture and beta plus transitions
- Log *ft* values

Main changes v1 → v2

- Bugs fixing and code structure.
- Uncertainty treatment: if no unc. in input file, null unc. considered (instead of 60% from flat distribution).
- All physical constants from CODATA 2018, names of elements up to Z=118 according to IUPAC recommendations.
- Q-values can be updated on-the-fly with AME2016 evaluation.
- Radiative corrections from superallowed beta decay studies.
- Experimental shape factors: ^{14}O, ^{36}Cl, ^{138}La. Continuation record in ENSDF file.
- Fixing a constant energy step for the calculated spectra now possible.
- Calculation of electron capture transitions, information for each subshell given. ENSDF file is updated.
- Splitting of the branch between capture and beta plus can be updated or fixed from input data.

Single transition file: beta decay

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: electron capture

```
----------------------------------------
Ratios of relative capture probabilities

PL1/PK =  0.1073 (7)
PL2/PK =  2.472E-4 (16)
PL3/PK =  6.973E-4 (31)
PM1/PK =  0.01419 (18)
PM2/PK =  2.562E-5 (15)
PM3/PK =  5.72E-5 (7)

L/K =  0.1083 (7)
M/K =  0.01427 (18)


------------------------------
Relative capture probabilities

PK  =  0.8908 (7)
PL1 =  0.0956 (5)
PL2 =  2.202E-4 (16)
PL3 =  6.211E-4 (32)
PM1 =  0.01264 (15)
PM2 =  2.282E-5 (12)
PM3 =  5.09E-5 (6)

K =  0.8908 (7)
L =  0.0965 (5)
M =  0.01271 (15)
```

```
---------------------------
Capture-to-positron ratios

K/b+ =  188.1 (26)
L1/b+ =  20.19 (15)
L2/b+ =  0.0465 (9)
L3/b+ =  0.1311 (24)
M1/b+ =  2.669 (8)
M2/b+ =  0.004818 (38)
M3/b+ =  0.010749 (37)

K/b+ =  188.1 (26)
L/b+ =  20.37 (15)
M/b+ =  2.684 (8)

EC/b+ =  211.1 (28)
```

```
---------------------
Capture probabilities

PK  =  0.89 (44)
PL1  =  0.095 (47)
PL2  =  2.2E-4 (11)
PL3  =  6.2E-4 (31)
PM1  =  0.013 (6)
PM2  =  2.3E-5 (11)
PM3  =  5.1E-5 (25)

K =  0.89 (44)
L =  0.096 (48)
M =  0.013 (6)
```

Detailed information for subshells
Combined for shells

```
----------------------------------------
Input log ft value (ec & beta +): 21.35

Log ft value (ec)     =  21.33 (22)
with log f            =  2.033 (5)
and log partial T1/2 =  19.30 (22)
```

```
Splitting of the branch between capture and beta plus decays

Input data: Iec tot. =   0.20 (10) %   Iec =   0.20 (10) %   Ib+ =   10.0E-4 (12) %
Iec       =   0.20 (10) %
Ib+       =   9.5E-4 (48) %
```

Report file

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

130CS  P 0.0         1+                29.21 M   4              2979      8     - PARENT
130XE  N 0.039     4  1.0      0.984     1.0163                                - NORMALIZATION
130XE PN                                                                3   - PRODUCTION NORMALIZATION
130XE  L 0.0         0+                                                      - LEVEL

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

From calculation
K =  0.4706 (30) | L =  0.06182 (39) | M =  0.01340 (10) | N =  0.003458 (47) | O =  5.73E-4 (9)
K/b+ =  1.045 (19) | L/b+ =  0.1373 (24) | M/b+ =  0.02977 (40) | N/b+ =  0.00768 (15) | O/b+ =  0.001273 (29)

Branch splitting:  Iec 52.0 (5) %  and  Ib+ 42.5 (5) %
EC component of log ft 5.096 (6)

*    log ft
130XE  E              43.0  5   51.5  5   5.073  6             94.5      6     - OLD CARD
130XE  E            42.5     552.0     55.096    6             94.5       7    - NEW CARD

*    Probabilities
130XES E EAV=879 4 $CK=0.466 3 $CL=0.0623 4 $CM+=0.01692 10                    - OLD CARD
130XES E EAV= $CK=0.4706 30$CL=0.06182 39$CM+=0.01743 11                       - NEW CARD

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

Additional beta continuation record

```
40K    P 0.0          4-                    1.2504E9 Y30              1311.07    11
40CA   N 1.12E0       1.12E0     0.8925      1.12E0
40CA   L 0            0+                   STABLE
40CA   B 1311.07    1189.25    17            20.5944 13                          3U
40CAS  B EAV=583.982 48
40CA2  B C1=6.3 $C2=6.25 $C3=0.95 $C4=1.05 (1965LE15)
40CA CB $C(W) = C4*q^6 + C1*q^4*p^2 + C2*q^2*p^4 + C3*p^6
```

Parameters (with uncertainties, if any)

Comment for the correct use

Experimental shape factor is given as continuation record.

Application to radionuclide metrology

Primary activity measurements

Counting efficiency in Liquid Scintillation Counting directly depends on beta spectrum

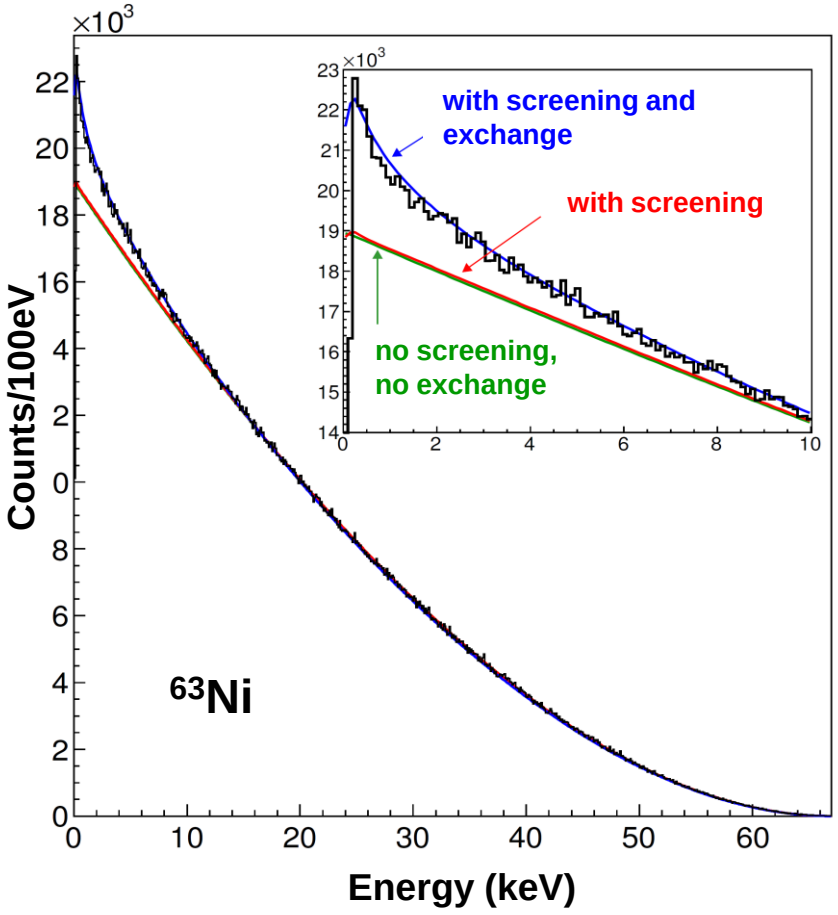
- **System with 2 PMTs**: CIEMAT/NIST (tracer)

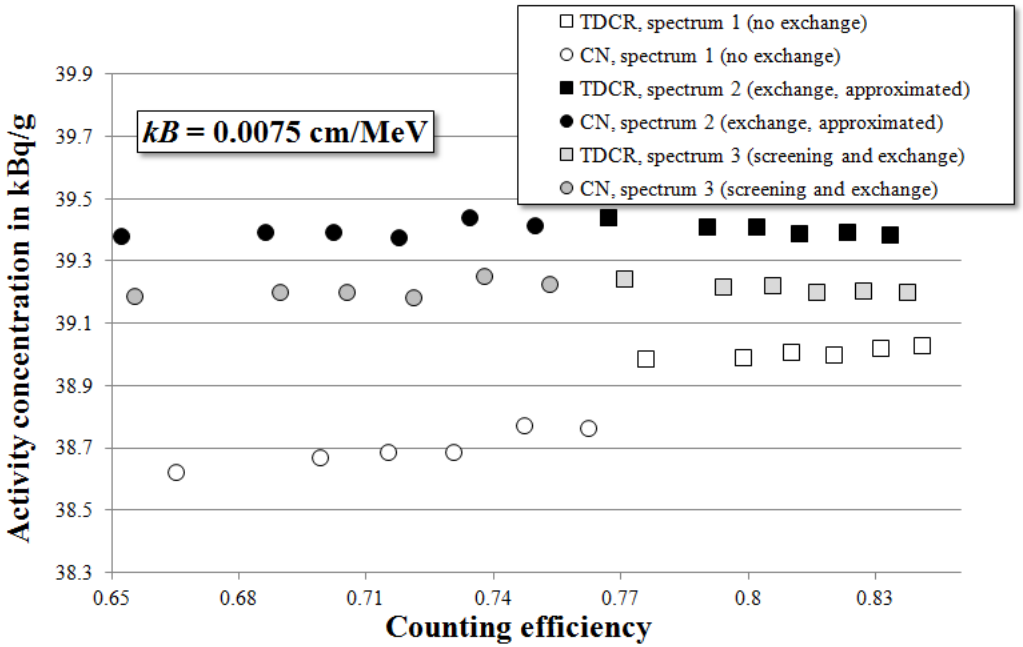
$$\varepsilon = \int_0^{E_{max}} S(E)(1-e^{-\eta})^2 dE \qquad \eta = \frac{\nu}{n}\int_0^E \frac{AdE}{1+kB\frac{dE}{dx}}$$

- **System with 3 PMTs**: TDCR (Triple to Double Coincidence Ratio)

$$TDCR = \frac{R_T}{R_D} = \frac{\int_0^{E_{max}} S(E)(1-e^{-\eta})^3 dE}{\int_0^{E_{max}} S(E)((3(1-e^{-\eta})^2 - 2(1-e^{-\eta})^3))dE}$$

^{63}Ni

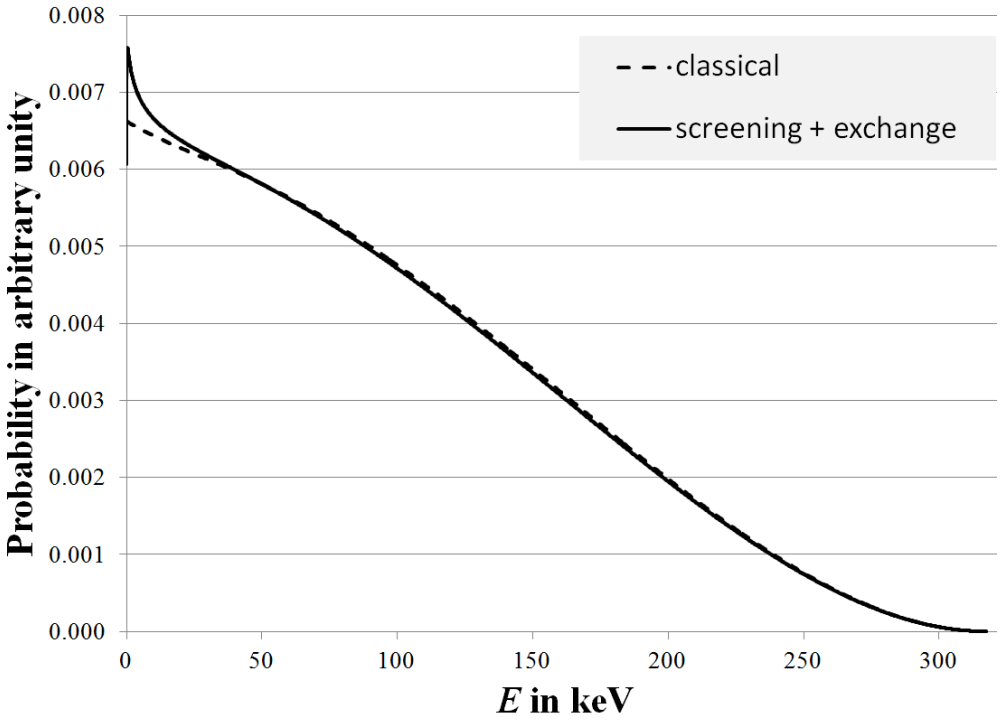




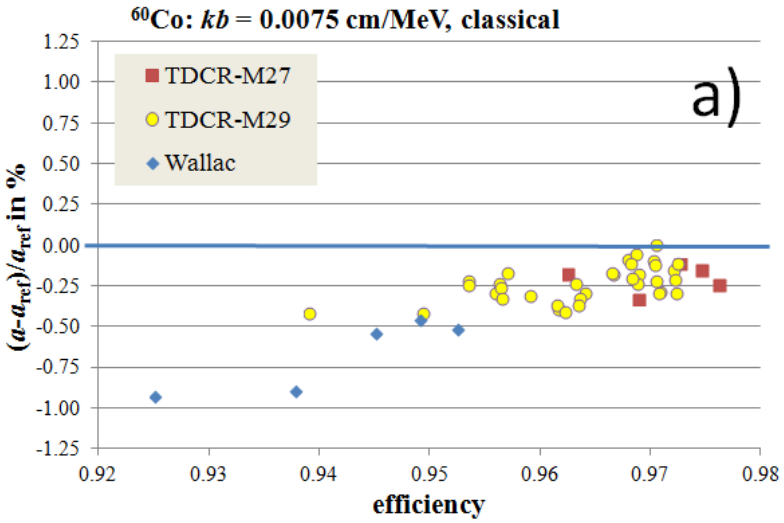
K. Kossert, X. Mougeot, Appl. Radiat. Isot. 101, 40 (2015)

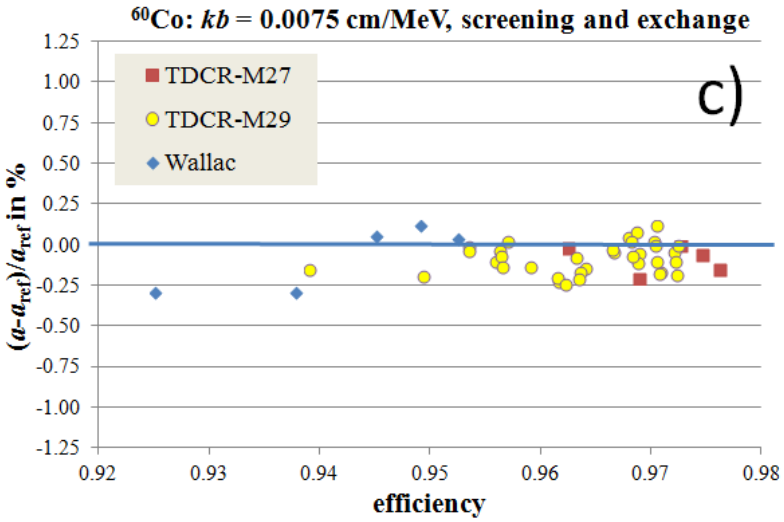
^{60}Co

Reference activity with 4πβ-γ coinc. counting



K. Kossert et al., Appl. Radiat. Isot. 134, 212 (2018)





Ongoing reanalysis

Preliminary results for ^{14}C, $^{32}Si/^{32}P$, ^{59}Fe and ^{99}Tc

→ Identical conclusion

Capture probabilities for ^{55}Fe

→ Strong impact on primary activity determination

November 7th-8th, 2019

→ Ongoing discussion at BIPM to adopt BetaShape results as the unique reference for future international intercomparisons

Ongoing developments and perspectives

Atomic effects

Next developments in BetaShape

- Inclusion of precise screening effect using a hybrid method.
- Inclusion of precise exchange effect using tabulated exchange factors for all Z.

Ongoing work

- New high-precision measurements to analyze: ^{14}C, ^{99}Tc, ^{151}Sm.
- Extension of theoretical formalism to forbidden beta transitions.
- High-precision atomic wave functions: relativistic DFT code in development within the European project MetroMMC with IPCMS, Strasbourg, France.

Nuclear structure

Calculation of theoretical shape factor

- For both beta decay and electron capture.
- For transition of every nature: allowed, forbidden unique and non-unique.
- Impulse approximation, spherical symmetry, single particle matrix elements.
- Very simple nuclear modelling: harmonic oscillators.

Future

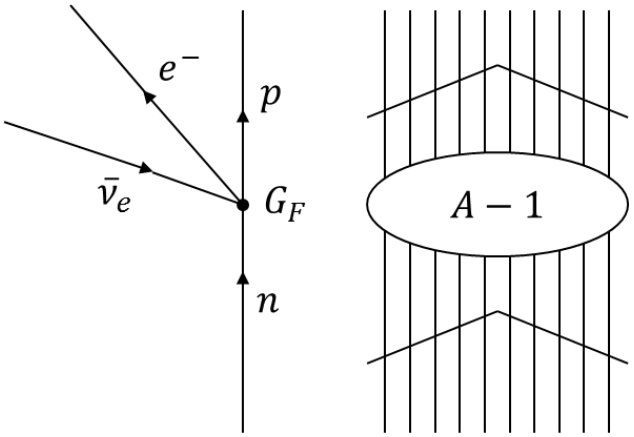
- Nuclear component: nuclear deformation, pairing correlations and configuration mixing using already existing codes. Looking for collaborations.
- Uncertainties: estimate of theoretical components and propagation using a Monte Carlo method.

Theoretical shape factor

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

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

Multipole expansion of hadron and lepton currents. Calculation of shape factors, half-lives, branching ratios, log *ft* values.



Fermi theory

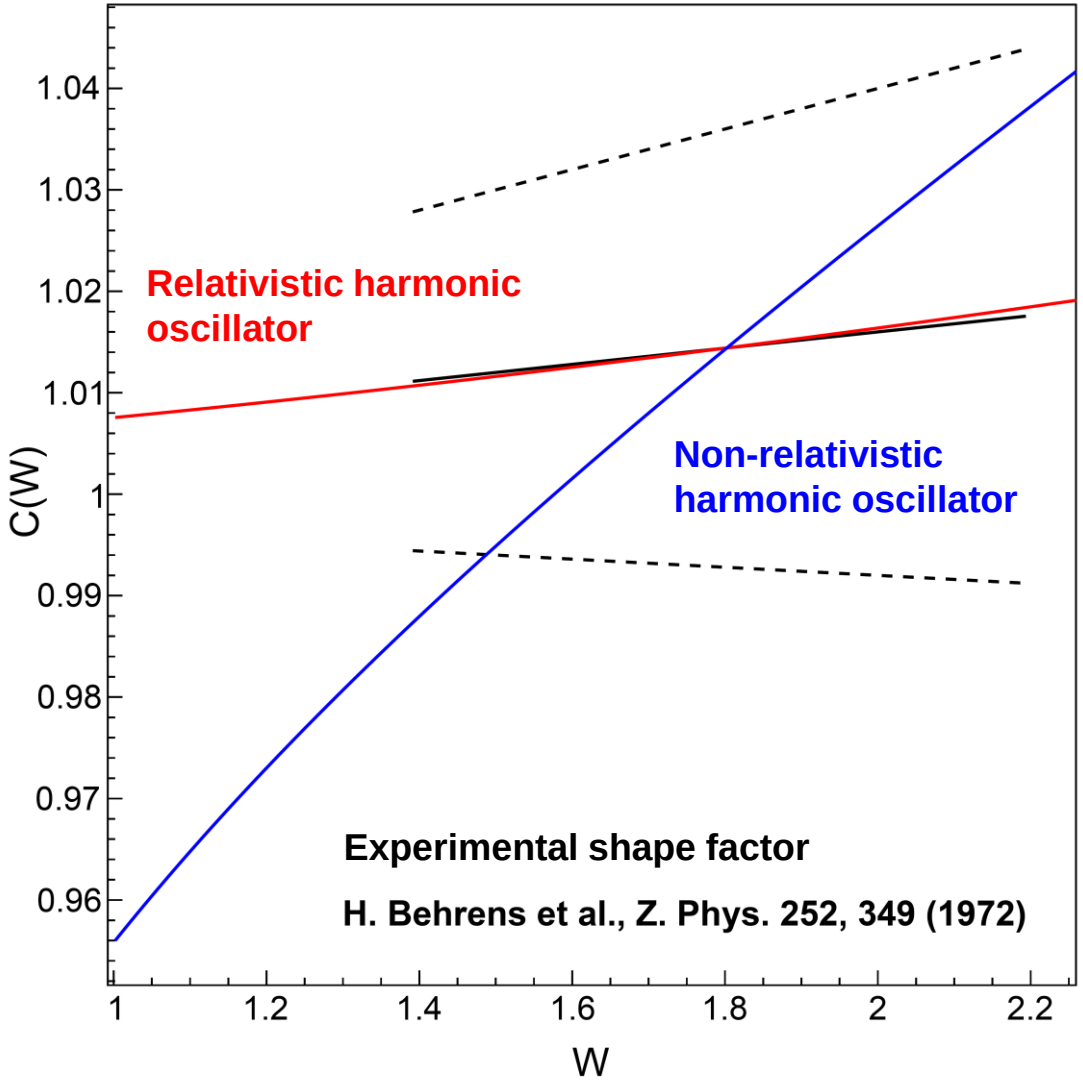
- Vertex of the weak interaction is assumed to be pointlike. No propagation of $W^\pm$ boson.
- Effective coupling constant G_F.

Impulse approximation

- The nucleon is assumed to feel only the weak interaction.
- Other nucleons are spectators.

Spherical symmetry. Single particle matrix elements. Multipole moments are selected according to the required precision. Two simple nuclear models: **non-relativistic and relativistic harmonic oscillators**.

^{209}Pb: first forbidden non-unique



$$^{209}_{82}\mathrm{Pb}_{127} \rightarrow {}^{209}_{83}\mathrm{Bi}_{126}$$

$$9/2^{+} \rightarrow 9/2^{-}$$

$$\left|\nu, 2g_{9/2}\right\rangle \rightarrow \left|\pi, 1h_{9/2}\right\rangle$$

E_0 = 644.0(11) keV

Evaluated from exp.
$t_{1/2}$ = 3.234(7) h
Non-rel. Harm. Osc.
$t_{1/2}$ = 2.874 h
Rel. Harm. Osc.
$t_{1/2}$ = 252.2 h

Beta decay to and from an even-even ground state

Many particle matrix elements in the $j-j$ coupling scheme are 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.

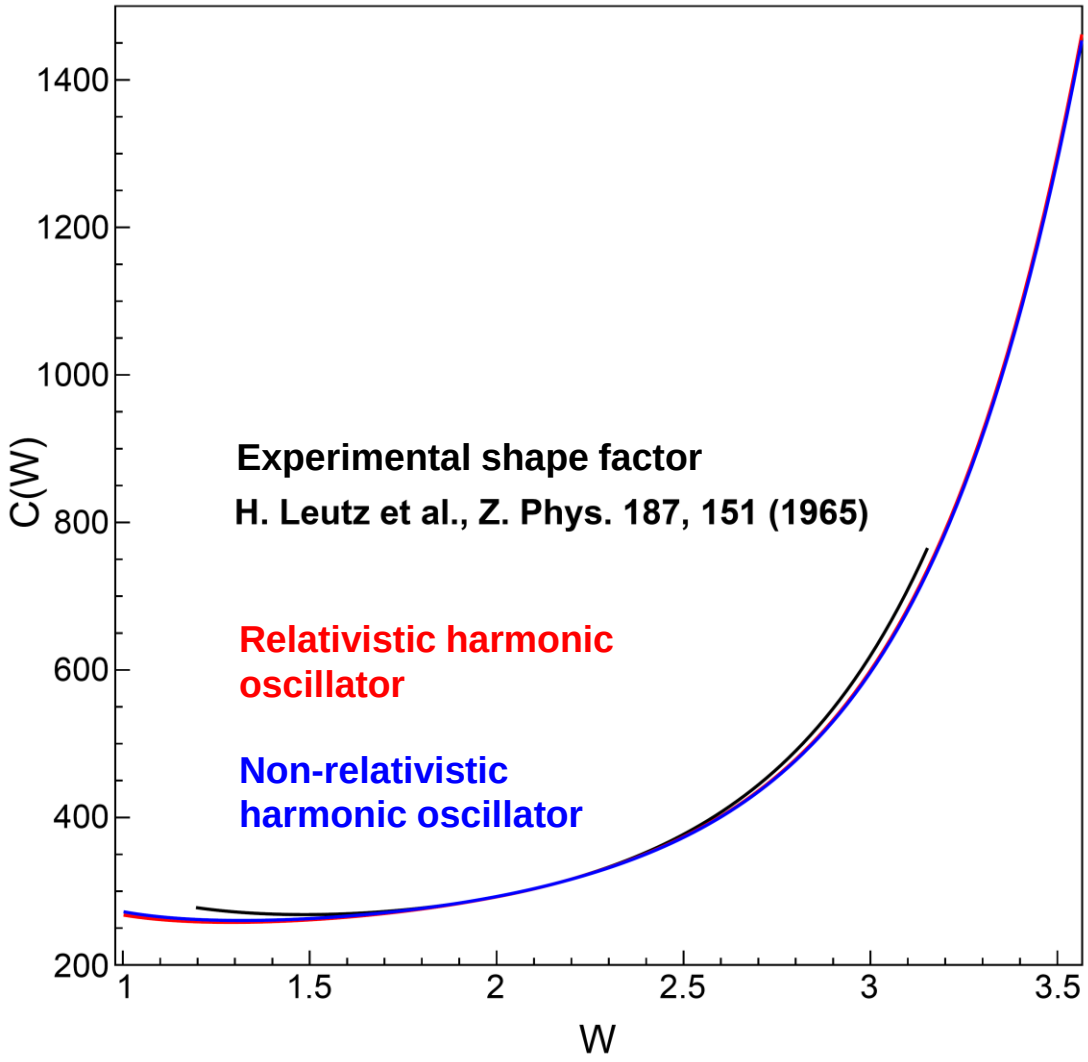
An even-even nucleus can be considered as the vacuum of particle-hole excitations used to describe adjacent nuclei.

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

^{40}K: third forbidden unique



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

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

^{40}Ca: vacuum state for particle-hole state describing ^{40}K

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

E_0 = 1310.89(6) keV

Evaluated from exp.
$t_{1/2}$ = 1.4010(43)·10^9 a
Non-rel. Harm. Osc.
$t_{1/2}$ = 2.748·10^7 a
Rel. Harm. Osc.
$t_{1/2}$ = 1.281·10^8 a

Conclusion

Conclusion

BetaShape v2

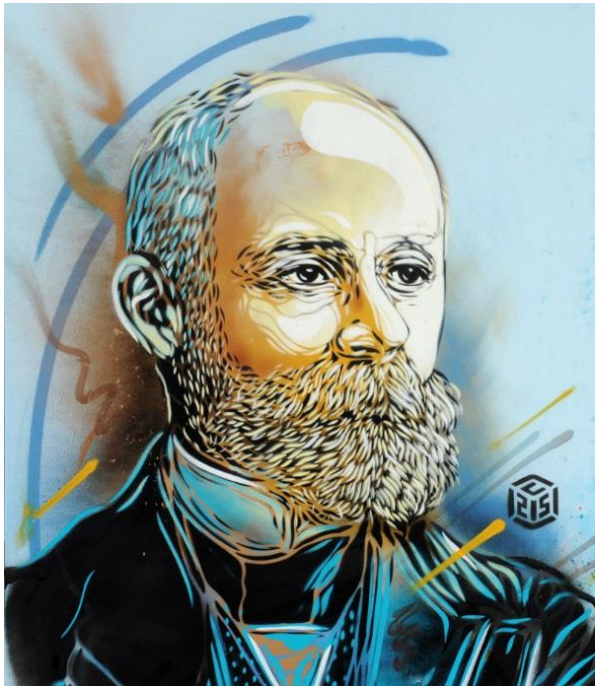
- ✓ Available at http://www.lnhb.fr/rd-activities/spectrum-processing-software/
- ✓ Executables for Windows and Linux, MacOS still pending.
- ✓ Now able to treat beta and capture decays.
- ✓ Provision of improved information needed for nuclear decay data evaluations.
- ✓ Provision of additional detailed information needed for various applications.

→ Feedback on the results, comments, suggestions and bug reports are highly expected

ENSDF evaluations

BetaShape v2 can improve nuclear decay data if used instead of LogFT. This code will be maintained and regularly improved.

→ Would you like to adopt it for the future evaluations?



Thank you for your attention

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