Reliability of information in nuclear databases through comprehensive tests

The example of beta decays

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Outline

- Overview of nuclear decay databases
- Why beta decays?
- Current situation
- The BetaShape code
- Comprehensive test of the ENSDF nuclear structure database
- Focus on well-defined beta transitions

Atomic and nuclear decay data

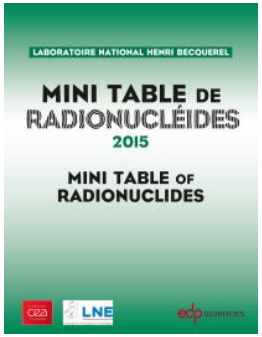
First nuclear data evaluation: M. Curie, H. Geiger, O. Hahn, St. Meyer, E. Rutherford, *et al.*

The radioactive constants as of 1930, Rev. Mod. Phys. 3, 427 (1930)

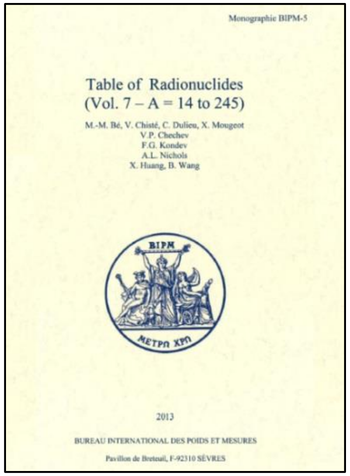
Still of importance. For instance ^{228}Ac (+1 meas. in 1985) and ^{234}Pa (+2 meas. in 1954, 1962)

DDEP – International collaboration
Decay Data Evaluation Project

Data recommended by the BIPM



www.nucleide.org
http://laraweb.free.fr

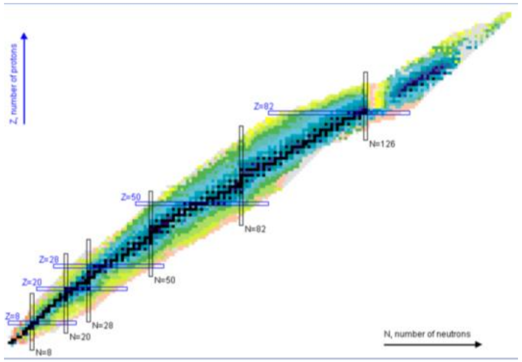


ENSDF – NNDC (IAEA)

Aims for completeness

Mass chain evaluations

Interactive chart of nuclides



Atomic and nuclear decay data

Lot of work for one radionuclide

Radionuclide production, radiochemistry, isotopic separation, impurity quantification, experimental methodology, primary measurements with different techniques, absolute activity and intensity measurements, manpower, depreciation of building and equipment, data evaluation process, etc.

→ ~ 200 k€ for one good published measurement of the complete decay scheme

→ At least x5 for a good evaluation, from different laboratories

→ **Low estimate of ~ 1 M€ / radionuclide evaluation** (short half-lives, ion beams, etc.)

DDEP – 220 radionuclides → 220 M€

ENSDF – ~ 3500 radionuclides → 3.5 B€

Evaluations available for free!

No evaluation → No recommended value

→ *Each physicist would have to manage alone the data published in the literature*

Pb #1: feeding the databases with new and updated evaluations

Pb #2: testing the data and their consistency in a comprehensive manner

→ the case of beta decays

Impact of beta decays

Users' request: **Improve the accuracy of the nuclear data related to beta and neutrino emission properties**

Scientific research

New detectors ($BrLa_3$), monitoring and safeguards applications, fundamental physics (weak magnetism, astrophysics, sterile neutrino, etc.)

Ionizing radiation metrology

Activity measurements

Better knowledge of the beta spectra → better uncertainties

Medical uses

Internal dosimetry, internal radiotherapy, etc.

Nuclear fuel cycle

Residual power of nuclear reactors, nuclear waste, fusion, etc.

Current situation in nuclear databases

If no experimental data → Theoretical estimates

LogFT program 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

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

The BetaShape code

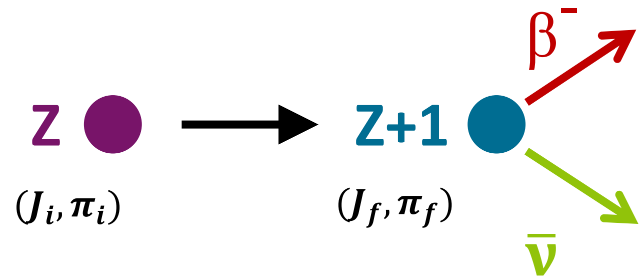
- Fast calculations → no fine atomic effects → For exchange effect, see X. Mougeot, C. Bisch, Phys. Rev. A 90, 012501 (2014)
- Ease-of-use for both evaluators and users
- Reads and writes ENSDF files

Physics modelling in BetaShape

Electroweak interaction: $M_{W+,W-,Z0} \sim 80$ GeV and $E_{\max}(\beta) \lesssim 50$ MeV

→ **Fermi theory**: 4 particles interacting at the same vertex

Beta spectrum $$\frac{dN}{dW} \propto \underbrace{\boxed{p\,W\,q^2}}_{\text{Phase space}}\ \overbrace{\boxed{F_0 L_0}}^{\text{Fermi function}}\ \underbrace{\boxed{C(W)}}_{\text{Shape factor}}$$



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

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

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

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.

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

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

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

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

Electron wave function
→ spherical symmetry

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)

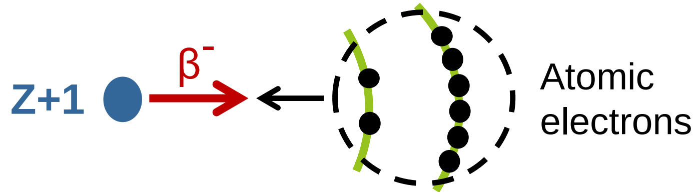
All quantities depend on the normalization of the electron wave functions

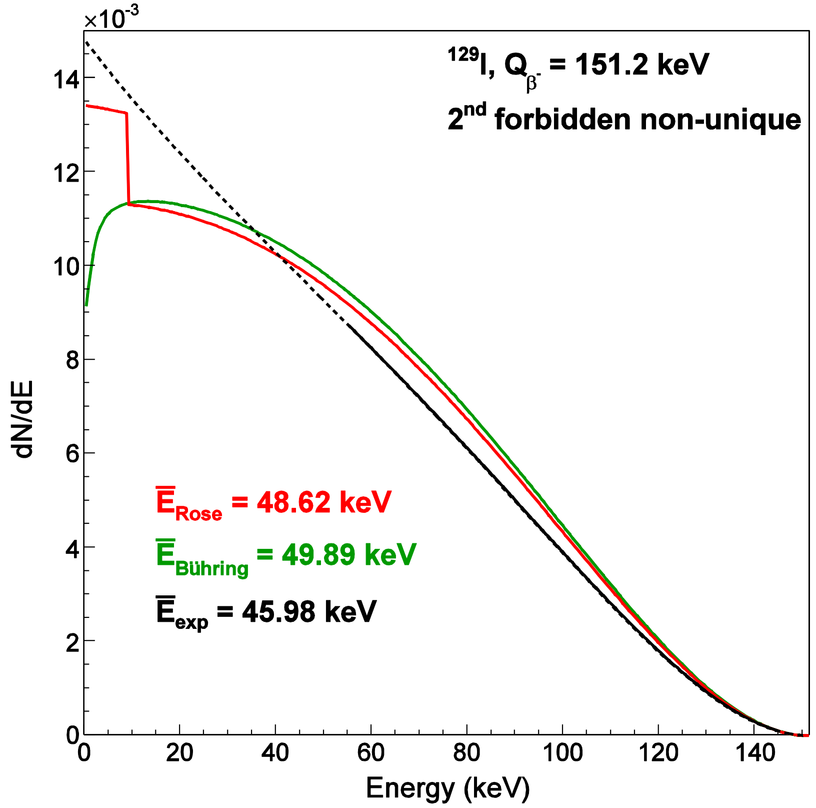
⇒ **Analytical solutions** and **leading order** at the nucleus + **asymptotic** solutions

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 refined** + **no breakdown** at low energy
- Rose's correction can be deduced

Radiative corrections

Electrons $\rightarrow \quad \times[1+\delta_R(W,Z)]$

$$\delta_R(W,Z) = \delta_1(W) + \delta_2(Z) + \delta_3(Z) + \delta_4(Z)$$

$$\delta_1(W) = \frac{\alpha}{2\pi} g(W,q)$$

$$\begin{aligned} g(W,q) = {} & 3\ln\left(\frac{m_p}{m_e}\right) - \frac{3}{4} + \frac{4}{\beta} L\left(\frac{2\beta}{1+\beta}\right) \\ & + 4\left(\frac{\tanh^{-1}\beta}{\beta} - 1\right)\left[\frac{q}{3W} - \frac{3}{2} + \ln(2q)\right] \\ & + \frac{\tanh^{-1}\beta}{\beta}\left[(1+\beta^2)\frac{q^2}{3W^2} - 4\tanh^{-1}\beta\right] \end{aligned}$$

$$\delta_2(Z) = 1.1\,|Z|\alpha^2 \frac{m_p}{m_e}$$

$$\delta_3(Z) = \frac{Z^2\alpha^3}{\pi}\left(3\ln 2 - \frac{3}{2} + \frac{\pi^2}{3}\right)\frac{m_p}{m_e}$$

$$\delta_4(Z) = \frac{|Z|\alpha^3}{2\pi}\frac{m_p}{m_e}$$

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

Virtual photons, internal bremsstrahlung.

Only **outer** radiative corrections influence the energy dependence of the β spectrum.

Analytical solutions from QED for **allowed** transitions.

Neutrinos $\rightarrow \quad \times[1+\delta_\nu(q)]$

$$\delta_\nu(q) = \frac{\alpha}{2\pi} h(W)$$

$$\begin{aligned} h(W) = {} & 3\ln\left(\frac{m_p}{m_e}\right) + \frac{23}{4} + \frac{8}{\beta} L\left(\frac{2\beta}{1+\beta}\right) \\ & + 8\left(\frac{\tanh^{-1}\beta}{\beta} - 1\right)\ln(2W\beta) \\ & + 4\frac{\tanh^{-1}\beta}{\beta}\left(\frac{7+3\beta^2}{8} - 2\tanh^{-1}\beta\right) \end{aligned}$$

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

$\beta = p/W$

Spence function $\quad L(x) = \displaystyle\int_0^x \frac{\ln(1-t)}{t}\,\mathrm{d}t$

Calculated quantities in BetaShape

- **Experimental shape factors** (database of 130 elements)
- **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**
  ☑ $f_{\beta^-} = \int_1^{W_0} N(W)\mathrm{d}W$
  ☒ $f_{\varepsilon/\beta^+} = \boldsymbol{f_\varepsilon} + \boldsymbol{f_{\beta^+}}$
  Partial half-life: $t_i = T_{1/2}/I_\beta \quad \longrightarrow \log ft$

provided that $f_{\beta^+} \neq 0$ and $I_{\beta^+} \neq 0$ $\rightarrow \log ft = \log\left(\frac{f_{\beta^+}}{I_{\beta^+}} T_{1/2}\right) + \log\left(\frac{1+f_\varepsilon/f_{\beta^+}}{1+I_\varepsilon/I_{\beta^+}}\right)$

However

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

C_x: lepton dynamics

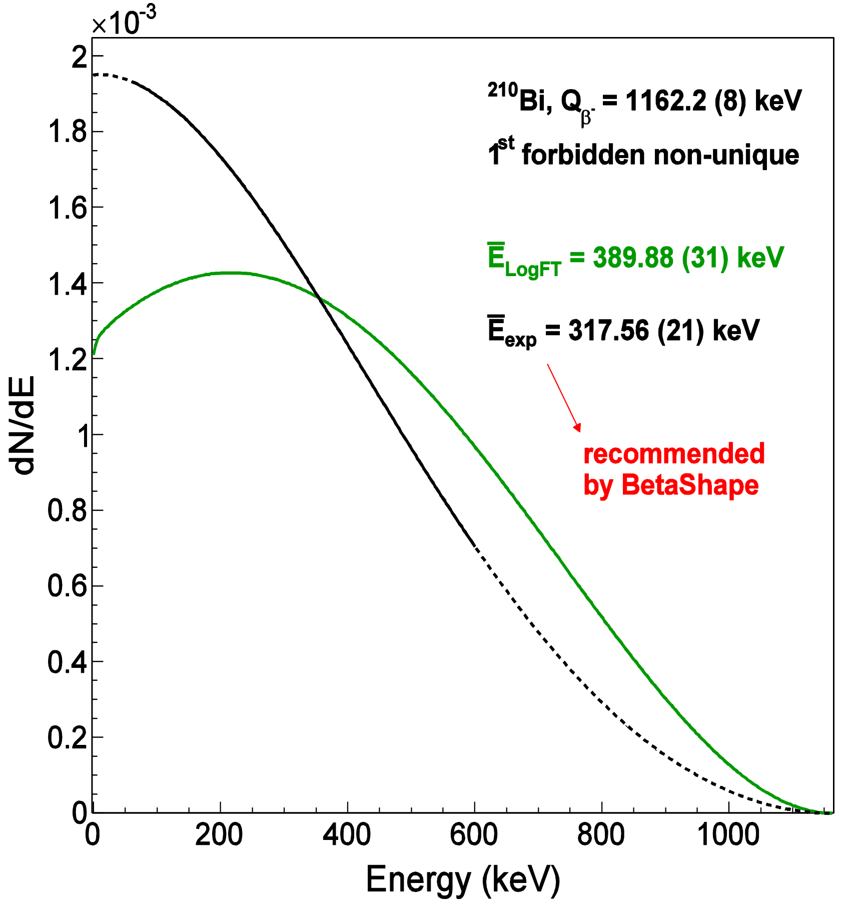
K_{nuc}: nuclear structure (allowed, forbidden unique)

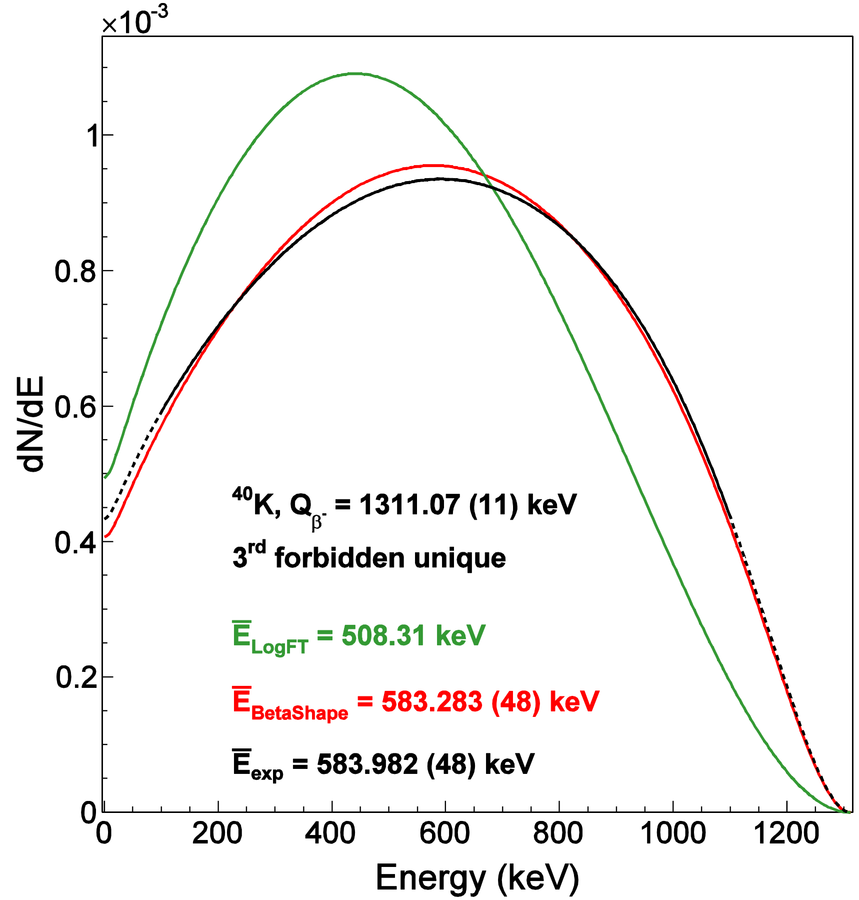
n_x: relative occupation number of the orbital, not accounted for in the LogFT program

For allowed and forbidden unique electron capture transitions, one might expect

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

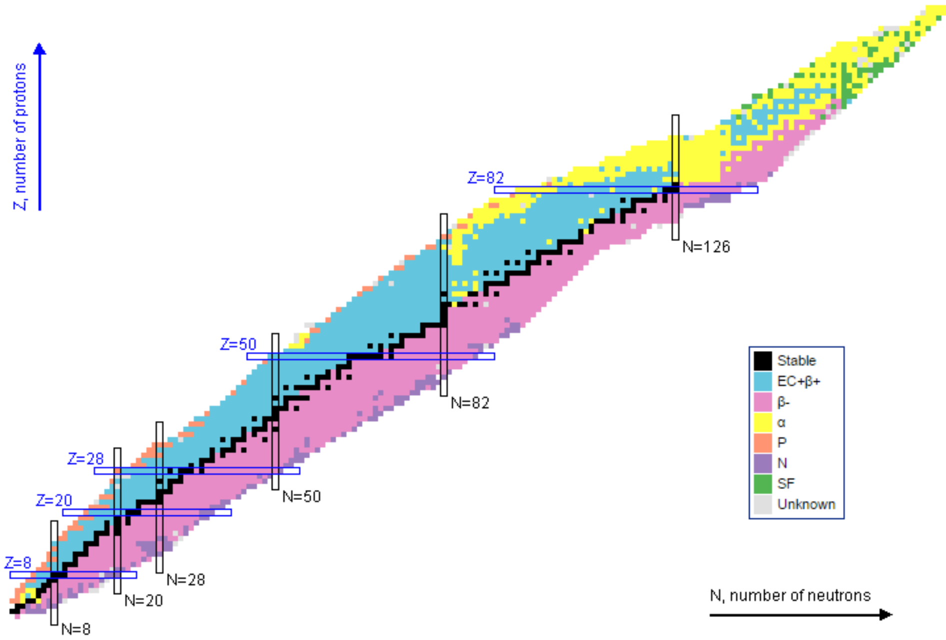
Examples of improved calculations

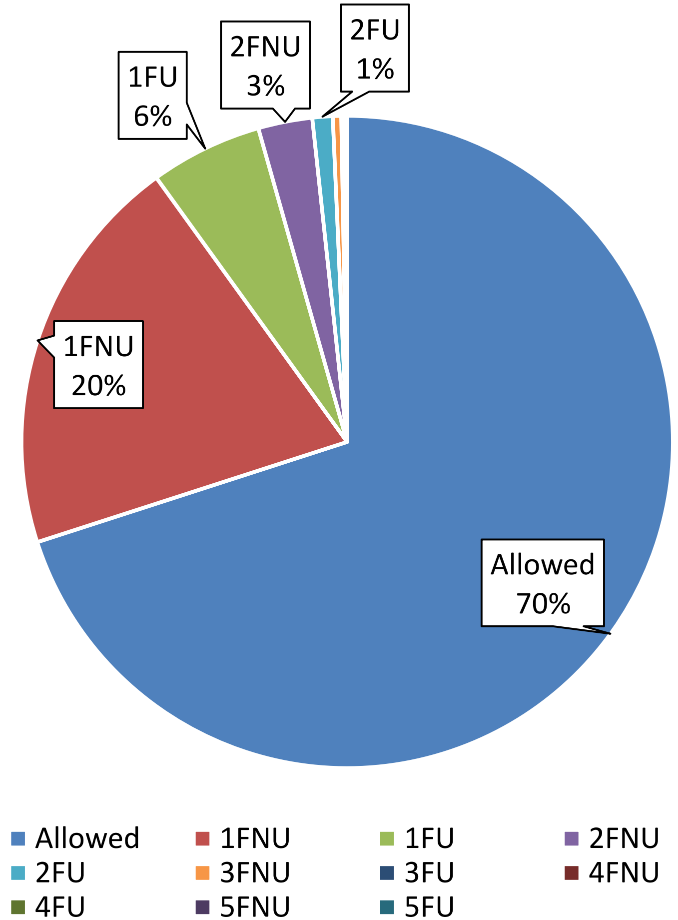




These two transitions are calculated as allowed by the LogFT program.

ENSDF database analysis

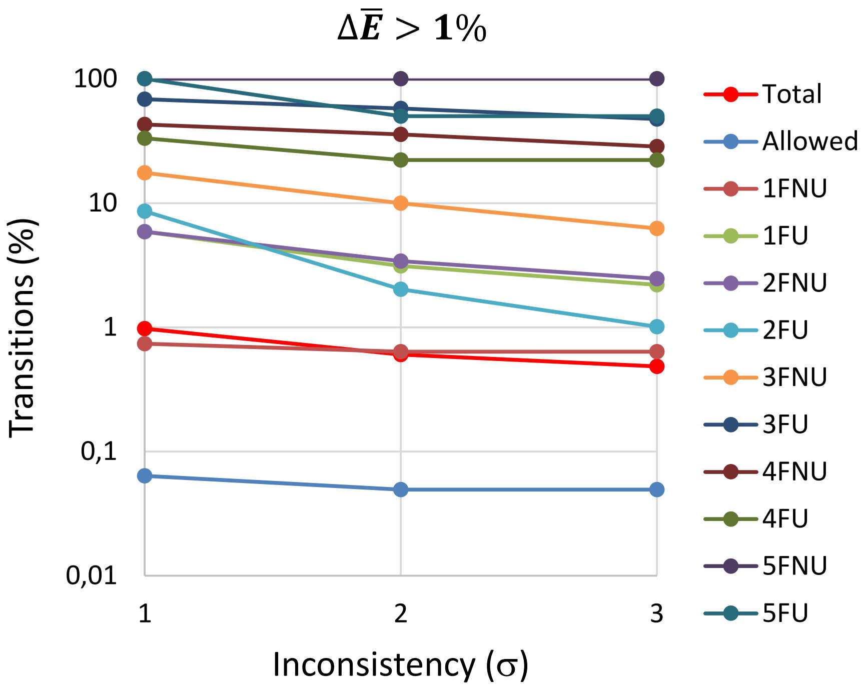




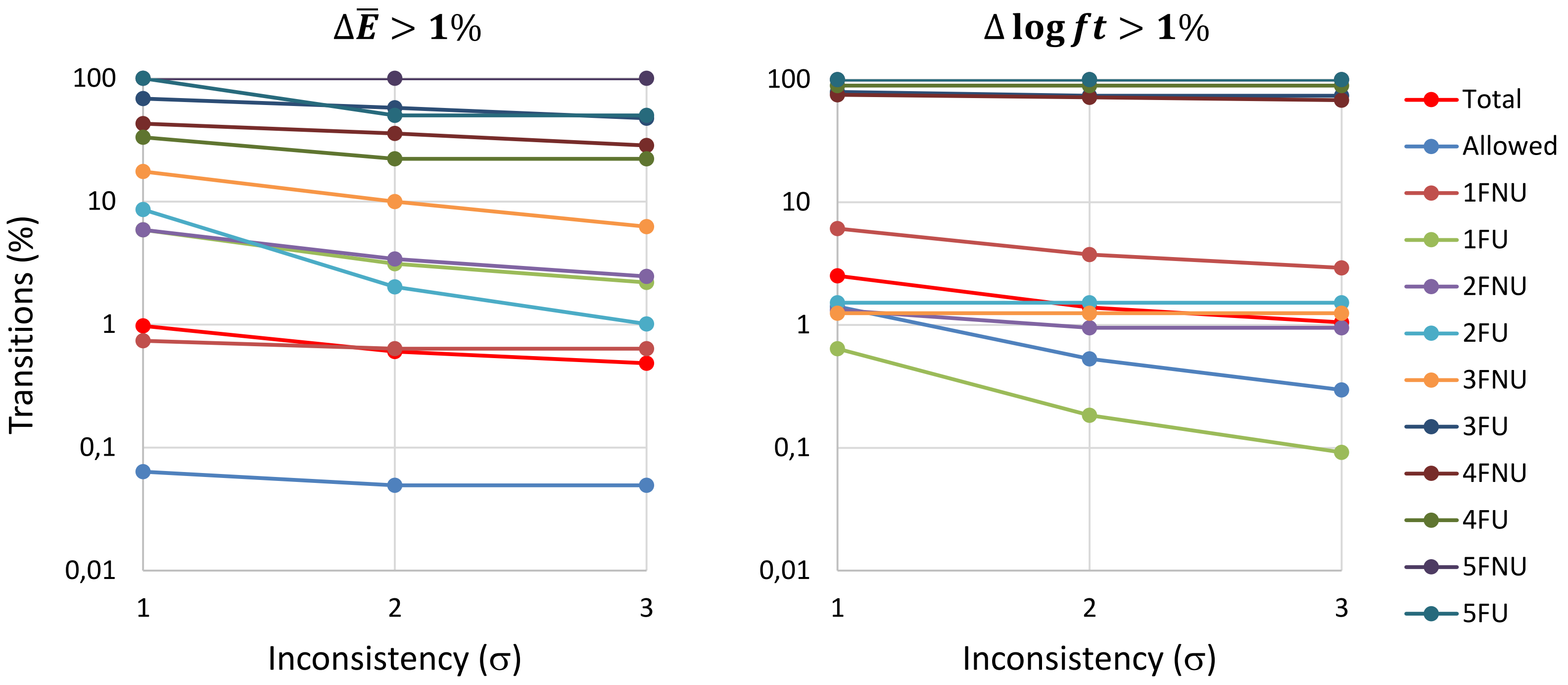
- 21 768 $\beta^{\pm}$ transitions read from ENSDF database
- 19 602 $\beta^{\pm}$ transitions with $I_\beta \geq 0$ and $E_{\max} \geq 0$ keV
- 4 529 transitions calculated as allowed due to lack of spins and parities

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

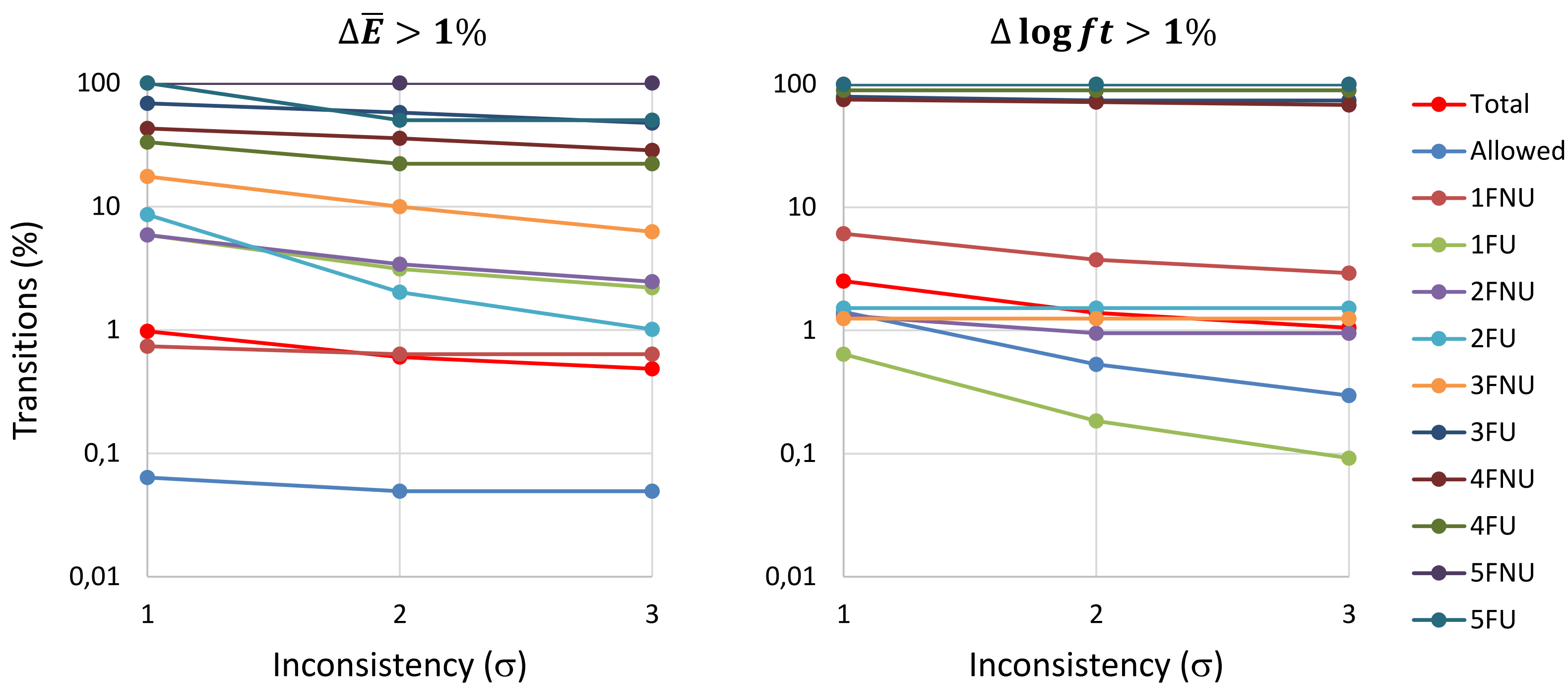
Validation: BetaShape vs LogFT



Validation: BetaShape vs LogFT



Validation: BetaShape vs LogFT



For allowed and forbidden unique β^+/ε transitions

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

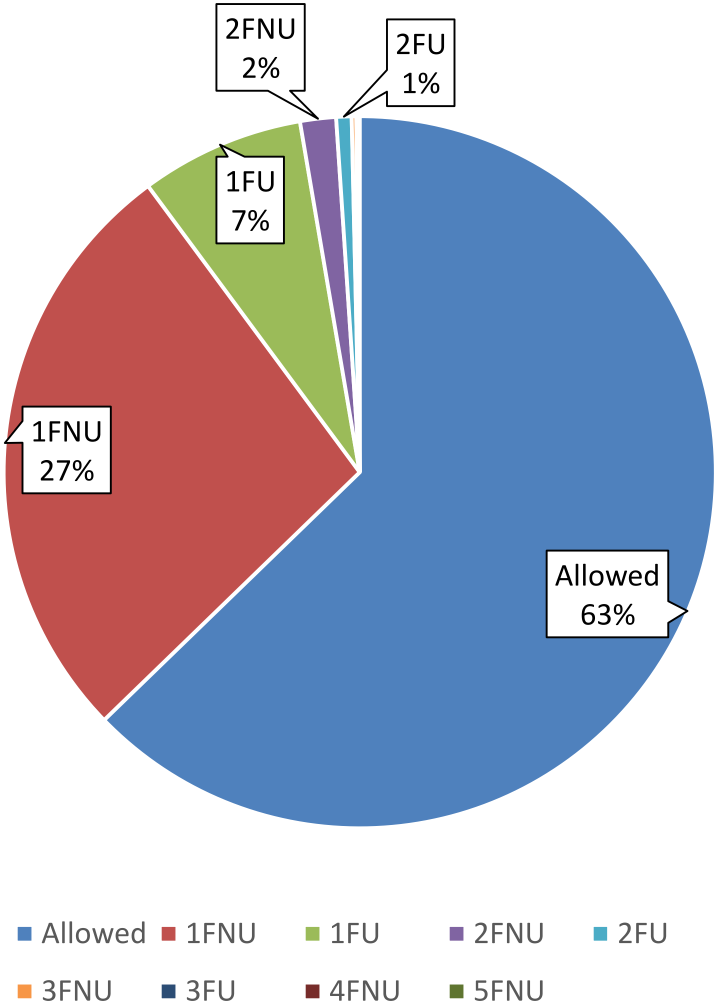
→ 21 of 8 506 β^+ transitions with inconsistent log *ft* at 1σ (experimental shape factors, no uncertainty on intensities, disagreement ≤ 2.5%)

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

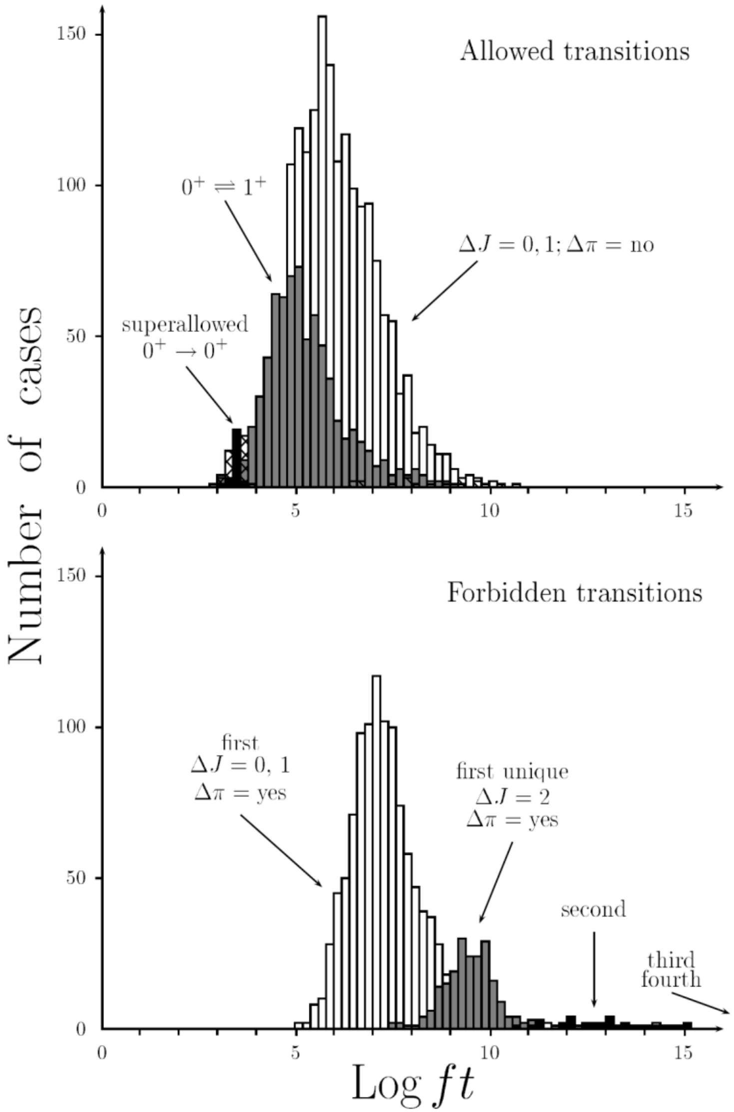
Well-defined transitions

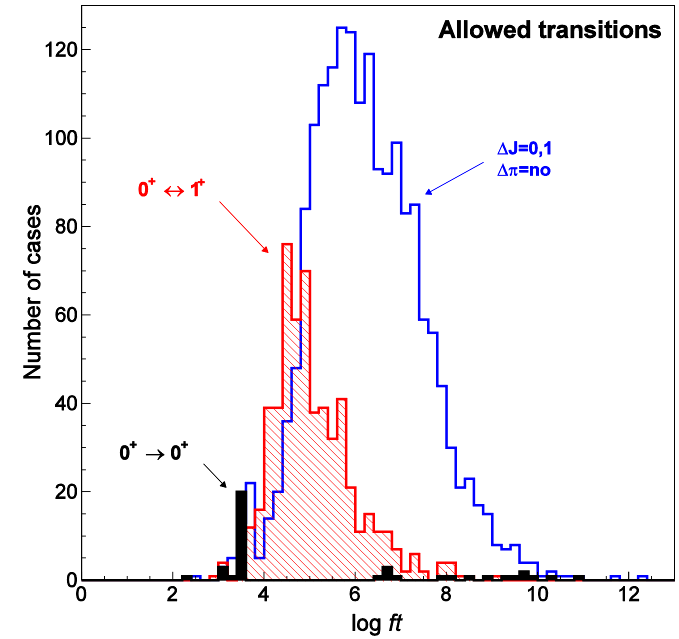
- Well-defined forbiddenness: spins and parities firmly assigned.
- Well-defined Q-values, parent half-life, energies, intensities and their uncertainties.
- Ionized or excited atomic states, uncertain or questionable states and decays, and decays with more than one parent (mixed source) are not considered.

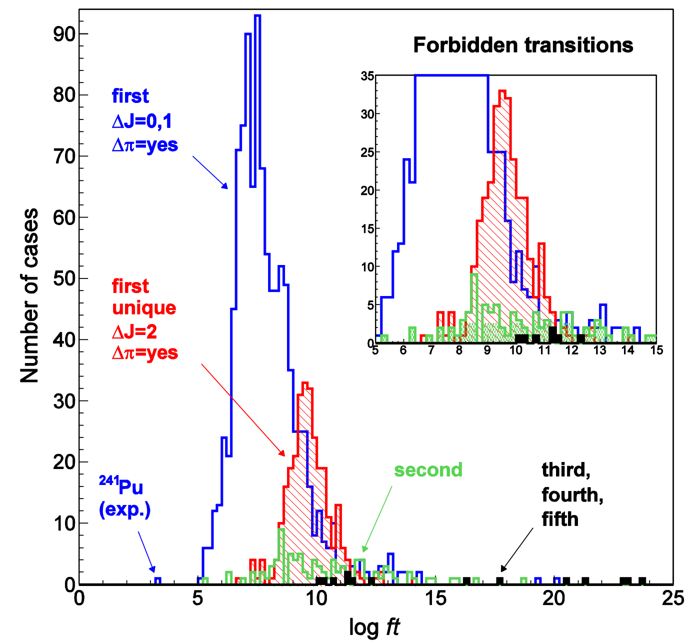
Type	Transitions
Total	3868
Allowed	2427
1FNU	1049
1FU	288
2FNU	63
2FU	27
3FNU	8
3FU	2
4FNU	3
5FNU	1



Well-defined transitions



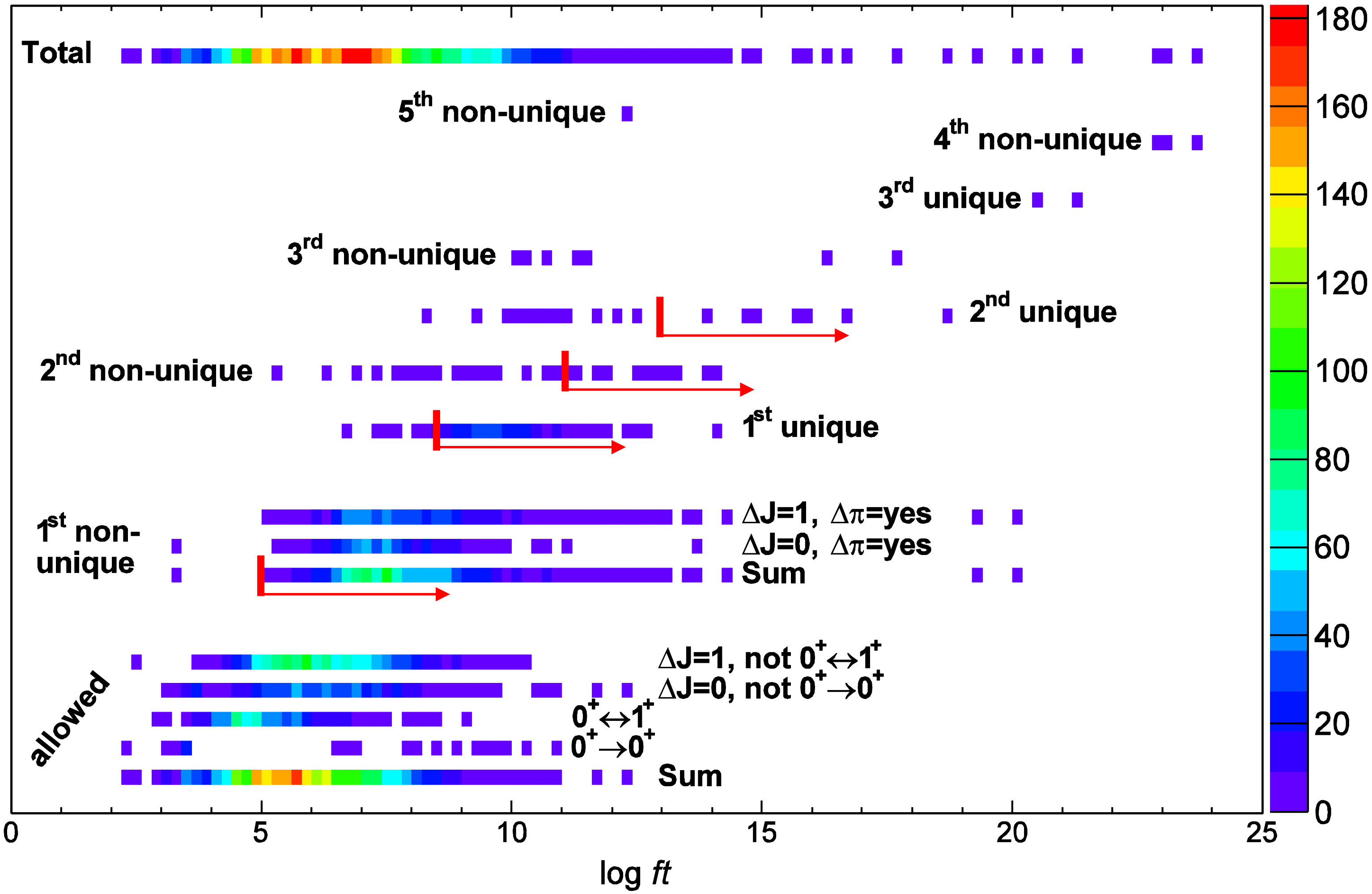




B. Singh *et al.*, *Review Of Logft Values In β Decay*, Nuclear Data Sheets 84, 487 (1998)

Well-defined transitions: Summary $\log ft$

S. Raman, N.B. Gove, *Rules for spin and parities assignments based on* Logft *values*, Phys. Rev. C 7, 1995 (1973)



Conclusion

- Comprehensive analysis of beta emission properties demonstrates the validity of BetaShape and highlights the expected improvement of the data.

- The BetaShape program is available at http://www.nucleide.org/logiciels.htm and is now the reference code for DDEP evaluations.

- Preliminary results for **electron capture transitions**, including atomic effects, seem very promising.

F.G.A. Quarati, P. Dorenbos, X. Mougeot, Appl. Radiat. Isot. 109, 172 (2016)

- **Inclusion of the nuclear structure** is in progress in collaboration with Pr. J. Dudek within the European Metrology project MetroBeta.

- Nuclear data are of importance for fundamental research as well as for applications. We need expertise from all walks for improving them.

  → **Experimentalists** for a fine understanding of the published measurements.

  → **Theorists** for providing the best estimates when no measurement is available.

We need YOU to improve nuclear data!

Thank you for your attention

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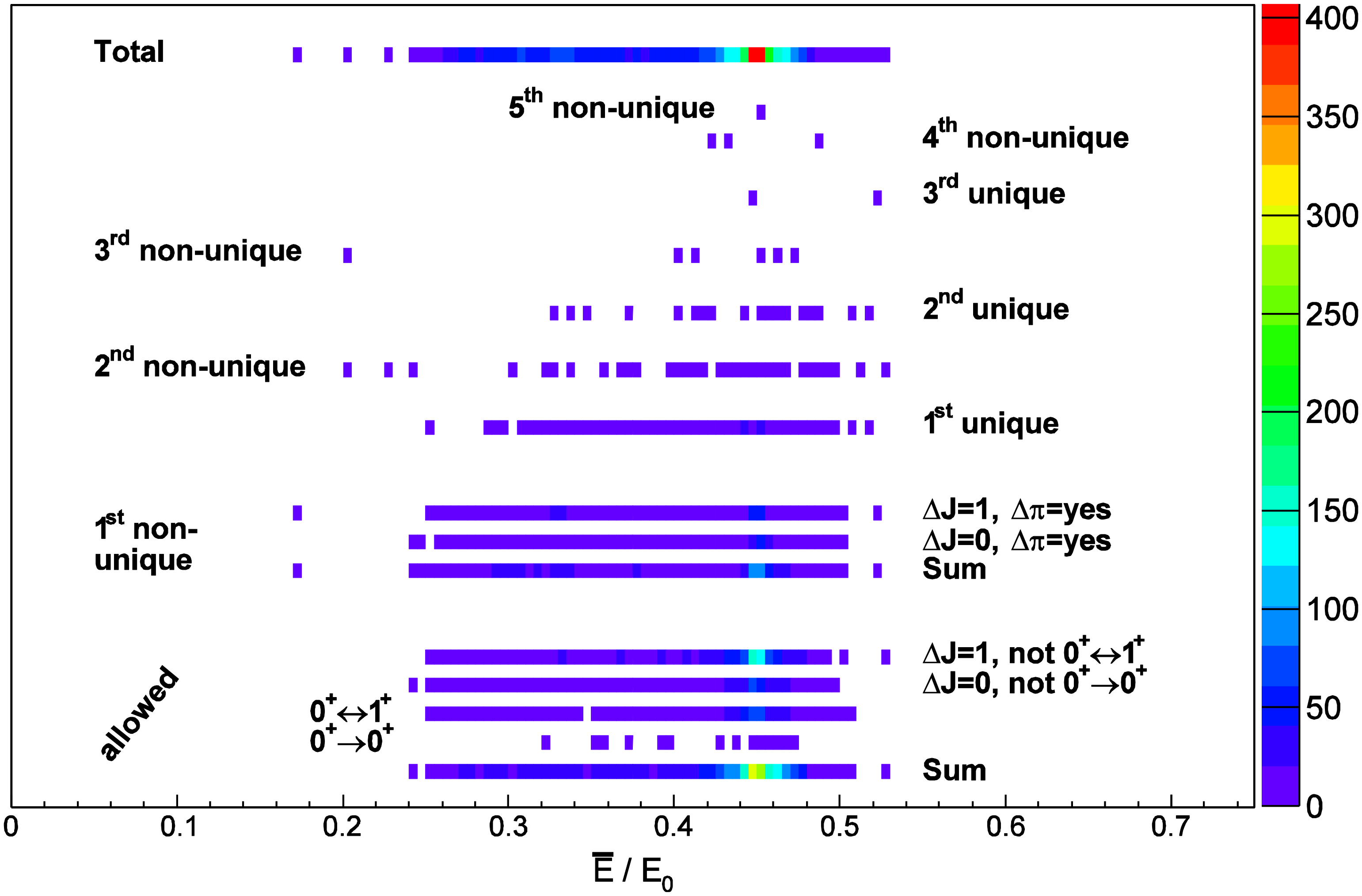
Well-defined transitions: Summary $\overline{E}$



Bühring's screening correction

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

Nucleus region

$$\begin{Bmatrix} F_\kappa(r) \\ G_\kappa(r) \end{Bmatrix} = N(\kappa) \begin{Bmatrix} (\kappa+\gamma)/(\alpha Z) \\ 1 \end{Bmatrix} r^\gamma [1+\mathrm{O}(r)]$$

$$[N(\kappa)]^2 = \tfrac{1}{2}[(\kappa-\gamma)(\kappa\tilde{W}-\gamma m)+\tfrac{1}{2}(\gamma/\kappa)(m+W)(\tilde{\kappa}-\kappa)^2]R_{\mathrm{AB}}^{-1}[\Gamma(1+2\gamma)]^{-2}$$
$$\times|\Gamma(\gamma+i\tilde{y})|^2|\Gamma(\gamma+2i\tilde{P})|^2|\Gamma(k+2iP)|^{-2}\beta^{2\gamma-2k}(2p)^{2k-1}$$

Imaginary momentum without any physical significance as in Rose's correction

$$\tilde{W} = W - \tfrac{1}{2}\alpha Z\beta$$

$$\tilde{p} = \tfrac{1}{2}p + \tfrac{1}{2}[p^2 - 2\alpha Z\tilde{W}\beta]^{1/2}$$

→ **no breakdown at low energy**

Asymptotic region

$$\begin{Bmatrix} F_\kappa(r) \\ G_\kappa(r) \end{Bmatrix} \sim \begin{Bmatrix} -[T/2p]^{1/2}\sin\{pr-\tfrac{1}{2}\pi[l(\kappa)+1]+\Delta_\kappa\} \\ [(2m+T)/2p]^{1/2}\cos\{pr-\tfrac{1}{2}\pi[l(\kappa)+1]+\Delta_\kappa\} \end{Bmatrix}[1+\mathrm{O}(1/r)]$$

$$[N^{\mathrm{Coul}}(\kappa)]^2 = \tfrac{1}{2}(\kappa-\gamma)(\kappa W-\gamma m)[\Gamma(1+2\gamma)]^{-2}|\Gamma(\gamma+iy)|^2$$
$$\times\exp(\pi y)(2p)^{2\gamma-1},$$

Screening correction

Fermi function

$$Q(Z,W) = F(Z,W)/F^{\mathrm{u.s.}}(Z,W)$$

$$Q(Z,W) = \{[N(-1)]^2 + [(1+\gamma_1)^2/(\alpha Z)^2][N(+1)]^2\}$$
$$\times\{[N^{\mathrm{Coul}}(-1)]^2 + [(1+\gamma_1)^2/(\alpha Z)^2][N^{\mathrm{Coul}}(+1)]^2\}^{-1}$$

λ_k parameters

$$Q_k = \{(\alpha Z)^2[N(-k)]^2 + (k+\gamma_k)^2[N(+k)]^2\}$$
$$\times\{(\alpha Z)^2[N^{\mathrm{Coul}}(-k)]^2 + (k+\gamma_k)^2[N^{\mathrm{Coul}}(+k)]^2\}^{-1}$$

$$\lambda_k/\lambda_k^{\mathrm{u.s.}} = Q_k/Q$$

Hulthén screened potential

$$V(r) = -\alpha Z\beta[\exp(\beta r)-1]^{-1}.$$

$$V(r) = -\alpha Z/r + \tfrac{1}{2}\alpha Z\beta + \mathrm{O}(r)$$

→ leading order in nucleus region

Salvat screened potential

$$V(r) = -\frac{Z}{r}\sum_{i=1}^{3} A_i e^{-\alpha_i r} = \left(-\frac{\alpha Z}{r}\right) + (\alpha Z)\sum_{i=1}^{3} A_i\alpha_i + O(r)$$

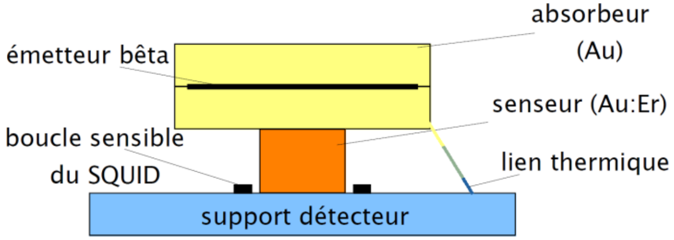
F. Salvat *et al.*, Phys. Rev. A 36, 467 (1987)

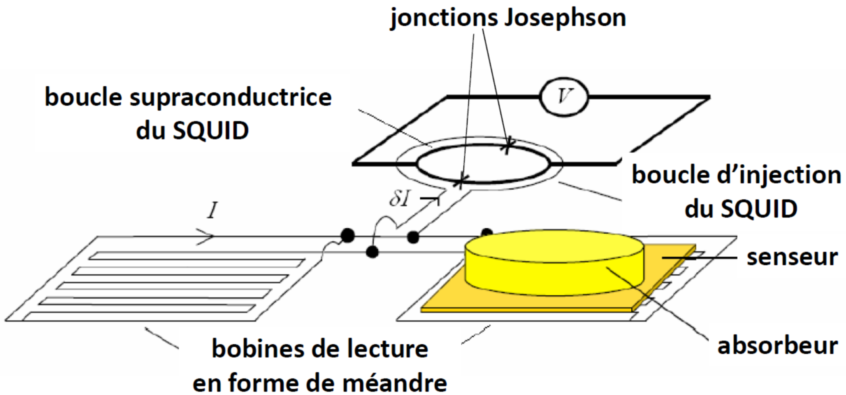
Excellent agreement with tabulated parameters

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

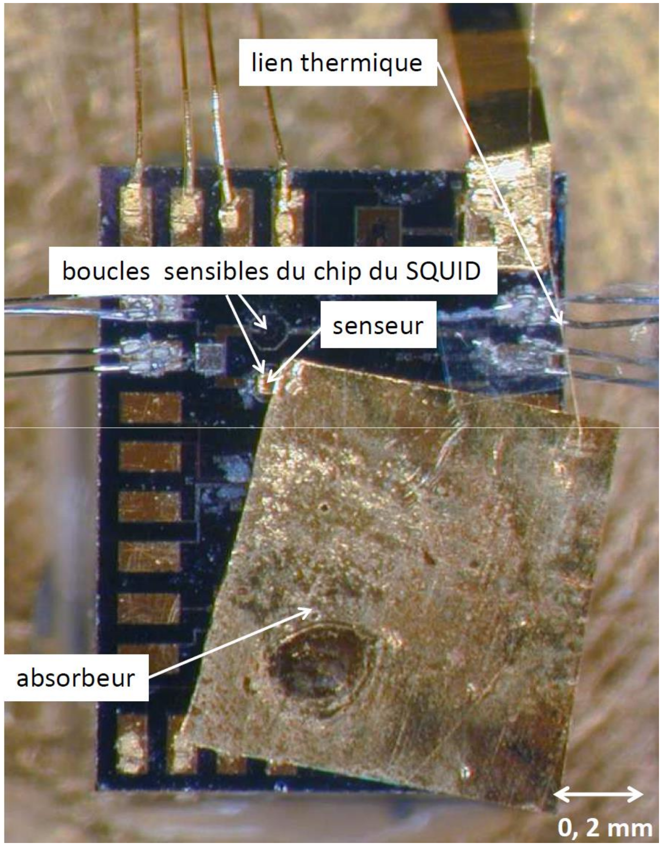
Metallic magnetic calorimeters

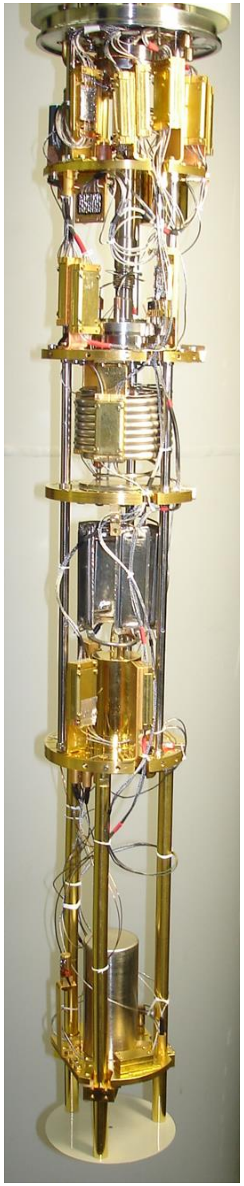
Direct magnetic coupling





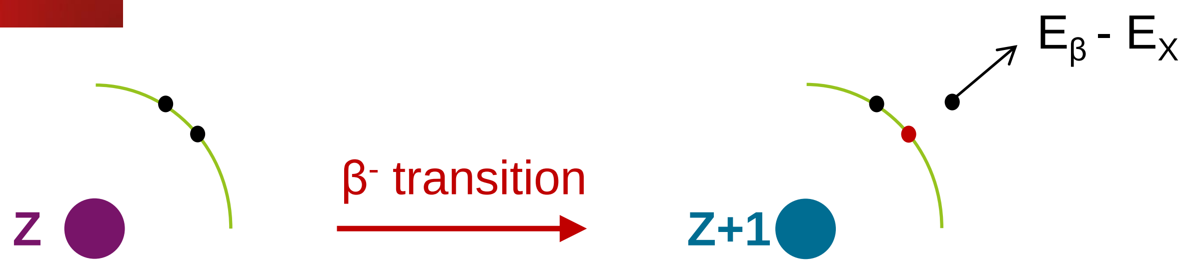
Indirect magnetic coupling





System cooled down to 10 mK

The atomic exchange effect



N.C. Pyper, M.R. Harston, Proc. Roy. Soc. Lond. A 420, 277 (1988)

X. Mougeot *et al.*, Phys. Rev. A 86, 042506 (2012)

First work using analytical wave functions

Atomic exchange effect

→ Indistinguishable from the direct decay to a final continuum state

→ Depends on the **overlap of the continuum and bound electron wave functions**

→ **Allowed transitions**: only the ***ns* orbitals** are reachable

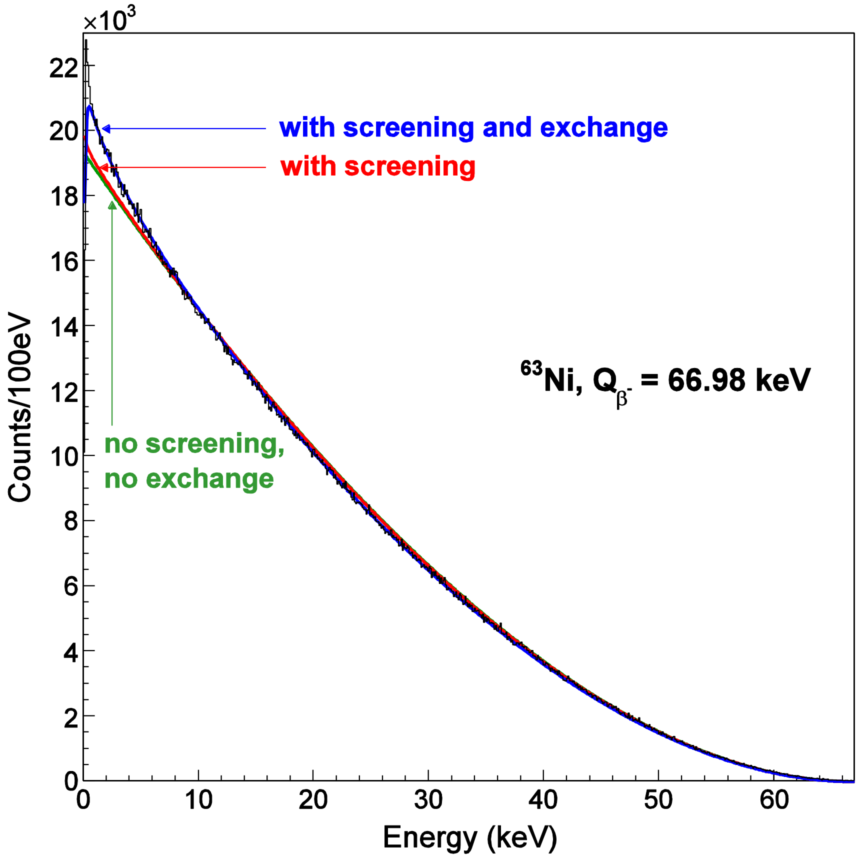
Spectrum correction factor $\left[1+\eta^T_{ex}(E)\right]$

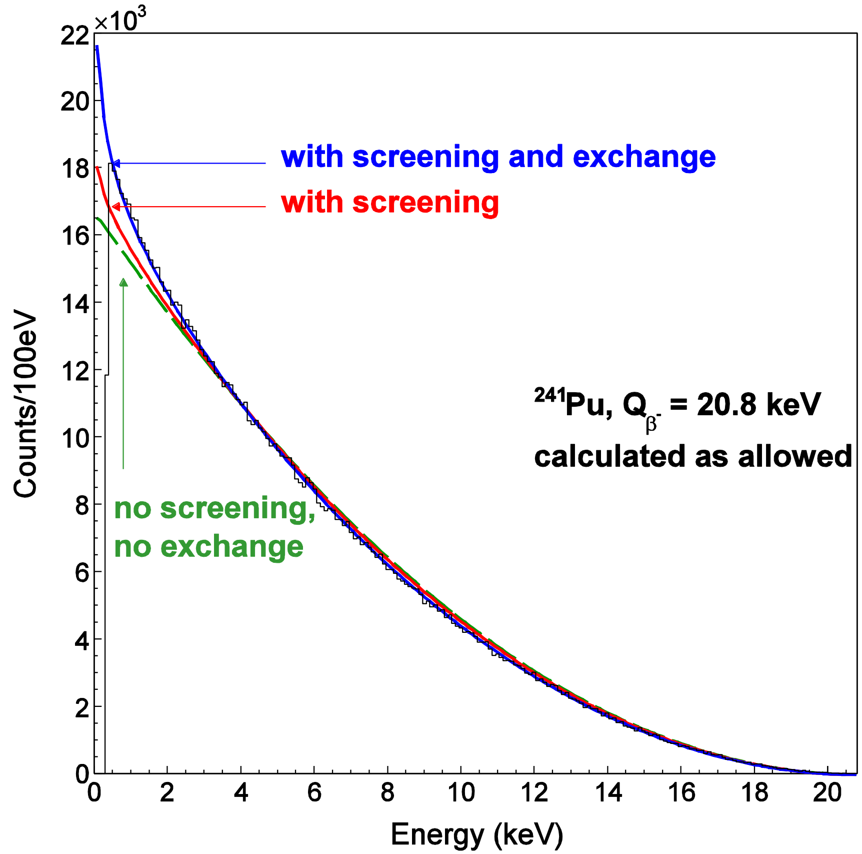
Total exchange factor $$\eta^T_{ex}(E) = \sum_n \eta^{ns}_{ex}(E) + \sum_{\substack{m,n \\ (m\neq n)}} \mu_m \mu_n$$

Subshell contribution $$\eta^{ns}_{ex}(E) = f\left(\mu_n^2 - 2\mu_n\right)$$

with $$\mu_n = \langle Es'|ns\rangle \frac{g^b_{n,\kappa}(R)}{g^c_\kappa(R)}, \quad f = \frac{g^c_\kappa(R)^2}{g^c_\kappa(R)^2 + f^c_\kappa(R)^2}$$

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





With precise calculation of atomic effects

$$(1 - R^2) = 0.028\ \%$$

Mean energy decreased by **1.8 %**

With precise calculation of atomic effects

$$(1 - R^2) = 0.040\ \%$$

Mean energy decreased by **4 %**

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