

Calculation of beta decays

*The most common assumptions
and how to go beyond*

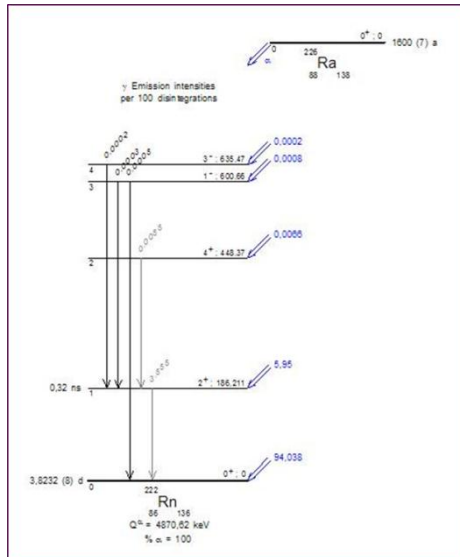
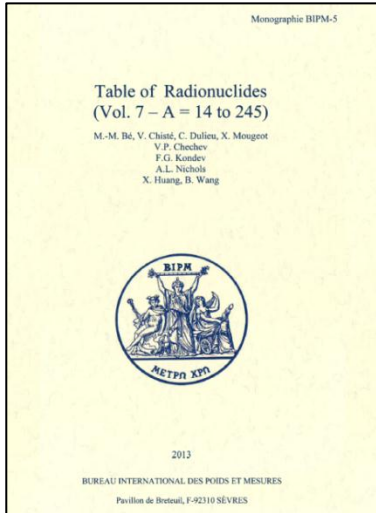
CEA Saclay – LNHB

M.-M. Bé, C. Dulieu, M. A. Kellett, **X. Mougeot**

list

Decay Data Evaluation Project (DDEP)

→ Recommended data by BIPM



This introduction presents a brief description of the radioactivity physical processes, the enumeration of the evaluation rules leading to the recommended values, and a summary of the symbols and terms used in all the publications.

Explanation on recommended data and their evaluation (in various languages):

updated: 19th November 2013
 newly added: Co-58, Cu-61, Pm-148m, Zr-93
 recently updated: Nb-93m
 ASCII files updated on: 26/04/2013
 (205 nuclides in table, sorted by [edition date](#) / [alphabetical order](#) / [atomic number](#) / [mass number](#))

([History of older evaluations](#), sorted by [alphabetical order](#))

Subscribe to DDEP RSS feed

(Type of updates: N - new evaluation, 1 - update in comments only, 2 - minor update in table, 3 - major update in table)

Nuclide	Tables	Comments	ENSDF	ASCII	In	UpDate	Type
Co-58	58Co	table	comments	ensdf	txt	8	19/11/2013 N
Zr-93	93Zr	table	comments	ensdf	txt	8	18/11/2013 N
Nb-93m	93mNb	table	comments	ensdf	txt	8	18/11/2013 2

Nuclide	Tables	Comments	ENSDF	ASCII	In	UpDate	Type
Te-132	132Te	table	comments	ensdf	txt	6	22/01/2010 2
Pa-233	233Pa	table	comments	ensdf	txt	6	11/01/2010 2
Np-237	237Np	table	comments	ensdf	txt	6	7/01/2010 2

www.nucleide.org

α and γ libraries
<http://laraweb.free.fr/>

All published data are considered and carefully analyzed (provided they exist!).

Values may be rejected, uncertainties may be expanded.

The decay scheme will be based as much as possible on the available measured data.

Otherwise, calculation codes are used.

→ $\log ft$ for β and electron capture processes.



Ionizing radiation metrology

Activity measurements by Liquid Scintillation, MetroMRT, MetroRWM
Better knowledge of the β spectra → **better uncertainties**



Medical uses, nuclear fuel cycle

Residual power of nuclear reactors, nuclear waste, internal dosimetry, internal radiotherapy, imaging, etc.



Scientific research

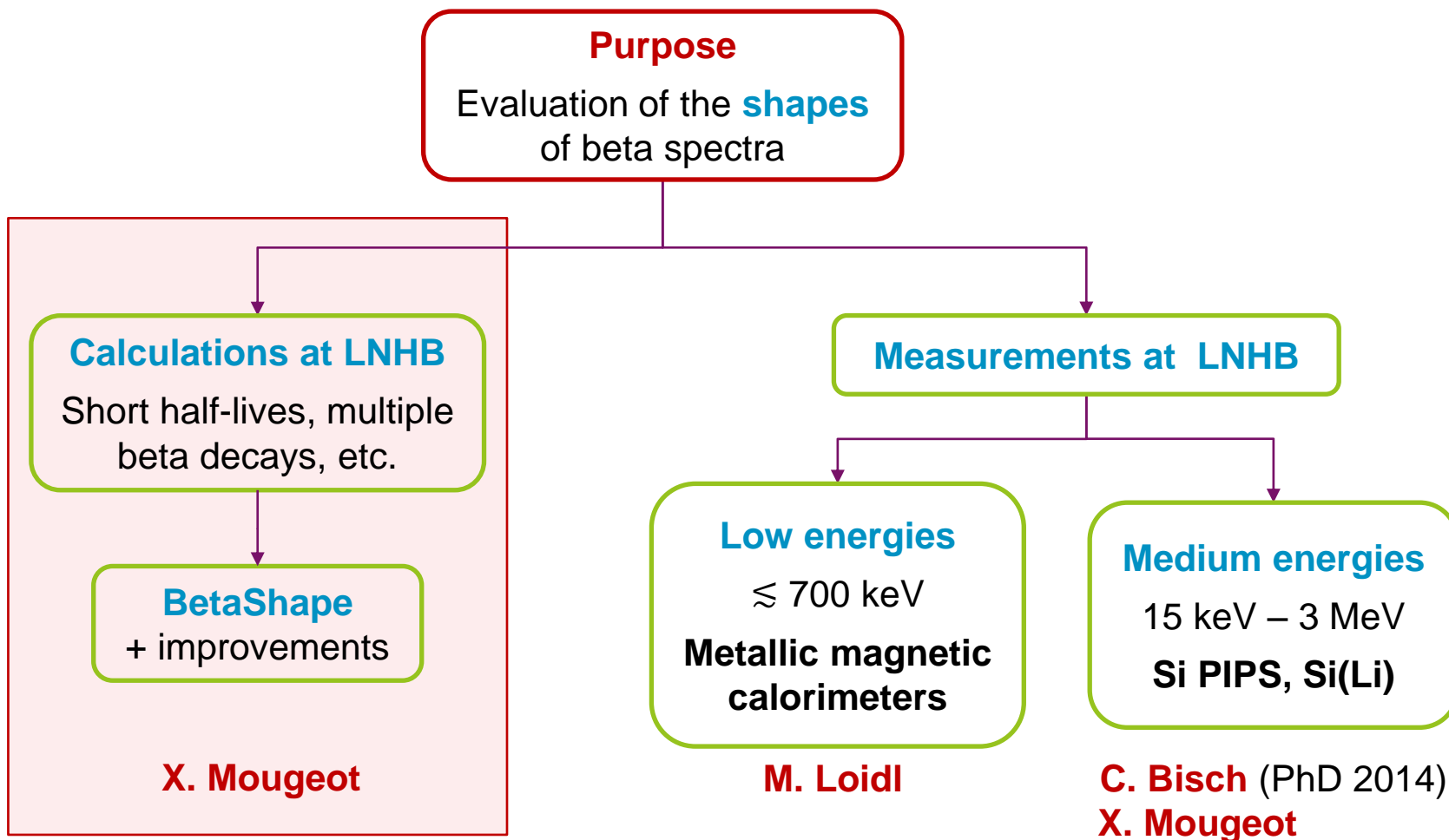
New detectors (BrLa₃), monitoring and safeguards applications, fundamental physics (CeLAND, etc.)



AIEA (Nuclear Data Section), DDEP, NNDC

Atomic and nuclear data

Our users need **a precise knowledge of β spectra**,
coupled with **well-established uncertainties**.



Basics of beta decay, the **most common assumptions**

→ **Systematic comparison** with 130 **experimental shape factors**

Recent precise measurements of **^{63}Ni** and **^{241}Pu** beta spectra

→ **Improvements** of the calculation to include **atomic effects**

Basics of beta decay

Similarly we obtain for the space components

$$\langle p | \mathbf{V} + \mathbf{A} | n \rangle = i u_p^\dagger \gamma_4 \gamma_\mu (1 + \lambda \gamma_5) u_n = \sqrt{\frac{(W_n + M_n)}{2W_n}} \sqrt{\frac{(W_p + M_p)}{2W_p}} \begin{pmatrix} 0 & i\boldsymbol{\sigma} \\ i\boldsymbol{\sigma} & 0 \end{pmatrix} \lambda \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \times \left\{ \left(\frac{\boldsymbol{\sigma} \mathbf{p}}{W_p + M_p} \chi_p^{m'} \right)^+ \boldsymbol{\sigma} \chi_n^m + \left(\chi_p^{m'} \right)^+ \boldsymbol{\sigma} \frac{\boldsymbol{\sigma} \mathbf{p}}{W_n + M_n} \chi_n^m - \lambda \left(\chi_p^{m'} \right)^+ \boldsymbol{\sigma} \chi_n^m - \lambda \left[\left(\frac{\boldsymbol{\sigma} \mathbf{p}}{W_p + M_p} \chi_p^{m'} \right)^+ \boldsymbol{\sigma} \frac{\boldsymbol{\sigma} \mathbf{p}}{W_n + M_n} \chi_n^m \right] \right\}. \quad (6.38)$$

This equals to

$$\langle p | \mathbf{V} + \mathbf{A} | n \rangle = \sqrt{\frac{(W_n + M_n)}{2W_n}} \sqrt{\frac{(W_p + M_p)}{2W_p}} \left\{ \left(\chi_p^{m'} \right)^+ \frac{\boldsymbol{\sigma} \mathbf{p}_p}{W_p + M_p} \boldsymbol{\sigma} \chi_n^m + \frac{\mathbf{p}_p + i(\boldsymbol{\sigma} \times \mathbf{p}_p)}{W_p + M_p} \left(\chi_p^{m'} \right)^+ \boldsymbol{\sigma} \frac{\boldsymbol{\sigma} \mathbf{p}_n}{W_n + M_n} \chi_n^m - \lambda \left(\chi_p^{m'} \right)^+ \boldsymbol{\sigma} \frac{\boldsymbol{\sigma} \mathbf{p}_n}{W_n + M_n} \chi_n^m - \lambda \left[\left(\chi_p^{m'} \right)^+ \frac{\boldsymbol{\sigma} \mathbf{p}_p}{W_p + M_p} \boldsymbol{\sigma} \frac{\boldsymbol{\sigma} \mathbf{p}_n}{W_n + M_n} \chi_n^m \right] - \frac{(\mathbf{p}_p \cdot \mathbf{p}_n) \boldsymbol{\sigma} + (\boldsymbol{\sigma} \mathbf{p}_p) \mathbf{p}_n + \mathbf{p}_p (\boldsymbol{\sigma} \mathbf{p}_n) - i(\mathbf{p}_p \times \mathbf{p}_n)}{(W_p + M_p)(W_n + M_n)} \right\}. \quad (6.39)$$

Finally we obtain for the space components

$$\langle p | \mathbf{V}(0) + \mathbf{A}(0) | n \rangle = \sqrt{\frac{(W_n + M_n)}{2W_n}} \sqrt{\frac{(W_p + M_p)}{2W_p}} \times \left\{ \left[\frac{\mathbf{p}_p}{W_p + M_p} + \frac{\mathbf{p}_n}{W_n + M_n} \right] \left(\chi_p^{m'} \right)^+ \chi_n^m + \left(\chi_p^{m'} \right)^+ \times \left[\frac{i(\boldsymbol{\sigma} \times \mathbf{p}_p)}{W_p + M_p} - \frac{i(\boldsymbol{\sigma} \times \mathbf{p}_n)}{W_n + M_n} \right] \chi_p^{m'} - \lambda \left(\chi_p^{m'} \right)^+ \boldsymbol{\sigma} \chi_n^m + \lambda \frac{\mathbf{p}_p \mathbf{p}_n}{(W_p + M_p)(W_n + M_n)} \left\{ \left(\chi_p^{m'} \right)^+ \boldsymbol{\sigma} \chi_n^m \right\} + \lambda \frac{i(\mathbf{p}_p \times \mathbf{p}_n)}{(W_p + M_p)(W_n + M_n)} \times \left\{ \left(\chi_p^{m'} \right)^+ \chi_n^m - \lambda \left[\left(\chi_p^{m'} \right)^+ \frac{(\boldsymbol{\sigma} \mathbf{p}_p) \mathbf{p}_n + \mathbf{p}_p (\boldsymbol{\sigma} \mathbf{p}_n)}{(W_p + M_p)(W_n + M_n)} \chi_n^m \right] \right\}. \quad (6.40)$$

$$\frac{i}{2M_\Lambda} F_M(q^2) (\mathbf{P} \times \mathbf{q}) \boldsymbol{\sigma} - F_S(q^2) q_0 + \frac{1}{4(2M_\Lambda)^2} F_S(q^2) q_0 (\mathbf{P}^2 - \mathbf{q}^2) - \frac{i}{2(2M_\Lambda)^2} F_S(q^2) q_0 (\mathbf{P} \times \mathbf{q}) \boldsymbol{\sigma} \left\} \chi^M, \quad (9.15)$$

$$\langle \phi_f(p_f) | A_0(0) | \phi_i(p_i) \rangle = N(\chi^M)^+ \left\{ -\frac{1}{2M_\Lambda} F_\Lambda(q^2) (\mathbf{P} \boldsymbol{\sigma}) - \frac{q_0}{2M_\Lambda} F_p(q^2) (\mathbf{q} \boldsymbol{\sigma}) - F_T(q^2) (\mathbf{q} \boldsymbol{\sigma}) + \frac{1}{4(2M_\Lambda)^2} F_T(q^2) \times [(\mathbf{P} \mathbf{q})(\boldsymbol{\sigma} \mathbf{P} + \boldsymbol{\sigma} \mathbf{q}) - (\boldsymbol{\sigma} \mathbf{q})(\mathbf{P}^2 + \mathbf{q}^2)] \right\} \chi^M, \quad (9.16)$$

$$\langle \phi_f(p_f) | \mathbf{V}(0) | \phi_i(p_i) \rangle = N(\chi^M)^+ \left\{ \frac{1}{2M_\Lambda} F_V(q^2) \mathbf{P} + \frac{i}{2M_\Lambda} F_V(q^2) (\boldsymbol{\sigma} \times \mathbf{q}) + i F_M(q^2) (\boldsymbol{\sigma} \times \mathbf{q}) - \frac{1}{2M_\Lambda} F_M(q^2) q_0 \mathbf{q} - \frac{i}{4M_\Lambda} F_M(q^2) q_0 (\boldsymbol{\sigma} \times \mathbf{P}) - F_S(q^2) \mathbf{q} + \frac{1}{4(2M_\Lambda)^2} F_S(q^2) \mathbf{q} (\mathbf{P}^2 - \mathbf{q}^2) - \frac{i}{2(2M_\Lambda)^2} F_S(q^2) \mathbf{q} \times ((\mathbf{P} \times \mathbf{q}) \boldsymbol{\sigma}) - \frac{i}{2(2M_\Lambda)^2} F_M(q^2) \mathbf{P} (\mathbf{P} \times \mathbf{q}) \boldsymbol{\sigma} - \frac{i}{4(2M_\Lambda)^2} \times F_M(q^2) (\mathbf{P}^2 + \mathbf{q}^2) (\boldsymbol{\sigma} \times \mathbf{q}) + \frac{i}{2(2M_\Lambda)^2} F_M(q^2) (\mathbf{P} \mathbf{q})(\boldsymbol{\sigma} \times \mathbf{P}) \right\} \chi^M, \quad (9.17)$$

$$\langle \phi_f(p_f) | \mathbf{A}(0) | \phi_i(p_i) \rangle = N(\chi^M)^+ \left\{ -F_\Lambda(q^2) \boldsymbol{\sigma} + \frac{1}{2(2M_\Lambda)^2} \times F_\Lambda(q^2) \mathbf{P}^2 \boldsymbol{\sigma} - \frac{1}{4(2M_\Lambda)^2} F_\Lambda(q^2) (\mathbf{P}^2 + \mathbf{q}^2) \boldsymbol{\sigma} - \frac{i}{2(2M_\Lambda)^2} \times F_\Lambda(q^2) (\mathbf{P} \times \mathbf{q}) - \frac{1}{2(2M_\Lambda)^2} F_\Lambda(q^2) [(\boldsymbol{\sigma} \mathbf{P}) \mathbf{P} - (\boldsymbol{\sigma} \mathbf{q}) \mathbf{q}] + \frac{1}{2M_\Lambda} F_T(q^2) [(\mathbf{P} \mathbf{p}) \boldsymbol{\sigma} - \mathbf{q} (\mathbf{P} \mathbf{p})] - F_T(q^2) q_0 \boldsymbol{\sigma} + \frac{1}{2(2M_\Lambda)^2} F_T(q^2) q_0 \mathbf{P}^2 \boldsymbol{\sigma} - \frac{1}{4(2M_\Lambda)^2} F_T(q^2) q_0 (\mathbf{P}^2 + \mathbf{q}^2) \boldsymbol{\sigma} - \frac{i}{2(2M_\Lambda)^2} F_T(q^2) q_0 (\mathbf{P} \times \mathbf{q}) - \frac{1}{2(2M_\Lambda)^2} F_T(q^2) q_0 [(\boldsymbol{\sigma} \mathbf{P}) \mathbf{P} - (\boldsymbol{\sigma} \mathbf{q}) \mathbf{q}] - \frac{1}{2M_\Lambda} F_p(q^2) (\boldsymbol{\sigma} \mathbf{q}) \mathbf{q} \right\} \chi^M. \quad (9.18)$$

$$+ \sqrt{\frac{2}{3}} \left\{ \left(\frac{r}{R} \right) r I'(r) \beta \gamma_5 T_{121} \right\} \mp \frac{f_p}{R} (W_0 R \pm \frac{2}{3} \alpha Z) {}^D \mathfrak{Y}_{110}^{(0)}(1, 1, 1, 1) \quad (14.101)$$

$${}^A F_{121}^{(0)} = \mp \lambda {}^A \mathfrak{Y}_{121}^{(0)} - \frac{f_T}{R} \left[\frac{5}{\sqrt{3}} {}^C \mathfrak{Y}_{111}^{(0)} - (W_0 R \pm \frac{2}{3} \alpha Z) {}^A \mathfrak{Y}_{121}^{(0)} \right] \mp \frac{f_p}{R} 5\sqrt{\frac{2}{3}} {}^D \mathfrak{Y}_{110}^{(0)} \quad (14.102)$$

$${}^A F_{121}^{(0)}(1, 1, 1, 1) = \mp \lambda {}^A \mathfrak{Y}_{121}^{(0)}(1, 1, 1, 1) - \frac{f_T}{R} \left\{ \sqrt{\frac{2}{3}} \left(\frac{r}{R} \right) [5I(r) + r I'(r)] \beta T_{111} \right\} - (W_0 R \pm \frac{2}{3} \alpha Z) {}^A \mathfrak{Y}_{121}^{(0)}(1, 1, 1, 1) \mp \frac{f_p}{R} \sqrt{\frac{2}{3}} \left(\frac{r}{R} \right) [5I(r) + r I'(r)] \beta \gamma_5 T_{110} \quad (14.103)$$

$${}^V F_{211}^{(0)} = -{}^V \mathfrak{Y}_{211}^{(0)} \frac{f_M}{R} (W_0 R \pm \frac{2}{3} \alpha Z) {}^C \mathfrak{Y}_{211}^{(0)} \quad (14.104)$$

$${}^V F_{220}^{(0)} = {}^V \mathfrak{Y}_{220}^{(0)} + \frac{f_M}{R} \sqrt{(10)} {}^C \mathfrak{Y}_{211}^{(0)} + \frac{f_S}{R} (W_0 R \pm \frac{2}{3} \alpha Z) {}^V \mathfrak{Y}_{220}^{(0)} \quad (14.105)$$

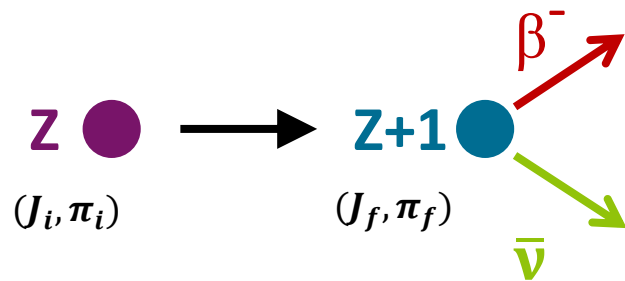
$${}^V F_{220}^{(0)}(1, 1, 1, 1) = {}^V \mathfrak{Y}_{220}^{(0)}(1, 1, 1, 1) + \frac{f_M}{R} \left\{ \sqrt{\frac{2}{3}} \left(\frac{r}{R} \right) [5I(r) + r I'(r)] \beta T_{211} \right\} + \sqrt{\frac{2}{3}} \left\{ \left(\frac{r}{R} \right) r I'(r) \beta T_{231} \right\} \pm \frac{f_S}{R} (W_0 R \pm \frac{2}{3} \alpha Z) {}^V \mathfrak{Y}_{220}^{(0)}(1, 1, 1, 1) \quad (14.106)$$

$${}^A F_{221}^{(0)} = \pm \lambda {}^A \mathfrak{Y}_{221}^{(0)} + \frac{f_T}{R} \left\{ \sqrt{(15)} {}^C \mathfrak{Y}_{211}^{(0)} - (W_0 R \pm \frac{2}{3} \alpha Z) {}^A \mathfrak{Y}_{221}^{(0)} \right\} \quad (14.107)$$

$${}^A F_{221}^{(0)}(1, 1, 1, 1) = \pm \lambda {}^A \mathfrak{Y}_{221}^{(0)}(1, 1, 1, 1) + \frac{f_T}{R} \left\{ \sqrt{\frac{2}{3}} \left(\frac{r}{R} \right) [5I(r) + r I'(r)] \beta T_{211} \right\} - \sqrt{\frac{2}{3}} \left\{ \left(\frac{r}{R} \right) r I'(r) \beta T_{231} \right\} - (W_0 R \pm \frac{2}{3} \alpha Z) {}^A \mathfrak{Y}_{221}^{(0)}(1, 1, 1, 1) \quad (14.108)$$

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

More than 600 p.!



Electroweak interaction

$$\left. \begin{aligned} M_{W^+, W^-, Z^0} &\sim 80 \text{ GeV} \\ E_{\text{max}}(\beta) &\lesssim 50 \text{ MeV} \end{aligned} \right\} \text{Fermi: 4 particles interacting at one vertex}$$

Free neutron decay

$$H_\beta = \frac{G_\beta}{\sqrt{2}} \left[\bar{\psi}_p \gamma_\mu (1 + \lambda \gamma_5) \psi_n \quad \text{nuclear current} \right. \\ \left. \times \bar{\psi}_e \gamma_\mu (1 + \gamma_5) \psi_\nu + \text{h.c.} \right] \quad \text{leptonic current}$$

Neutrino

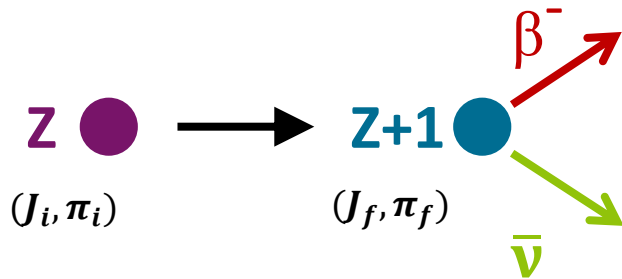
$m_{\bar{\nu}} \sim 0 \rightarrow \beta$ spectrum very poorly modified, in the endpoint region

Nucleus

- **Point charge, spherical symmetry**
 \rightarrow no deformation of the nucleus
- $M_{\text{nucleus}} \sim \infty \rightarrow E_{\text{recoil}} \sim 0$

ΔJ	$\pi_i \pi_f$	Classification
0, 1	1	Allowed
0, 1	-1	1 st fnu
> 1	$(-1)^{ \Delta J }$	$ \Delta J ^{\text{th}}$ fnu
> 1	$(-1)^{ \Delta J -1}$	$(\Delta J - 1)^{\text{th}}$ fu

$\Delta J = |J_f - J_i|$
fnu: forbidden non-unique
fu: forbidden unique



Beta spectrum

$$\frac{dN}{dW} \propto \underbrace{p W q^2}_{\text{Phase space}} \underbrace{F_0 L_0}_{\text{Coulomb part (Fermi function)}} \underbrace{C(W)}_{\text{Shape factor}}$$

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

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

$L = 1$ if $\Delta J = 0$
 $L = \Delta J$ otherwise

$\lambda_k = 1?$

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

if $2\xi = \alpha Z/R \gg E_{\max}$	
1 st fnu	→ allowed
2 nd fnu	→ 1 st fu
3 rd fnu	→ 2 nd fu

Assumptions → Corrections

- **Screening:** $W \rightarrow W \pm V_0(\beta^\pm)$, Thomas-Fermi potential such as $V_0(Z)$ only
- **Finite nuclear size**
- **Radiative corrections** (virtual photons, internal bremsstrahlung)

X. Mougeot *et al.*, Proceedings of the LSC2010 International Conference, Paris, France, p. 249 (2010)

Small database of **130 experimental shape factors**

- Allowed: 36
- Forbidden unique: 25 (1st), 4 (2nd), 1 (3rd)
- Forbidden non-unique: 53 (1st), 9 (2nd), 1 (3rd), 1 (4th)

But almost comprehensive!

→ Very few measurements below 50 keV (7)

→ Very few transitions of high forbidding order

→ 10 published shape factors since 1976!

This study will be published within the proceedings of the ICRM 2015 conference.

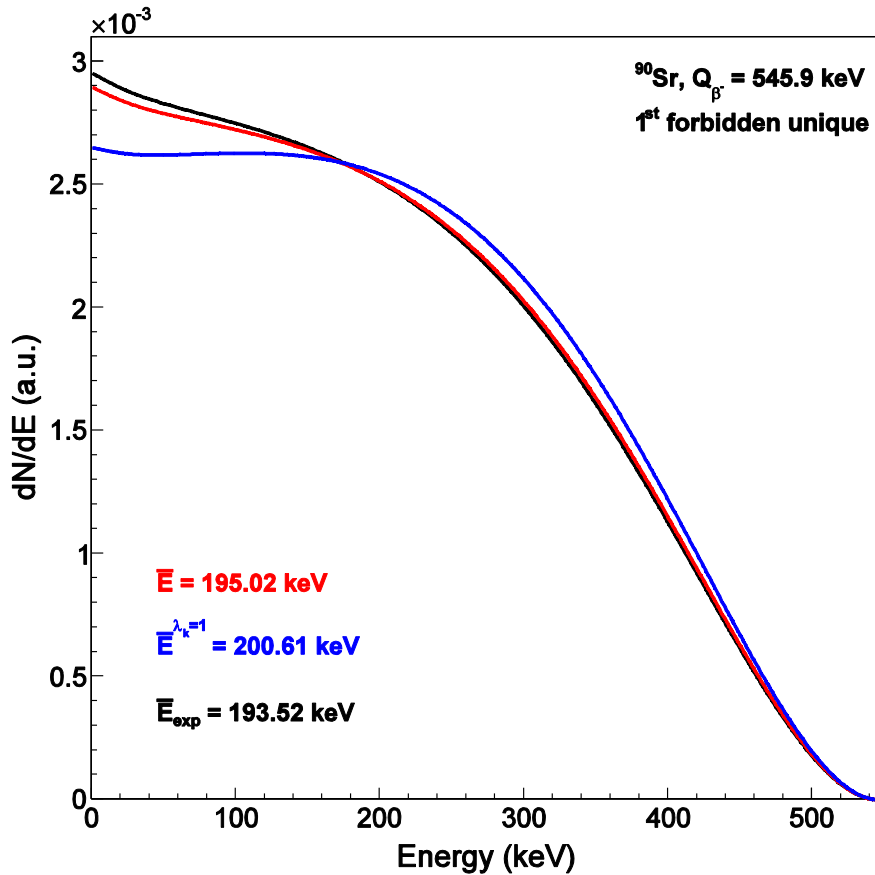
Results

→ $\lambda_k = 1$ is generally a bad approximation

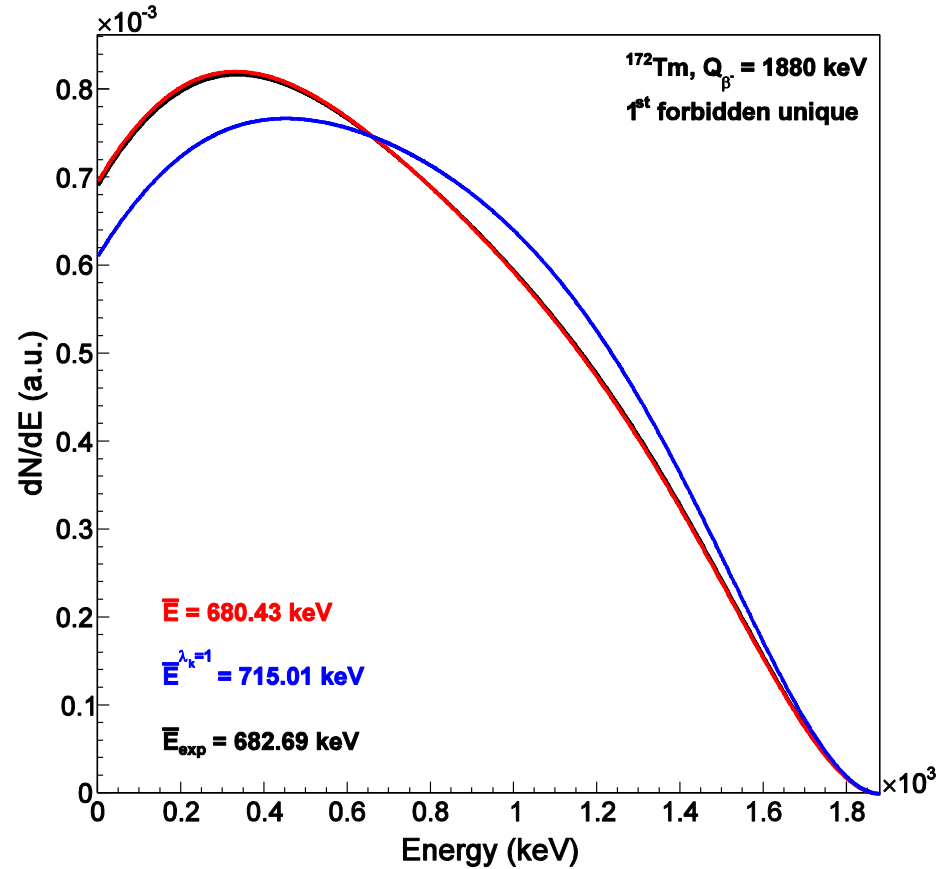
→ Allowed and forbidden unique spectra are generally reproduced well

→ ξ approximation is correct **only** for ~ 50 % of the 1st forbidden non-unique transitions, and **incorrect** for all other non-unique transitions

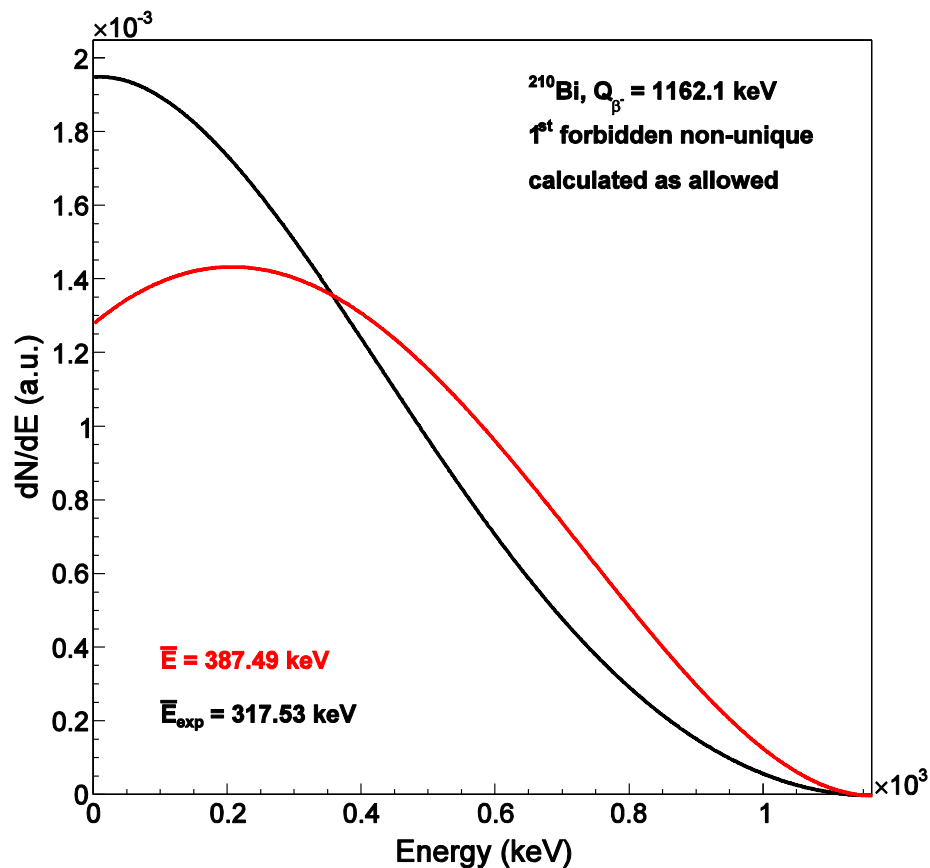
New measurements are needed to test the theoretical predictions



Mean energy disagrees by **3.6 %**
 High influence at low energy

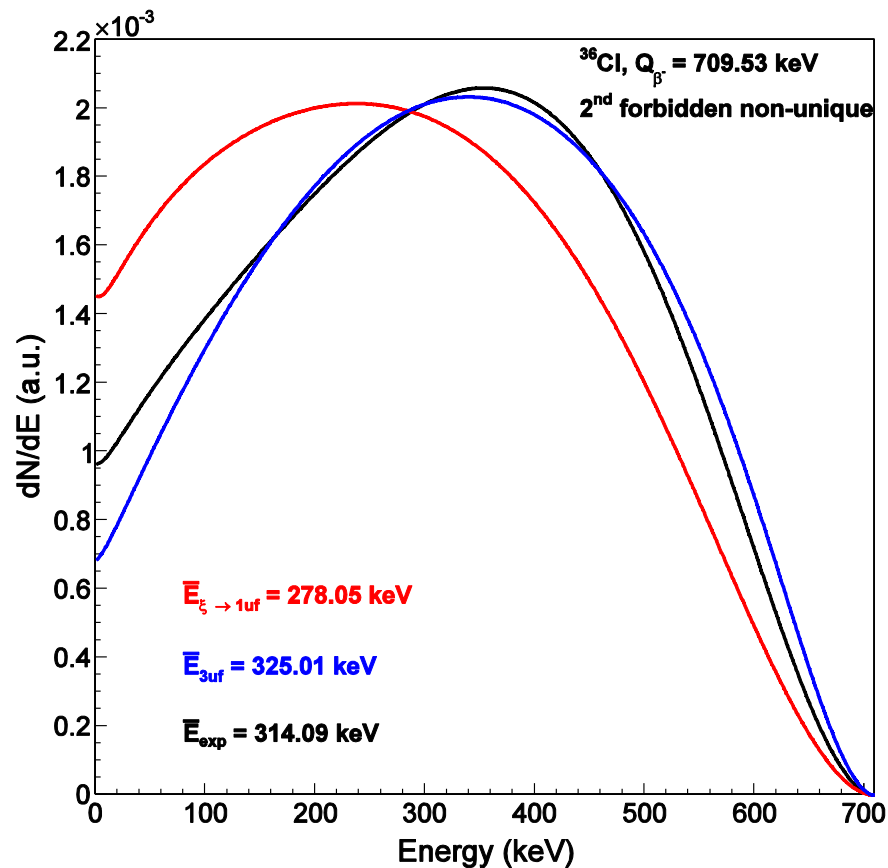


Mean energy disagrees by **4.6 %**
 High influence at low energy and on the overall shape of the spectrum



Calculated as **allowed**, this spectrum is **not correct**

Mean energy disagrees by **20 % (!)**



Calculated as 1^{st} forbidden unique, this spectrum is **not correct**

Mean energy disagrees by **14 % (!)**

Better as 3^{rd} forbidden unique \rightarrow **justification?**

Atomic effects

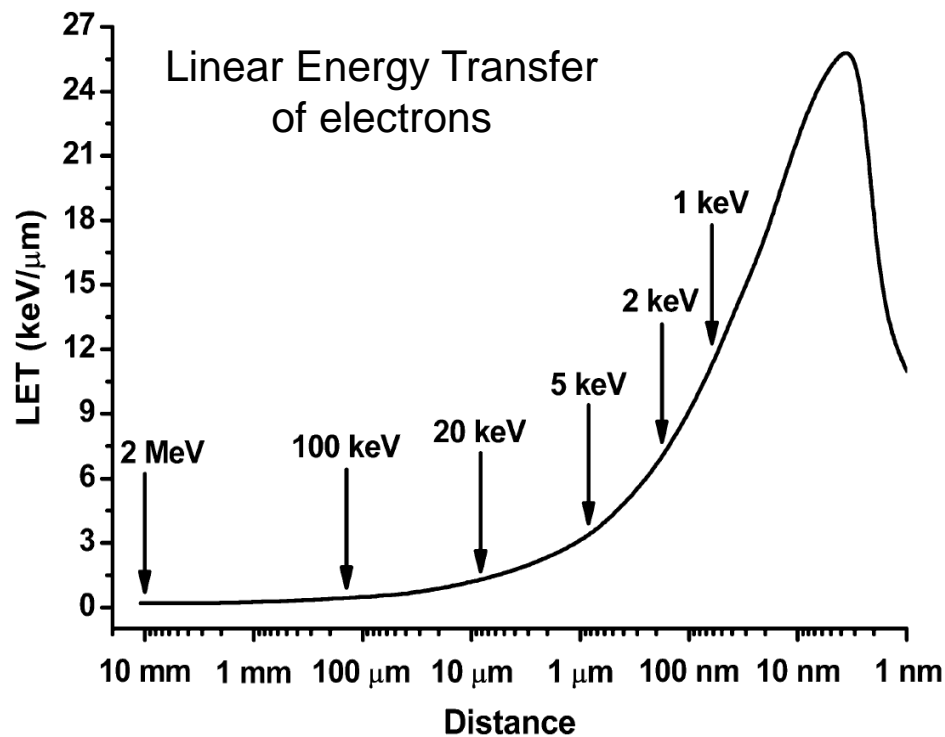
- **Activity measurements using Liquid Scintillation Counting technique**

R. Broda, P. Cassette, K. Kossert, Metrologia 44, S36-S52 (2007)

- Evaluation of the **dose deposited** in patient's cells

M. Bardiès, J.-F. Chatal, Phys. Med. Biol. 39, 961-981 (1994)

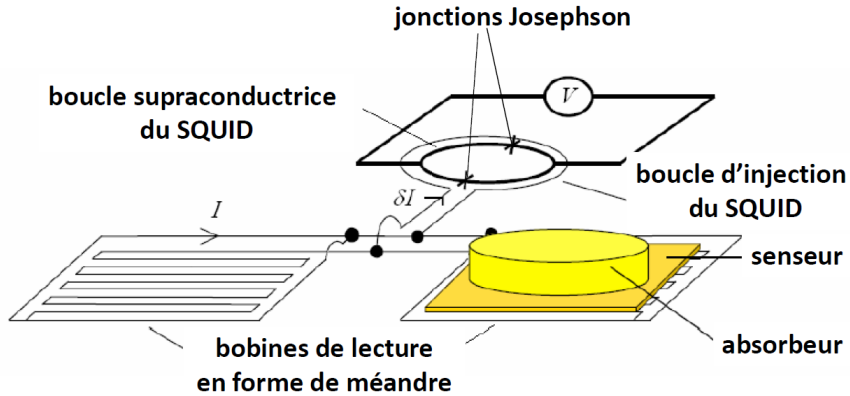
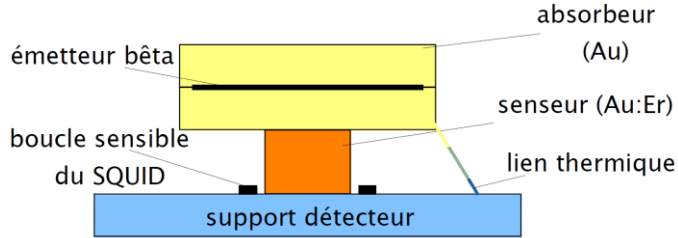
→ e.g. 1 electron of 2 keV
≠
2 electrons of 1 keV



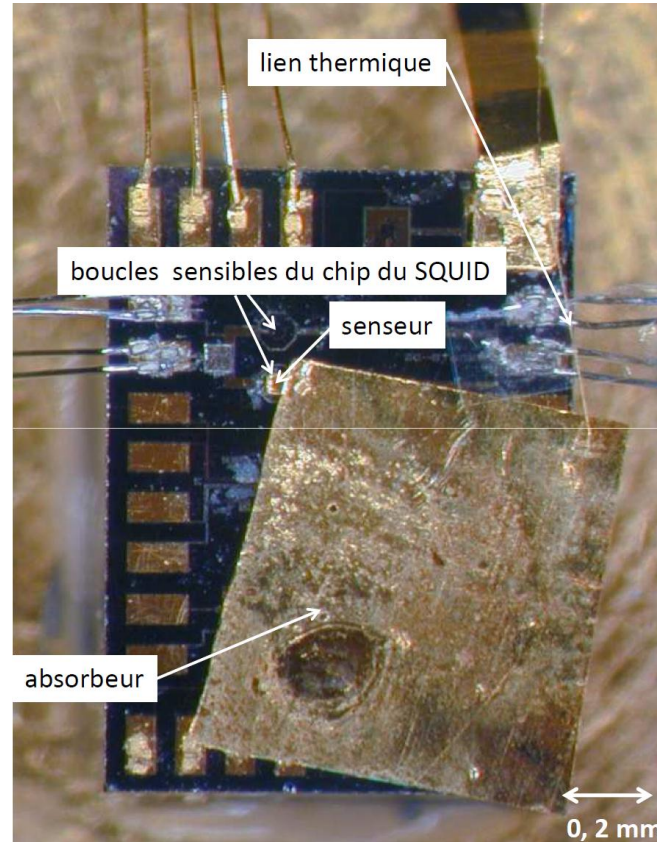
A.I. Kassis, Int. J. Radiat. Biol. 80, 789 (2004)

Precise knowledge of beta spectra shapes is needed at low energy

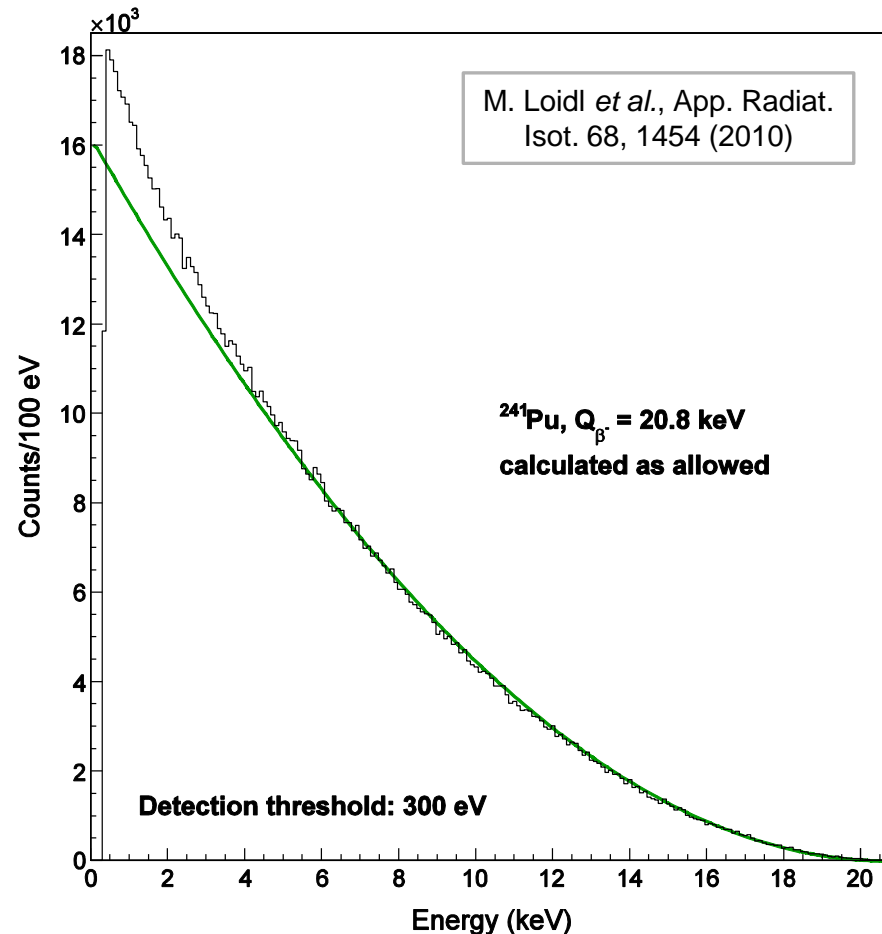
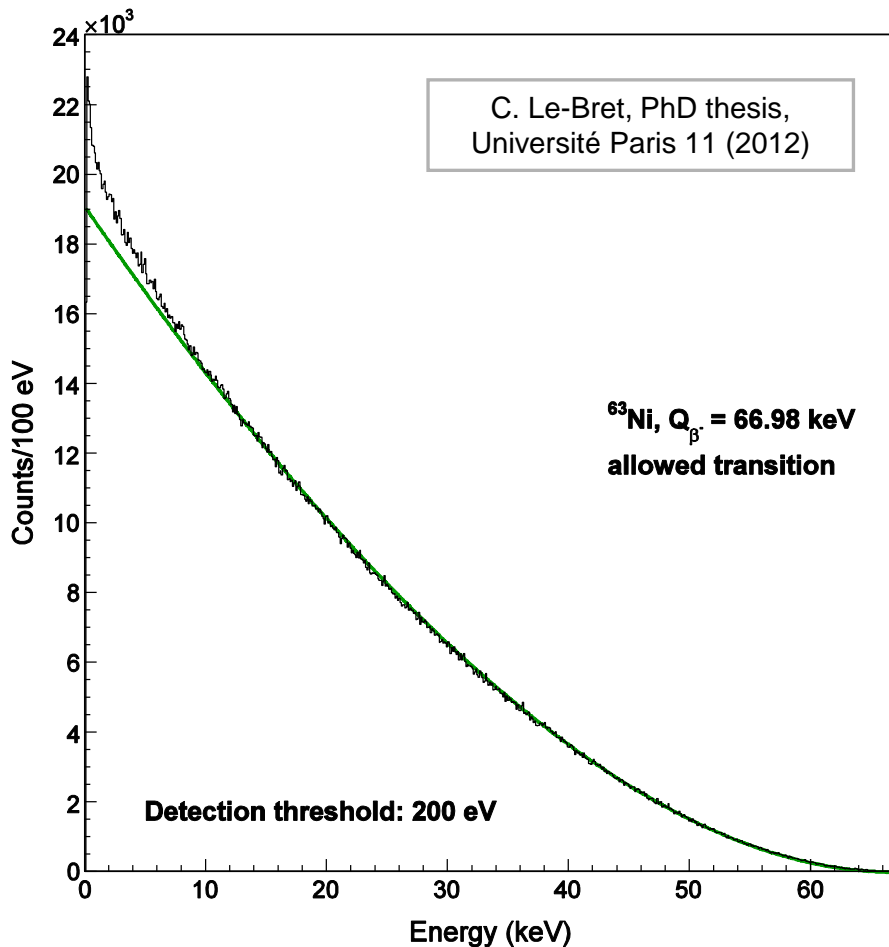
Direct magnetic coupling



Indirect magnetic coupling



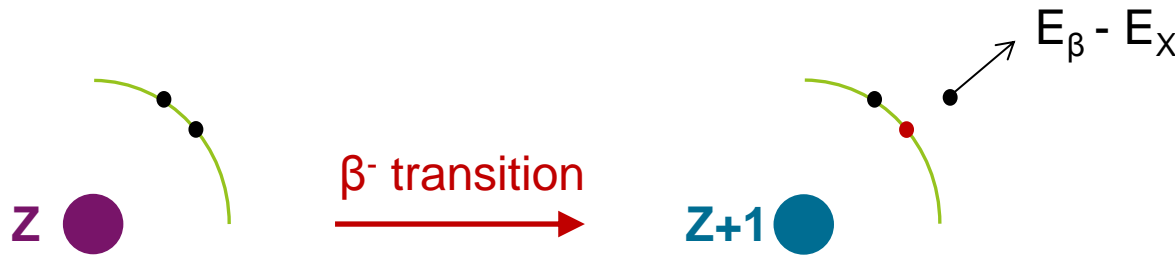
System cooled down to 10 mK



Classical beta calculations fail to reproduce these "simple" spectra

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

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



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

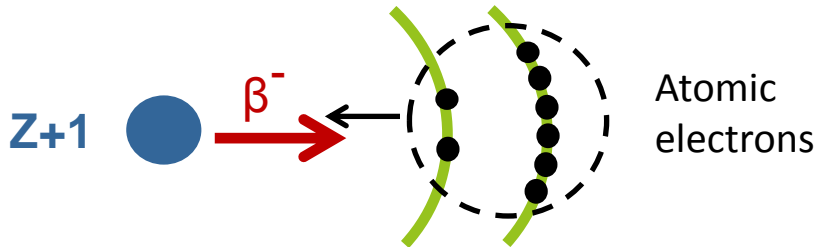
- Indistinguishable from the direct decay to a final continuum state
- Depends on the **overlap of the continuum and bound electron wave functions**
- **Allowed transitions**: only the ***ns* orbitals** are reachable

Spectrum correction factor $[1 + \eta_{ex}^T(E)]$

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

Subshell contribution $\eta_{ex}^{ns}(E) = f (\mu_n^2 - 2\mu_n)$

with $\mu_n = \langle Es' | ns \rangle \frac{g_{n,\kappa}^b(R)}{g_\kappa^c(R)}, \quad f = \frac{g_\kappa^c(R)^2}{g_\kappa^c(R)^2 + f_\kappa^c(R)^2}$



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

Screening

Generally corrected for using a constant Thomas-Fermi potential, which creates a **non physical discontinuity** in the spectrum.

Evaluating the **wave functions at the nuclear surface** cannot provide a good result because of the **weakness of the screened potentials** in this region.

→ Implementation of a **new screening correction** which:

- avoids complete calculation of leptonic and nuclear matrix elements
- is available only for allowed transitions up-to-now

$$C_{sc} = 1 - \frac{\Delta R_{unsc}}{\Delta R_{sc}} \cdot \left(1 - \frac{f_{sc}}{f_{unsc}} \right) \left\{ \begin{array}{l} \text{exchange formalism} \\ \rightarrow f \text{ factor} \\ \text{mean value} \\ \rightarrow \text{spatial extension} \end{array} \right. \quad \begin{array}{l} f^{-1} = \frac{\overline{g_{-1}^2}}{g_{-1}^2 + f_{-1}^2} \\ \overline{g_{\kappa}^2} = \frac{1}{\Delta R} \int_{\Delta R} g_{\kappa}^2(r) dr \end{array}$$

Electron wave function

→ spherical symmetry

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

Radial component → Spin-angular functions → spherical harmonics expansion

Dirac equation

→ system of coupled differential equations

$$\begin{cases} \frac{df_{\kappa}}{dr} = \frac{(\kappa - 1)}{r} f_{\kappa} - [W - 1 - V(r)] g_{\kappa} \\ \frac{dg_{\kappa}}{dr} = [W + 1 - V(r)] f_{\kappa} - \frac{(\kappa + 1)}{r} g_{\kappa} \end{cases}$$

Power series expansion (exact solutions)

regular singular $r = 0$ → ordinary $r = r_0$ → irregular singular $r = \infty$

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

$$\begin{Bmatrix} rf(r) \\ rg(r) \end{Bmatrix} = \sum_{n=0}^{\infty} \begin{Bmatrix} a_n \\ b_n \end{Bmatrix} (r - r_0)^n$$

$$\begin{Bmatrix} f_{\infty j}(r) \\ g_{\infty j}(r) \end{Bmatrix} = \frac{r^{-1+yt_0/p}}{W(W+1)} e^{t_0 r} \sum_{n=0}^{\infty} \begin{Bmatrix} a_n \\ b_n \end{Bmatrix} r^{-n}$$

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

Global potential

Point charge **Exchange potential**

$$V(r) = -\frac{\alpha Z}{r} \phi(r) - V_{ex}(r)$$

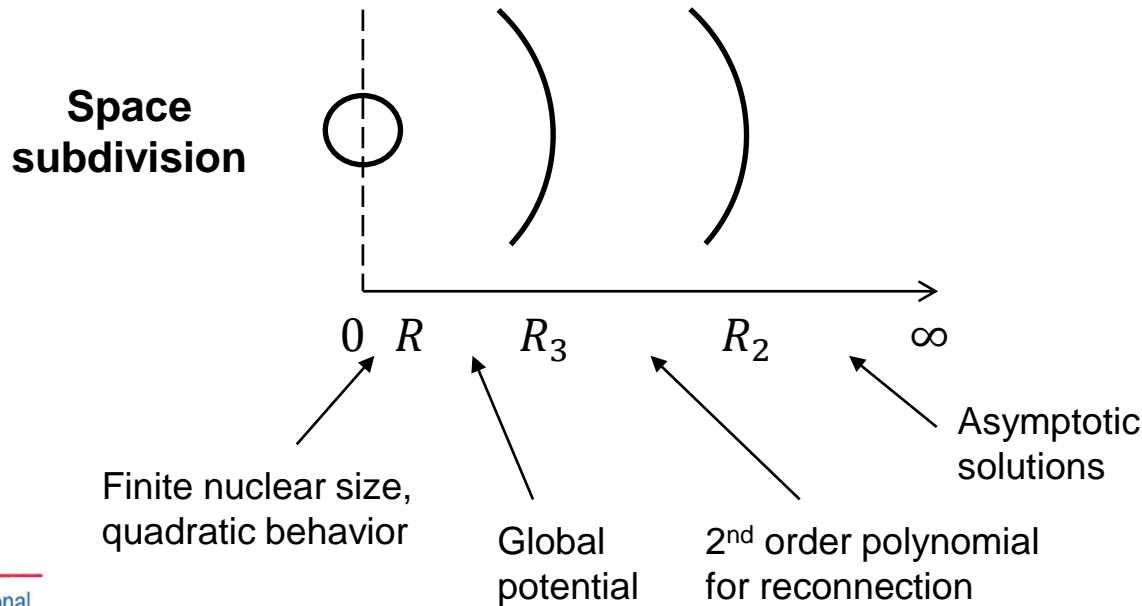
$$V_{ex}(r) = K \frac{3\alpha}{2} \left(\frac{3Z}{4\pi^2} \right)^{1/3} \left[\frac{1}{r} \frac{d^2 \phi(r)}{dr^2} \right]^{1/3}$$

for atomic electrons (**fermions**)

Screened potential

$$\phi(r) = \sum_{i=1}^N a_i e^{-\beta_i r}$$

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



A power series expansion of the global potential is required.

- For bound states, the **orbital energy** is **not known** in advance
→ **iterative procedure**
- **Orbital energy** → Oscillation frequency of the wave functions
→ **Accuracy** of the **overlap**

⇒ **Adjustment** of V_{ex} to reach the “good” energies in

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

Inspection

Useful **tabulated parameters** for β spectra, electron capture, electron polarization, β - γ angular correlation, etc.

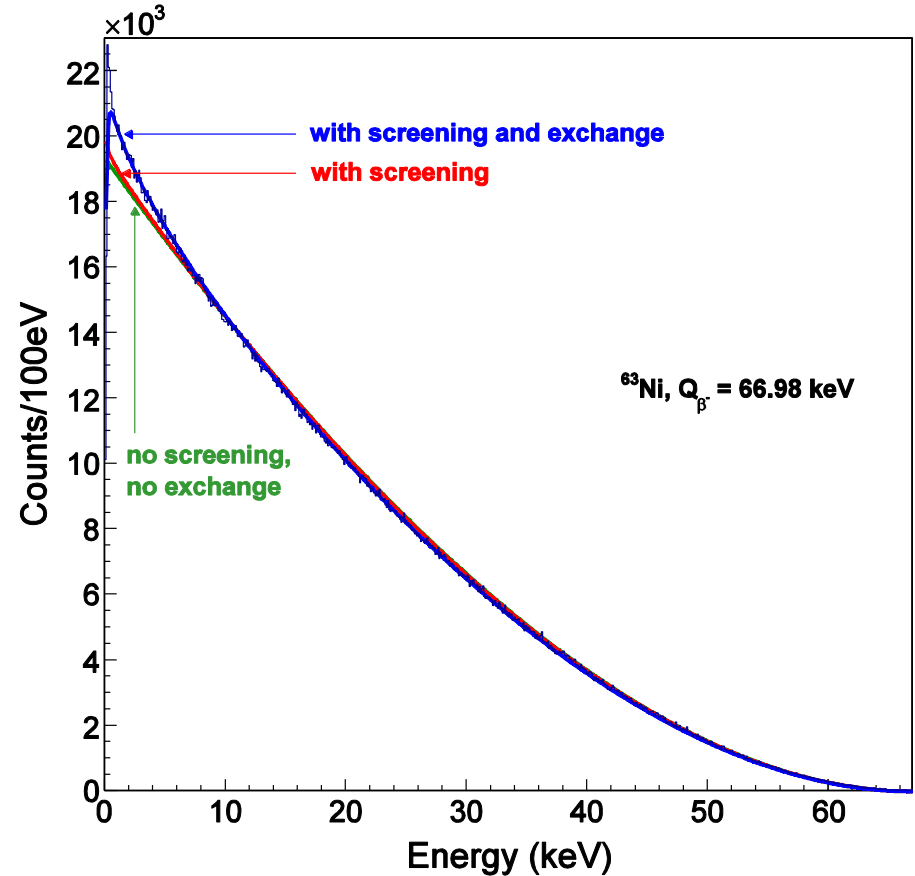
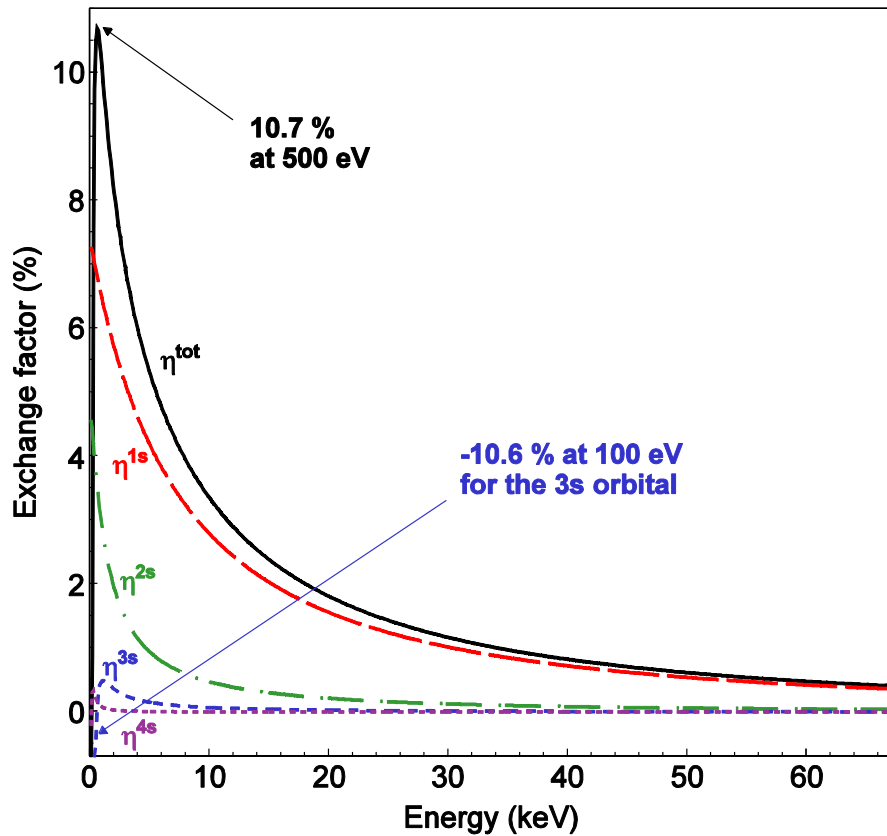
Tabulated **screened** parameters $F_0 L_0^*/F_0 L_0$ and λ_2^*/λ_2 **only**, but for **very few energies**

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

For both the continuum and bound wave functions,

Without screening: parameters perfectly reproduced

With screening: parameters in excellent agreement, despite different potentials



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

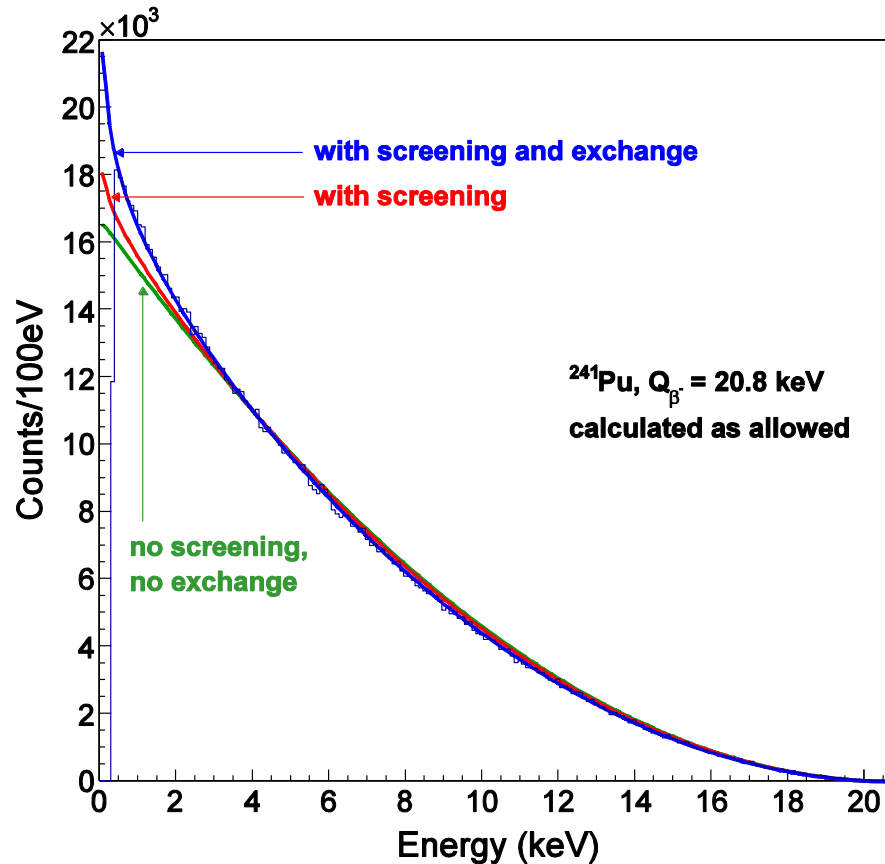
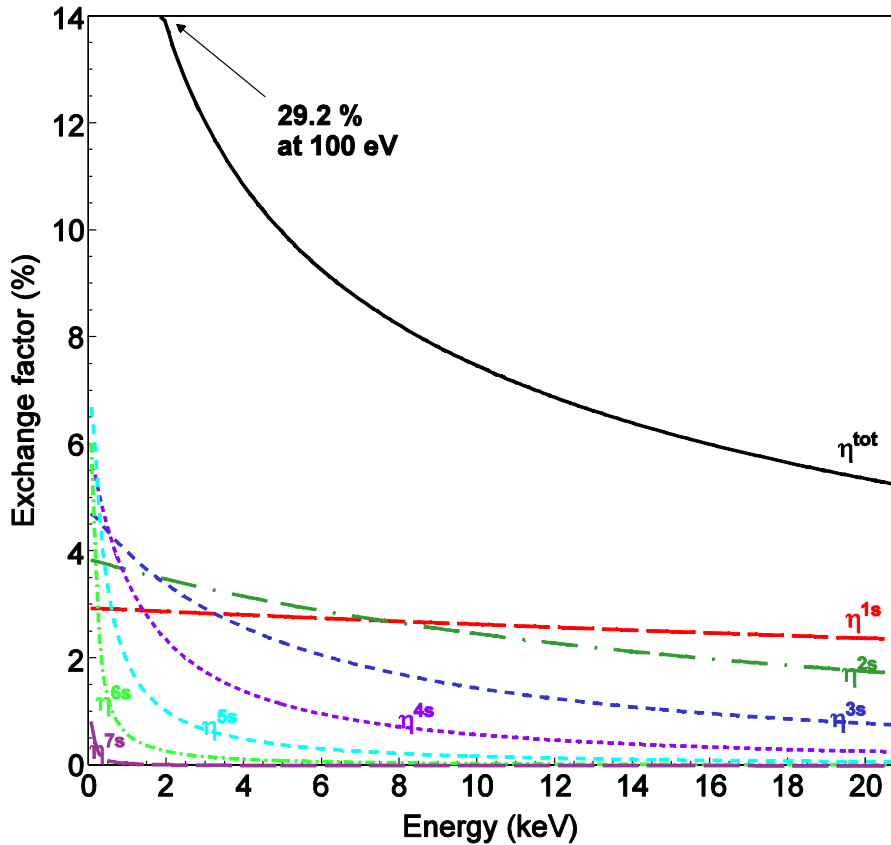
With screening: $\bar{E} = 17.40$ keV

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

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

Allowed transition
Experimental spectrum

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



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

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

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

Mean energy of the spectrum decreased by 4 %

Calculated as **allowed**
Experimental spectrum

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

Modelisation error $\hat{e}_i = y_i - y_i^{th}$

Fit quality $R^2 = 1 - \frac{\text{var}(\hat{e}_i)}{\text{var}(y_i)} \rightarrow (1 - R^2)$ is the **disagreement**

Here, 2 parameters: endpoint energy, global normalization on data

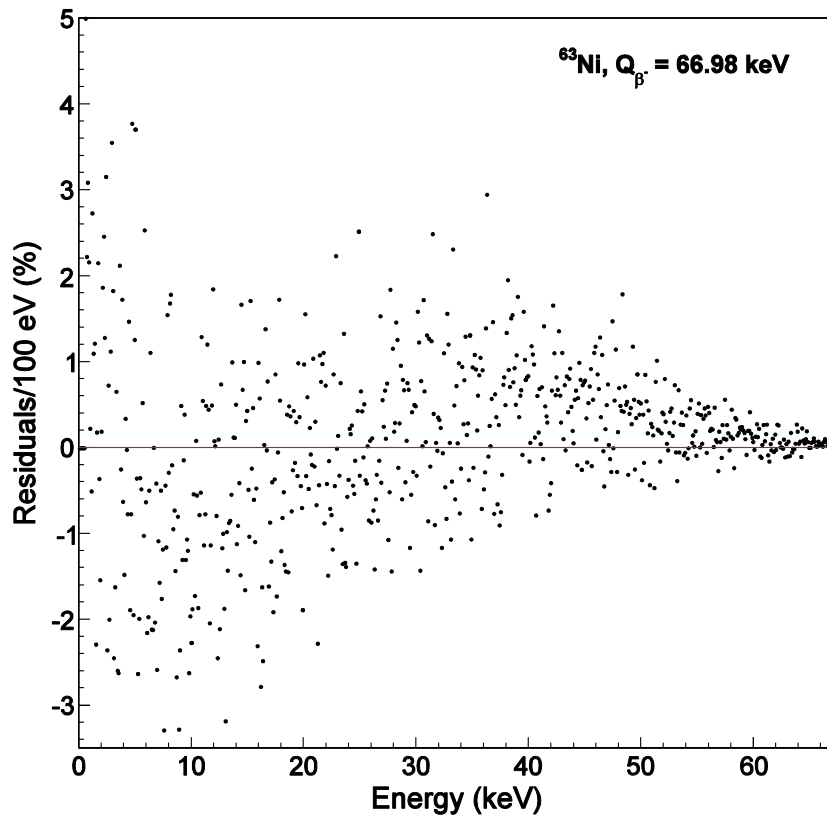
Standardized residuals $r_i = \frac{\hat{e}_i}{\sqrt{\text{var}(\hat{e}_i)}}$

If almost equally distributed around zero \rightarrow gaussian

$$\sigma_{r_i} = \sqrt{\text{var}(r_i)}$$

is an estimate of the **overall uncertainty** of the calculated spectrum

In $[500 \text{ eV}, E_{\max}]$ for both ^{63}Ni and ^{241}Pu beta spectra

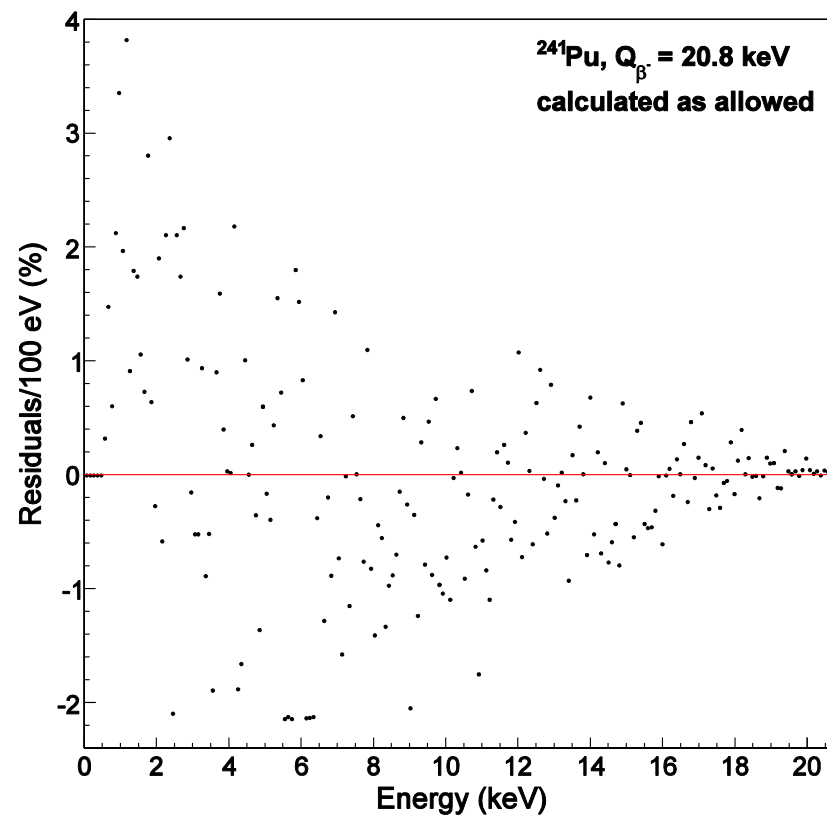


$$\bar{r}_i = 0.093 \%$$

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

$$\sigma_{r_i} = 1.03 \%$$

Residuals mean
Disagreement
Global uncertainty



$$\bar{r}_i = 0.0019 \%$$

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

$$\sigma_{r_i} = 0.99 \%$$

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

Conclusion

Exchange and **screening** effects have been demonstrated to have a **great influence** on the **spectrum shape at low energy**.

→ Explicit calculation of **exchange** and **screening** for **forbidden unique** transitions is needed and **must be compared to new measurements**.

$\lambda_k = 1$ is generally a bad approximation.

ξ approximation is correct **only** for ~ 50 % of the **1st forbidden non-unique** transitions, and **incorrect** for **all** other **non-unique** transitions.

Within 2 – 3 years (hopefully)

Collaboration with nuclear theorists from IPHC Strasbourg to evaluate the **influence** of the **nuclear matrix elements** in order to **calculate specifically** the **forbidden non-unique** transitions.

→ We aim for a code that accounts **consistently** for **the atomic and nuclear structure effects**.

Thank you for your attention



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