FROM RESEARCH TO INDUSTRY

cea tech

Calculation of beta decays

CEA Saclay – LNHB

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Outline

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

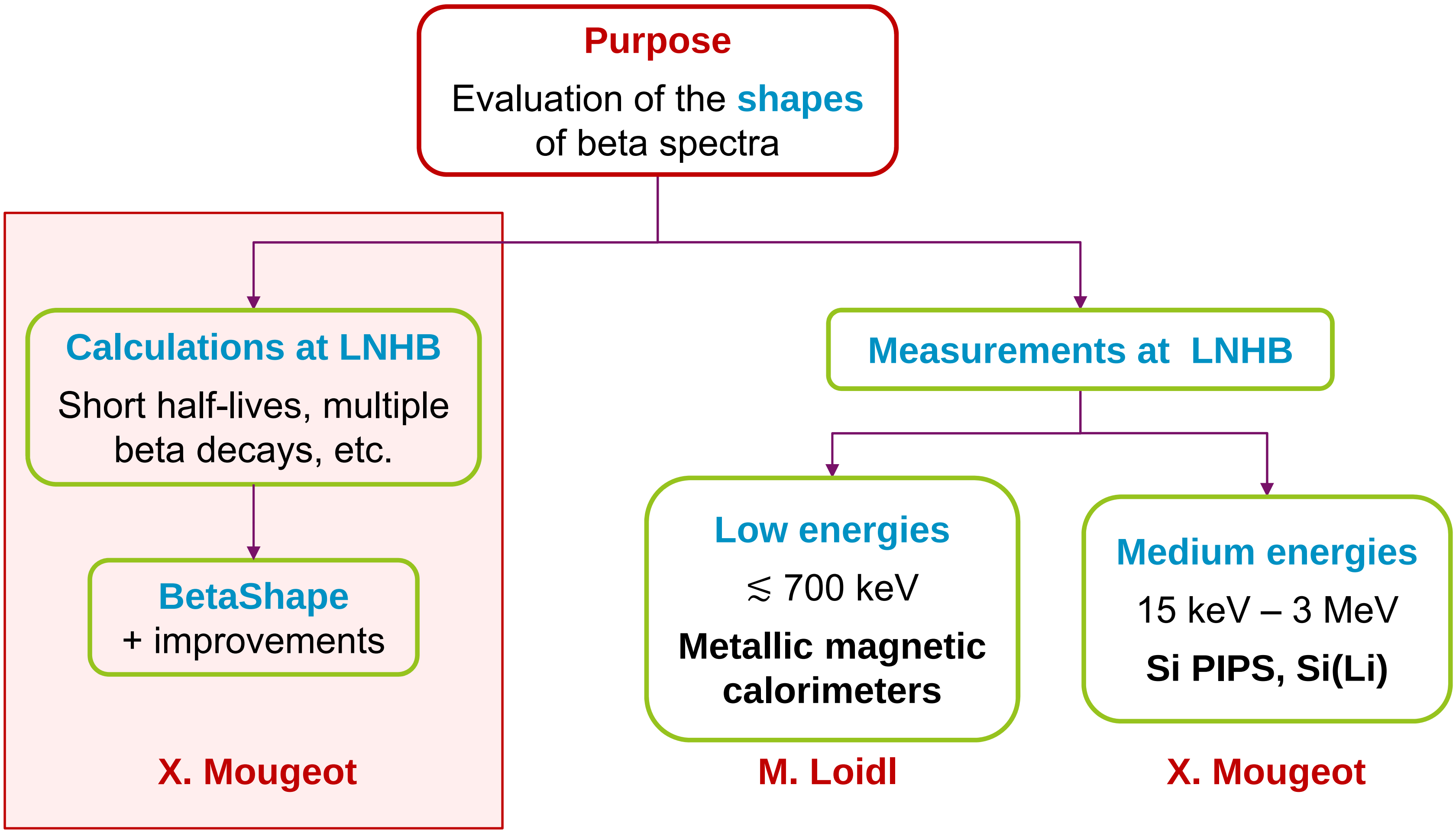
→ **Systematic comparison** with 130 **experimental shape factors**

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

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

Electron capture probabilities

Evaluation of beta spectra shapes



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Behrens & Bühring

Similarly we obtain for the space components

$$\langle p|\,\mathbf{V}+\mathbf{A}\,|n\rangle = iu_p^+\gamma_4\gamma_\mu(1+\lambda\gamma_5)u_n = \sqrt{\frac{(W_n+M_n)}{2W_n}}\sqrt{\frac{(W_p+M_p)}{2W_p}}\begin{pmatrix}0 & i\sigma\\ i\sigma & 0\end{pmatrix}\lambda\begin{pmatrix}0&1\\1&0\end{pmatrix}$$

$$\times\left\{\left(\frac{\sigma p}{W_p+M_p}\chi_p^{m'}\right)^+\sigma\chi_n^m+(\chi_p^{m'})^+\sigma\frac{\sigma p}{W_n+M_n}\chi_n^m-\lambda(\chi_p^{m'})^+\sigma\chi_n^m\right.$$

$$\left.-\lambda\left[\left(\frac{\sigma p}{W_p+M_p}\chi_p^{m'}\right)^+\sigma\frac{\sigma p}{W_n+M_n}\chi_n^m\right]\right\}. \quad (6.38)$$

This equals to

$$\langle p|\,\mathbf{V}+\mathbf{A}\,|n\rangle = \sqrt{\frac{(W_n+M_n)}{2W_n}}\sqrt{\frac{(W_p+M_p)}{2W_p}}\left\{(\chi_p^{m'})^+\underbrace{\frac{\sigma \mathbf{p}_p}{W_p+M_p}\sigma}_{\frac{\mathbf{p}_p+i(\sigma\times\mathbf{p}_p)}{W_p+M_p}}\chi_n^m\right.$$

$$+(\chi_p^{m'})^+\underbrace{\sigma\frac{\sigma \mathbf{p}_n}{W_n+M_n}}_{\frac{\mathbf{p}_n-i(\sigma\times\mathbf{p}_n)}{W_n+M_n}}\chi_n^m-\lambda(\chi_p^{m'})^+\sigma\chi_n^m$$

$$\left.-\lambda\left[(\chi_p^{m'})^+\underbrace{\frac{\sigma \mathbf{p}_p}{W_p+M_p}\sigma\frac{\sigma\mathbf{p}_n}{W_n+M_n}}_{\frac{-(\mathbf{p}_p\mathbf{p}_n)\sigma+(\sigma\mathbf{p}_p)\mathbf{p}_n+\mathbf{p}_p(\sigma\mathbf{p}_n)-i(\mathbf{p}_p\times\mathbf{p}_n)}{(W_p+M_p)(W_n+M_n)}}\chi_n^m\right]\right\}. \quad (6.39)$$

Finally we obtain for the space components

$$\langle p|\,\mathbf{V}(0)+\mathbf{A}(0)\,|n\rangle = \sqrt{\frac{(W_n+M_n)}{2W_n}}\sqrt{\frac{(W_p+M_p)}{2W_p}}$$

$$\times\left\{\left[\frac{\mathbf{p}_p}{W_p+M_p}+\frac{\mathbf{p}_n}{W_n+M_n}\right](\chi_p^{m'})^+\chi_n^m+(\chi_p^{m'})^+\right.$$

$$\times\left[\frac{i(\sigma\times\mathbf{p}_p)}{W_p+M_p}-\frac{i(\sigma\times\mathbf{p}_n)}{W_n+M_n}\right]\chi_n^m-\lambda(\chi_p^{m'})^+\sigma\chi_n^m$$

$$+\lambda\frac{\mathbf{p}_p\mathbf{p}_n}{(W_p+M_p)(W_n+M_n)}\{(\chi_p^{m'})^+\sigma\chi_n^m\}+\lambda\frac{i(\mathbf{p}_p\times\mathbf{p}_n)}{(W_p+M_p)(W_n+M_n)}$$

$$\left.\times(\chi_p^{m'})^+\chi_n^m-\lambda\left[(\chi_p^{m'})^+\frac{(\sigma\mathbf{p}_p)\mathbf{p}_n+\mathbf{p}_p(\sigma\mathbf{p}_n)}{(W_p+M_p)(W_n+M_n)}\chi_n^m\right]\right\}. \quad (6.40)$$

$$-\frac{i}{2M_A}F_M(q^2)(\mathbf{P}\times\mathbf{q})\sigma-F_S(q^2)q_0+\frac{1}{4(2M_A)^2}F_S(q^2)q_0(\mathbf{P}^2-\mathbf{q}^2)$$

$$-\frac{i}{2}\frac{1}{(2M_A)^2}F_S(q^2)q_0(\mathbf{P}\times\mathbf{q})\sigma\Big\}\chi^{M_i} \quad (9.15)$$

$$\langle\phi_f(p_f)|\,A_0(0)\,|\phi_i(p_i)\rangle = N(\chi^{M_f})^+\Big\{-\frac{1}{2M_A}F_A(q^2)(\mathbf{P}\sigma)$$

$$-\frac{q_0}{2M_A}F_P(q^2)(\mathbf{q}\sigma)-F_T(q^2)(\mathbf{q}\sigma)+\frac{1}{4}\frac{1}{(2M_A)^2}F_T(q^2)$$

$$\times[(\mathbf{Pq})(\sigma\mathbf{P}+\sigma\mathbf{q})-(\sigma\mathbf{q})(\mathbf{P}^2-\mathbf{q}^2)]\Big\}\chi^{M_i} \quad (9.16)$$

$$\langle\phi_f(p_f)|\,\mathbf{V}(0)\,|\phi_i(p_i)\rangle = N(\chi^{M_f})^+\Big\{\frac{1}{2M_A}F_V(q^2)\mathbf{P}+\frac{i}{2M_A}F_V(q^2)(\sigma\times\mathbf{q})$$

$$+iF_M(q^2)(\sigma\times\mathbf{q})-\frac{1}{2M_A}F_M(q^2)q_0\mathbf{q}-\frac{i}{4M_A}F_M(q^2)q_0(\sigma\times\mathbf{P})$$

$$-F_S(q^2)\mathbf{q}+\frac{1}{4(2M_A)^2}F_S(q^2)\mathbf{q}(\mathbf{P}^2-\mathbf{q}^2)-\frac{i}{2(2M_A)^2}F_S(q^2)\mathbf{q}$$

$$\times((\mathbf{P}\times\mathbf{q})\sigma)-\frac{i}{2(2M_A)^2}F_M(q^2)\mathbf{P}((\mathbf{P}\times\mathbf{q})\sigma)-\frac{i}{4(2M_A)^2}$$

$$\times F_M(q^2)(\mathbf{P}^2+\mathbf{q}^2)(\sigma\times\mathbf{q})+\frac{i}{2(2M_A)^2}F_M(q^2)(\mathbf{Pq})(\sigma\times\mathbf{P})\Big\}\chi^{M_i} \quad (9.17)$$

$$\langle\phi_f(p_f)|\,\mathbf{A}(0)\,|\phi_i(p_i)\rangle = N(\chi^{M_f})^+\Big\{-F_A(q^2)\sigma+\frac{1}{2(2M_A)^2}$$

$$\times F_A(q^2)\mathbf{P}^2\sigma-\frac{1}{4(2M_A)^2}F_A(q^2)(\mathbf{P}^2+\mathbf{q}^2)\sigma-\frac{i}{2(2M_A)^2}$$

$$\times F_A(q^2)(\mathbf{P}\times\mathbf{q})-\frac{1}{2(2M_A)^2}F_A(q^2)[(\sigma\mathbf{P})\mathbf{P}-(\sigma\mathbf{q})\mathbf{q}]$$

$$+\frac{1}{2M_A}F_T(q^2)[(\mathbf{Pp})\sigma-\mathbf{q}(\sigma\mathbf{P})]-F_T(q^2)q_0\sigma$$

$$+\frac{1}{2(2M_A)^2}F_T(q^2)q_0\mathbf{P}^2\sigma-\frac{1}{4(2M_A)^2}F_T(q^2)q_0(\mathbf{P}^2+\mathbf{q}^2)\sigma$$

$$-\frac{i}{2(2M_A)^2}F_T(q^2)q_0(\mathbf{P}\times\mathbf{q})-\frac{1}{2(2M_A)^2}F_T(q^2)q_0[(\sigma\mathbf{P})\mathbf{P}$$

$$-(\sigma\mathbf{q})\mathbf{q}]-\frac{1}{2M_A}F_P(q^2)(\sigma\mathbf{q})\mathbf{q}\Big\}\chi^{M_i}. \quad (9.18)$$

454 SPECIAL FORMULAE

$$+\sqrt{\tfrac{2}{3}}\left(\int rI'(r)\beta\gamma_5T_{121}\right)\Big\}$$

$$\mp\frac{f_P}{R}(W_0R\pm\tfrac{6}{5}\alpha Z)\,{}^{D}\mathfrak{M}^{(0)}_{110}(1,1,1,1) \quad (14.101)$$

$${}^{A}F^{(0)}_{121}=\mp\lambda\,{}^{A}\mathfrak{M}^{(0)}_{121}-\frac{f_T}{R}\left[\frac{5}{\sqrt{3}}\,{}^{C}\mathfrak{N}^{(0)}_{111}-(W_0R\pm\tfrac{6}{5}\alpha Z)\,{}^{A}\mathfrak{M}^{(0)}_{121}\right]\mp\frac{f_P}{R}5\sqrt{\tfrac{2}{3}}\,{}^{D}\mathfrak{N}^{(0)}_{110} \quad (14.102)$$

$${}^{A}F^{(0)}_{121}(1,1,1,1)=\mp\lambda\,{}^{A}\mathfrak{M}^{(0)}_{121}(1,1,1,1)$$

$$-\frac{f_T}{R}\Big\{\sqrt{\tfrac{1}{3}}\left(\int\left(\frac{r}{R}\right)[5I(r)+rI'(r)]\beta T_{111}\right)$$

$$-(W_0R\pm\tfrac{6}{5}\alpha Z)\,{}^{A}\mathfrak{M}^{(0)}_{121}(1,1,1,1)\Big\}$$

$$\mp\frac{f_P}{R}\sqrt{\tfrac{2}{3}}\left(\int\left(\frac{r}{R}\right)[5I(r)+rI'(r)]\beta\gamma_5T_{110}\right) \quad (14.103)$$

$${}^{V}F^{(0)}_{211}=-{}^{V}\mathfrak{M}^{(0)}_{211}-\frac{f_M}{R}(W_0R\pm\tfrac{6}{5}\alpha Z)\,{}^{C}\mathfrak{N}^{(0)}_{211} \quad (14.104)$$

$${}^{V}F^{(0)}_{220}={}^{V}\mathfrak{M}^{(0)}_{220}+\frac{f_M}{R}\sqrt{(10)}\,{}^{C}\mathfrak{N}^{(0)}_{211}\pm\frac{f_S}{R}(W_0R\pm\tfrac{6}{5}\alpha Z)\,{}^{V}\mathfrak{M}^{(0)}_{220} \quad (14.105)$$

$${}^{V}F^{(0)}_{220}(1,1,1,1)={}^{V}\mathfrak{M}^{(0)}_{220}(1,1,1,1)$$

$$+\frac{f_M}{R}\Big\{\sqrt{\tfrac{2}{3}}\left(\int\left(\frac{r}{R}\right)[5I(r)+rI'(r)]\beta T_{211}\right)$$

$$+\sqrt{\tfrac{1}{3}}\left(\int\left(\frac{r}{R}\right)rI'(r)\beta T_{231}\right)\Big\}$$

$$\pm\frac{f_S}{R}(W_0R\pm\tfrac{6}{5}\alpha Z)\,{}^{V}\mathfrak{M}^{(0)}_{220}(1,1,1,1) \quad (14.106)$$

$${}^{A}F^{(0)}_{221}=\pm\lambda\,{}^{A}\mathfrak{M}^{(0)}_{221}+\frac{f_T}{R}[\sqrt{(15)}\,{}^{C}\mathfrak{N}^{(0)}_{211}-(W_0R\pm\tfrac{6}{5}\alpha Z)\,{}^{A}\mathfrak{M}^{(0)}_{221}] \quad (14.107)$$

$${}^{A}F^{(0)}_{221}(1,1,1,1)=\pm\lambda\,{}^{A}\mathfrak{M}^{(0)}_{221}(1,1,1,1)$$

$$+\frac{f_T}{R}\Big\{\sqrt{\tfrac{2}{3}}\left(\int\left(\frac{r}{R}\right)[5I(r)+rI'(r)]\beta T_{211}\right)$$

$$-\sqrt{\tfrac{2}{3}}\left(\int\left(\frac{r}{R}\right)rI'(r)\beta T_{231}\right)$$

$$-(W_0R\pm\tfrac{6}{5}\alpha Z)\,{}^{A}\mathfrak{M}^{(0)}_{221}(1,1,1,1)\Big\} \quad (14.108)$$

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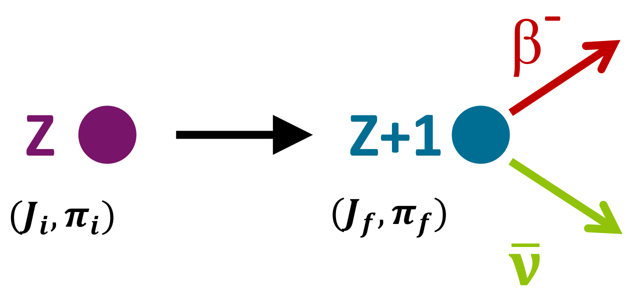
H. Behrens, W. Bühring, *Electron Radial Wave functions and Nuclear Beta Decay*, Oxford Science Publications (1982)

More than 600 p.!

BetaShape (almost analytical)



Beta spectrum $$\frac{dN}{dW} \propto \boxed{p\ W\ q^2}\ \boxed{F_0 L_0}\ \boxed{C(W)}$$

Phase space — Coulomb part (Fermi function) — Shape factor

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

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

$$L = 1 \text{ if } \Delta J = 0$$
$$L = \Delta J \text{ otherwise}$$

$\lambda_k = 1?$

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

if $2\xi = \alpha Z/R \gg E_{\text{max}}$

1^{st} fnu	→	allowed
2^{nd} fnu	→	1^{st} fu
3^{rd} fnu	→	2^{nd} fu

Assumptions → Corrections

- **Improved analytical screening correction** — W. Bühring, Nucl. Phys. A 430, 1 (1984)
- **Nucleus no longer considered as a point charge**
- **Radiative corrections** (virtual photons, internal bremsstrahlung)

Features

- β^-/β^+ spectra
- $\bar{\nu}/\nu$ spectra
- Database of experimental shape factors
- Calculation of individual transitions
- Reading of ENSDF files: total spectrum for all transitions; each spectrum is normalized to the branching ratio.

Systematic comparison

Small database of **130 experimental shape factors**

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

But almost comprehensive!

→ Very few measurements below 50 keV (7)

→ Very few transitions of high forbidding order

→ 10 published shape factors since 1976!

Recently submitted to Physical Review C

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 1^{st} forbidden non-unique transitions, and **incorrect** for all other non-unique transitions

New measurements are needed to test the theoretical predictions

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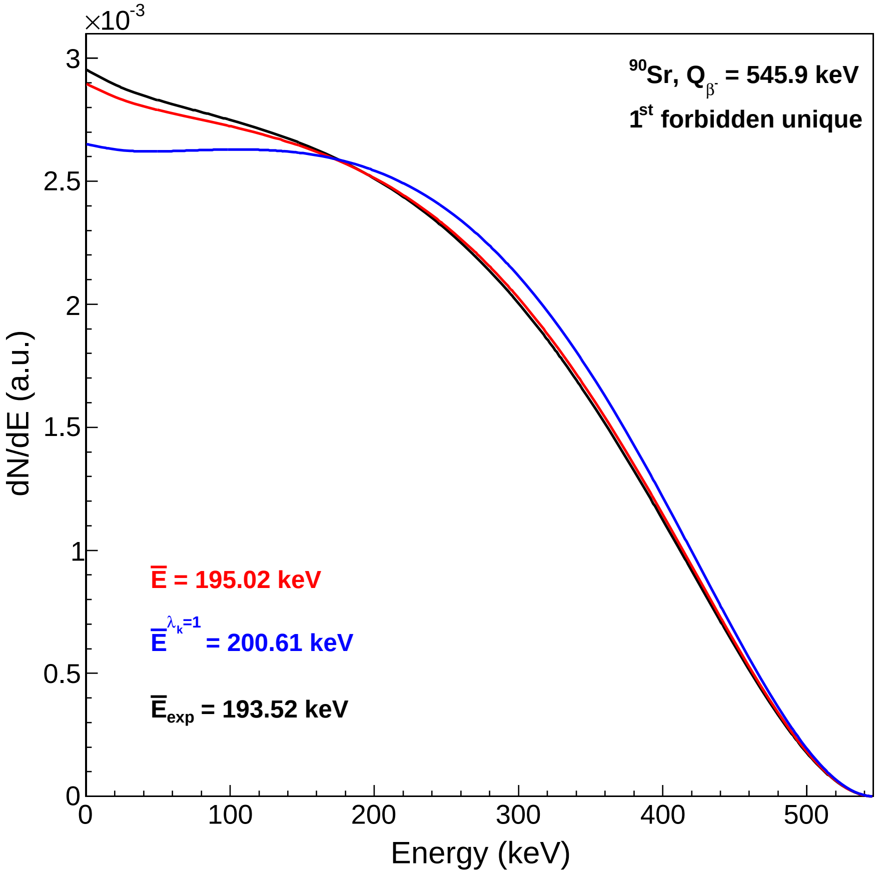
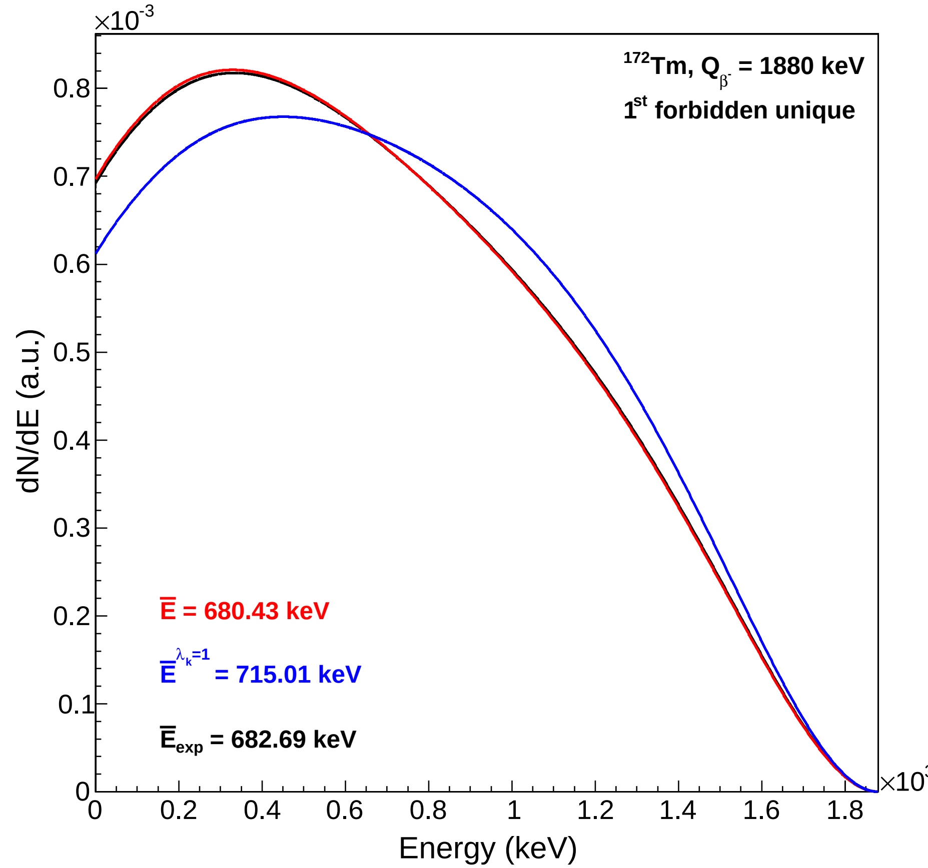
$\lambda_k = 1$ approximation





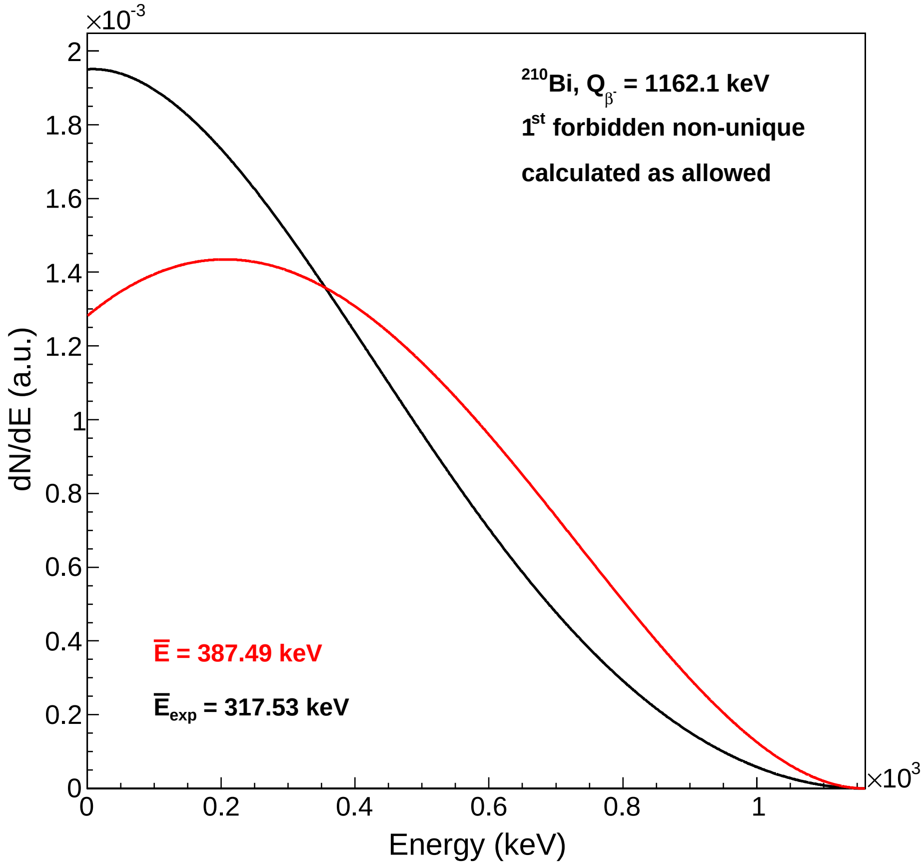
Mean energy disagrees by **3.6 %**

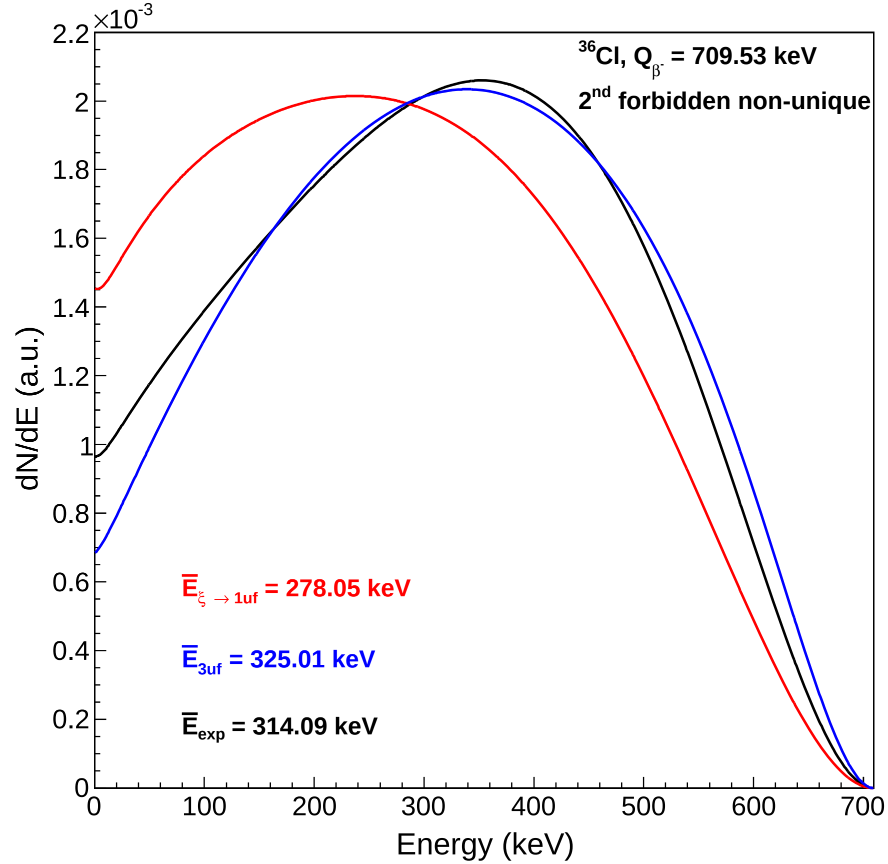
High influence at low energy

Mean energy disagrees by **4.6 %**

High influence at low energy and on the overall shape of the spectrum

ξ approximation





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

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

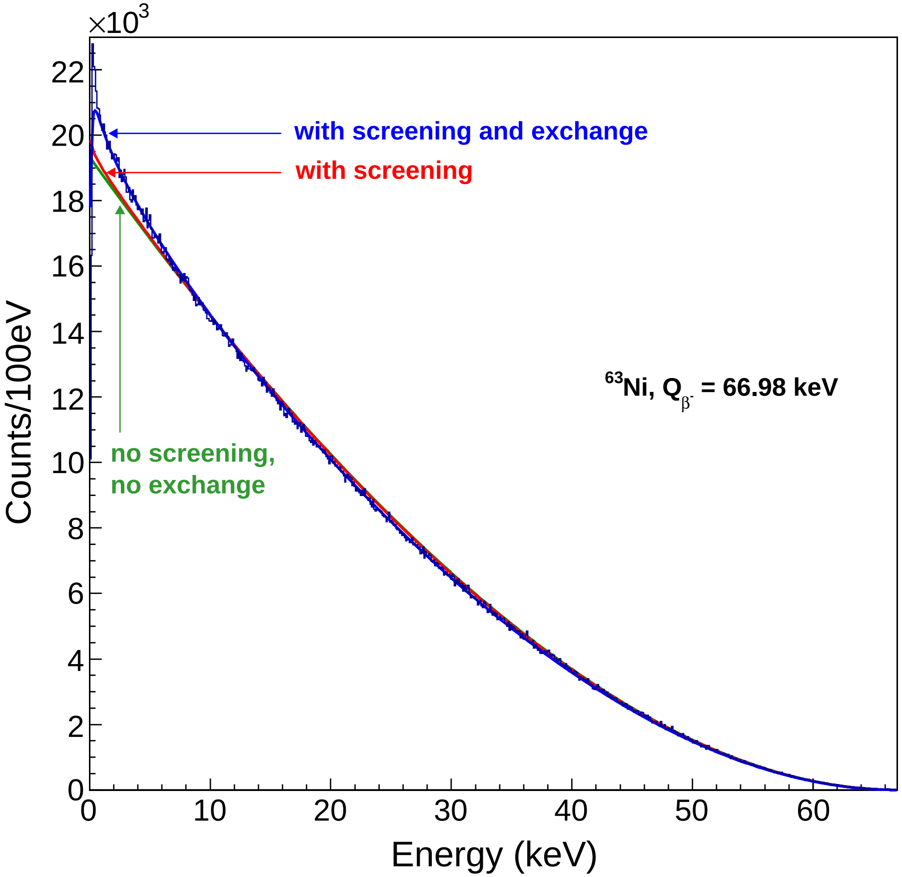
Calculated as **1st forbidden unique**, this spectrum **is not correct**

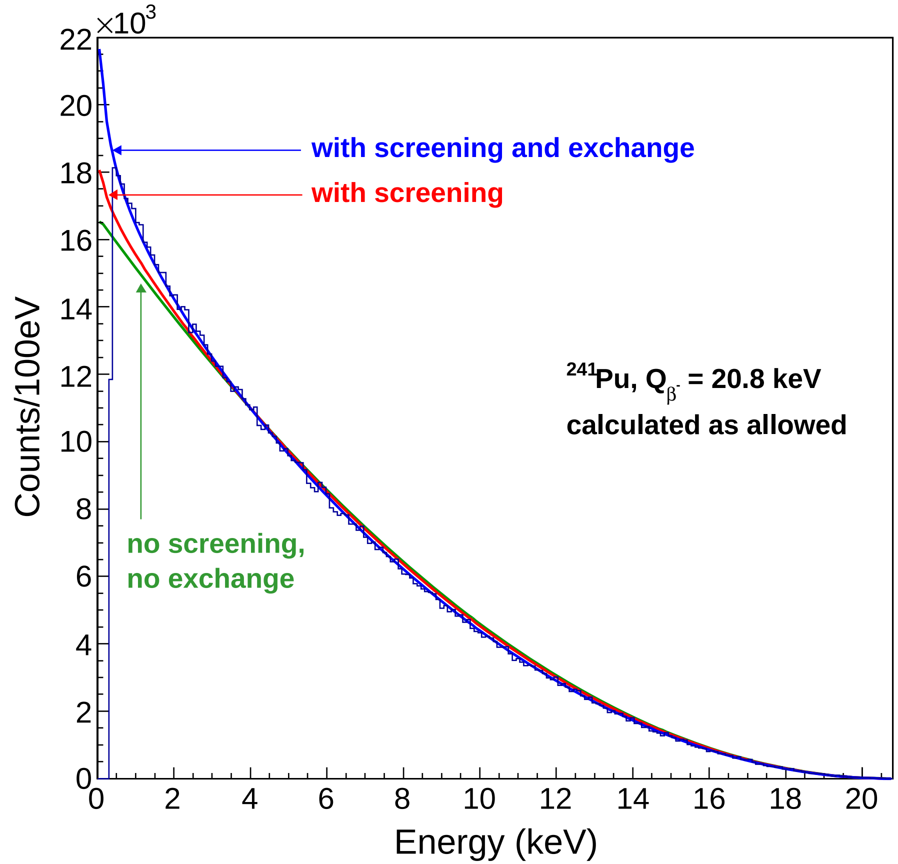
Mean energy disagrees by **14 %** (!)

Better as **3rd forbidden unique** → **justification?**

Further improvements
Atomic effects

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





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

Allowed transition

Experimental spectrum

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

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

Calculated as **allowed**

Experimental spectrum

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

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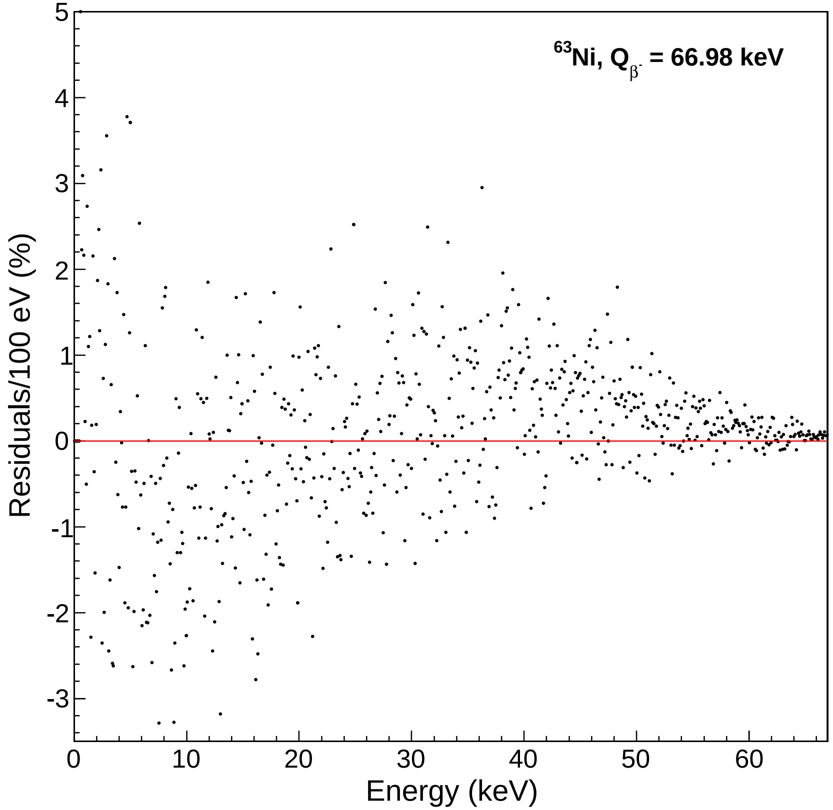
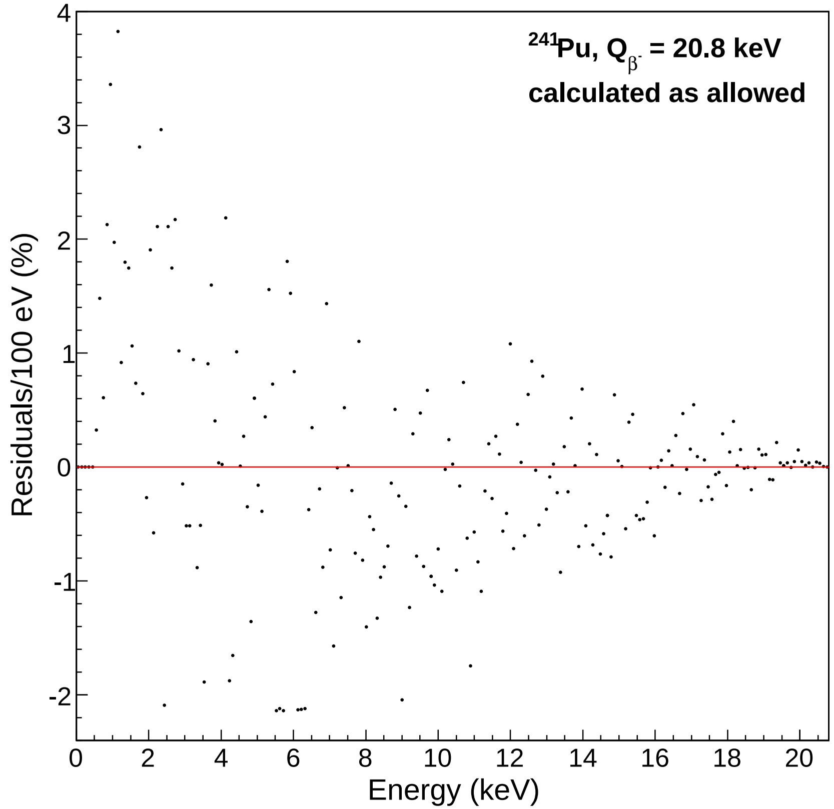
Quality of calculations for ^{63}Ni and ^{241}Pu





^{63}Ni		^{241}Pu
$\bar{r_i} = 0.093\ \%$	**Residuals mean**	$\bar{r_i} = 0.0019\ \%$
$(1 - R^2) = 0.028\ \%$	**Disagreement**	$(1 - R^2) = 0.040\ \%$
$\sigma_{r_i} = 1.03\ \%$	**Global uncertainty**	$\sigma_{r_i} = 0.99\ \%$

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

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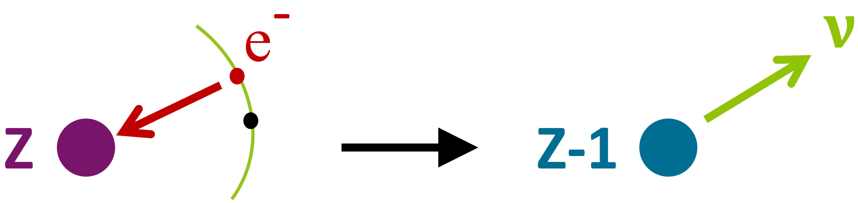
Electron capture probabilities

Electron capture decay



- **Same classification** as for β transitions
- **Allowed** and **forbidden unique** transitions can be calculated **exactly**, but **not forbidden non-unique** transitions

Total capture probability

$$\lambda \propto \sum_{\kappa_x} n_{\kappa_x} C_{\kappa_x} q^2_{\kappa_x} \beta^2_{\kappa_x} B_{\kappa_x}$$

- κ_x: shell quantum number
- n_{κ_x}: relative occupation number
- C_{κ_x}: "shape" factor → similar to $C(W)$
- q_{κ_x}: ν momentum
- β_{κ_x}: amplitude of wave function
- B_{κ_x}: overlap and exchange corrections

In fact, **ratios of relative probabilities** are calculated

$$P_K + P_{L_1} + P_{L_2} + P_{L_3} + P_{M_1} + \cdots = 1$$

$$\rightarrow \quad \frac{P_{L_1}}{P_K}, \quad \frac{P_{L_2}}{P_K}, \quad \frac{P_{L_3}}{P_K}, \ldots \quad \text{and} \quad \frac{\lambda_{EC}}{\lambda_{\beta+}}$$

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

Corrections

- Overlap and exchange corrections

Generalization of two approaches

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

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

- Effect of the inner hole: first order perturbation theory

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

→ **Influence** of the **hole** on the bound wave functions

- Shake-up and shake-off effects

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

Rough evaluation of the **shake-up (atomic excitations)** and **shake-off (internal ionizations)** effects, consecutive to an **electron capture** process
→ Creation of **secondary vacancies**

Conclusion

Conclusion

A dedicated code BetaShape has been developed for decay data evaluations.

- $\lambda_k = 1$ 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.
- **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**.

Preparation of an ENSDF friendly version is in progress in liaison with IAEA

Dedicated code for electron capture probabilities

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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