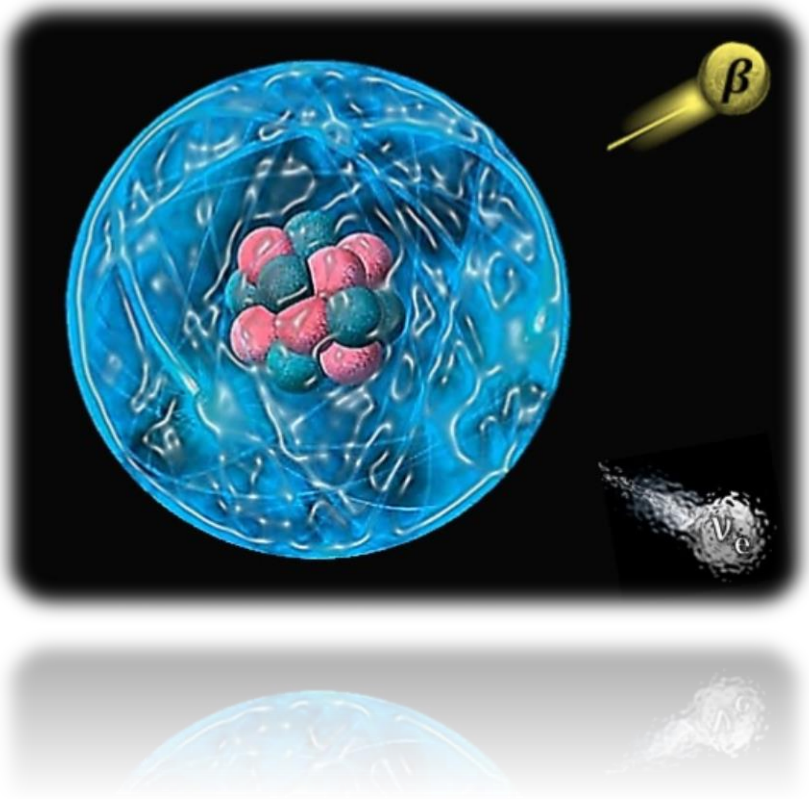

BetaShape

NSDD Meeting April 2019 | Xavier Mougeot

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LogFT

The LogFT program is the current reference code for ENSDF evaluations

- Handles β and ε transitions
- Provides mean energies of β spectra, log *ft* values, β^+ and ε probabilities
- Propagates uncertainties from input parameters
- Reads and writes ENSDF files (*Evaluated Nuclear Structure Data File*)

However

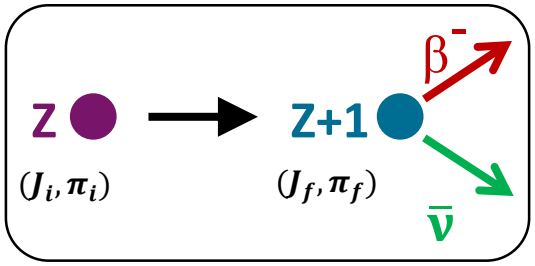
- Too simple analytical models → lack of accuracy
- Forbiddenness limitation (allowed, first- and second- forbidden unique)
- Users now require β spectra and correlated ν spectra
- Users now requires detailed information for many subshells in ε

Beta decays

Physics modelling

Beta spectrum

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



- Behrens and Bühring formalism
- Dirac equation solved numerically for beta particles (with spherical nucleus)
- Bühring screening correction with Salvat's potentials
- Allowed and forbidden unique transitions
- Forbidden non-unique transitions with ξ approximation
- Precise radiative corrections from Hardy's study of superallowed transitions
- Database of experimental shape factors (131 transitions)
- Propagation of uncertainties on Q-values and level energies
- Reads and writes to/from ENSDF files
- Provides beta and neutrino spectra for each transition, total spectrum for a radionuclide, mean energies, log *ft* values and report files

Relativistic electron wave functions

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

Radial component

Spin-angular functions
→ spherical harmonics expansion

Electron wave function
→ spherical symmetry

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

Dirac equation
→ coupled differential equations

Analytical solutions
(approximate)

M.E. Rose, *Relativistic Electron Theory*, Wiley and Sons (1961)

nucleus = point charge + very approximate correction for its spatial extension

LogFT treatment

Power series expansion
(exact solutions)

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

nucleus = uniformly charged sphere
→ fast computation of the solutions

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

BetaShape treatment

Excellent agreement with all the parameters tabulated in

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

Analytical screening corrections

Rose

M.E. Rose, Phys. Rev. 49, 727 (1936)

Thomas-Fermi $V_0(Z, \beta^{\pm})$

$\Rightarrow W \rightarrow W' = W \pm V_0$ in all quantities except in neutrino energy

→ **non-physical discontinuity** for β^- spectrum

→ **identical for all transitions**

N.B. Gove and M.J. Martin, Nucl. Data Tables 10, 205 (1971)

Bühring

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

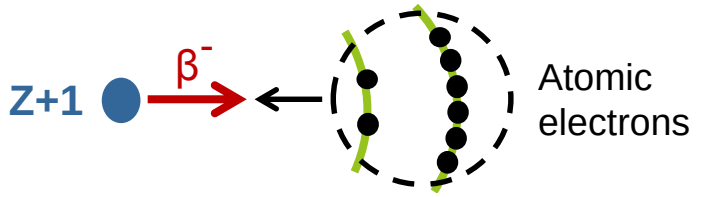
All quantities depend on the normalization of electron wave functions

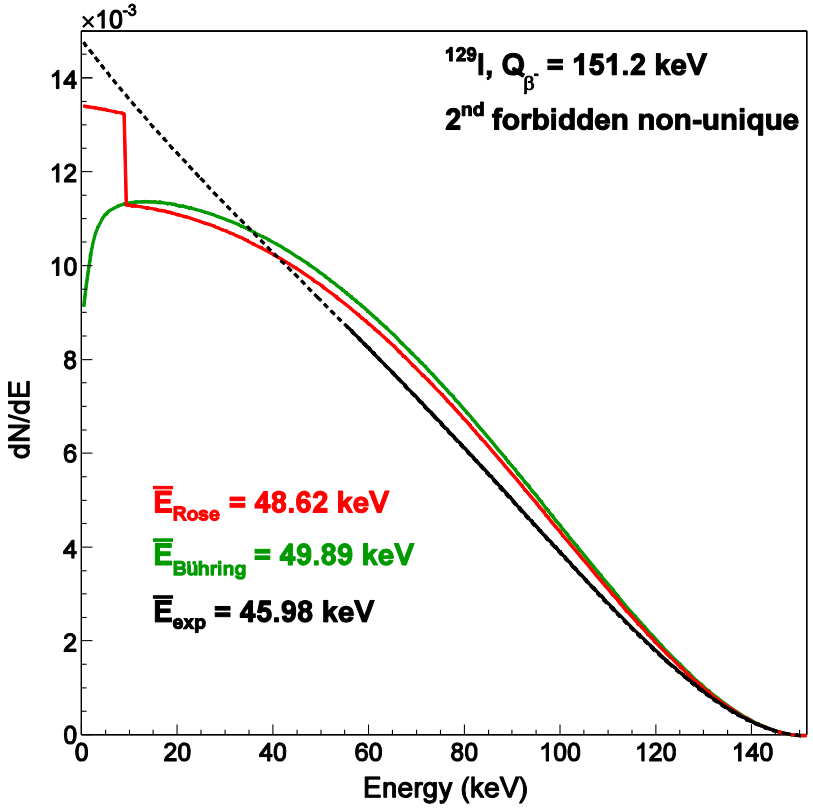
⇒ **Analytical solutions** and **leading order** at the nucleus + **asymptotic** solutions

Hulthén screened potentials → **Salvat's preferred**

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

→ **acting on Fermi function and λ_k parameters, thus different according to the forbiddenness**





More precise + **no breakdown** at low energy

Radiative corrections

Electrons – Old correction

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

Electrons – New correction

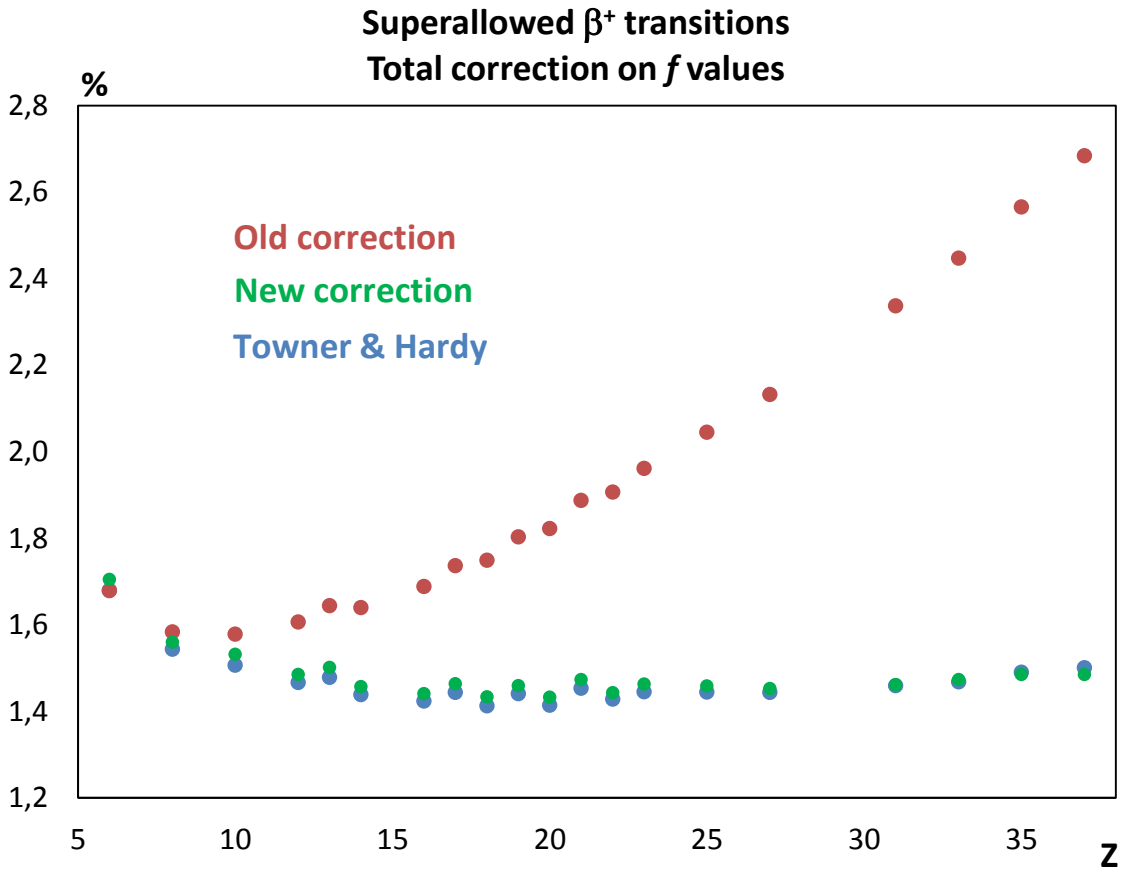
I.S. Towner, J.C. Hardy, PRC 77, 025501 (2008)
A. Czarnecki et al., PRD 70, 093006 (2004)

Neutrinos

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

First version of BetaShape

New version of BetaShape



Calculated quantities

- **Single and total β^+/β^- and $\nu_e/\bar{\nu}_e$ spectra**

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

- **Mean energy** $\bar{E} = \int_0^{E_0} E \cdot N(E)\mathrm{d}E \Big/ \int_0^{E_0} N(E)\mathrm{d}E$

- **Log *ft* value**

☑ $f_{\beta^-} = \int_1^{W_0} N(W)\mathrm{d}W$

☒ $f_{\varepsilon/\beta^+} = f_\varepsilon + f_{\beta^+}$

+ partial half-life from data: $t_i = T_{1/2}/P_\beta$

For allowed and forbidden unique transitions

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

C_x: lepton dynamics

C_{ns}: nuclear structure (allowed, forbidden unique)

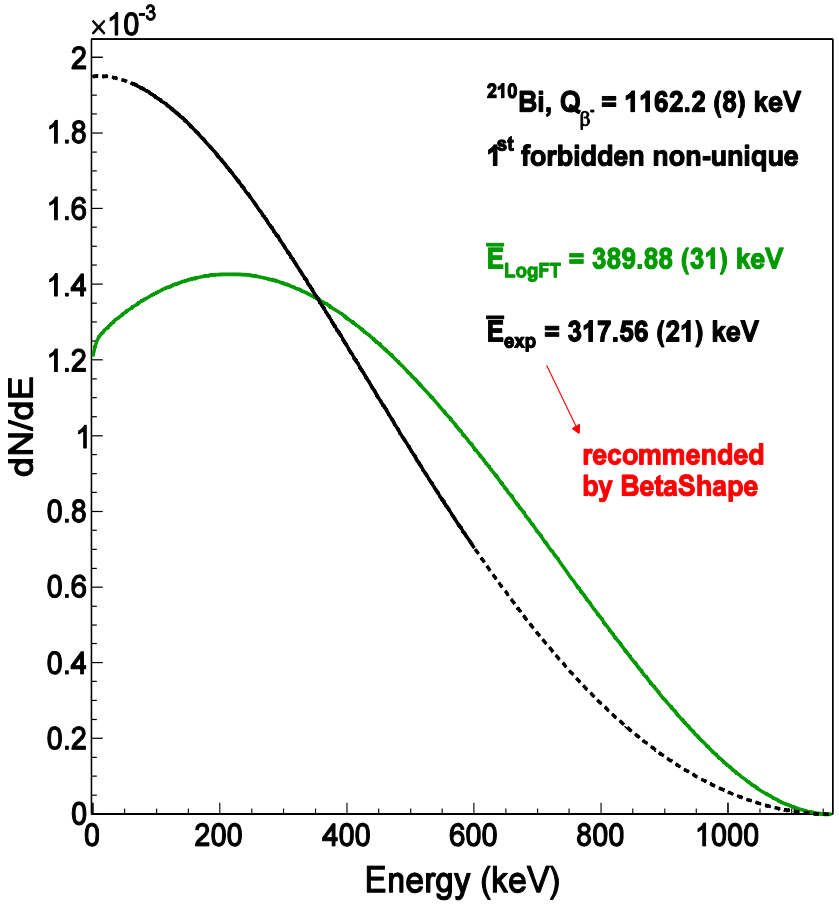
n_x: relative occupation number of the orbital, not accounted for in the LogFT program

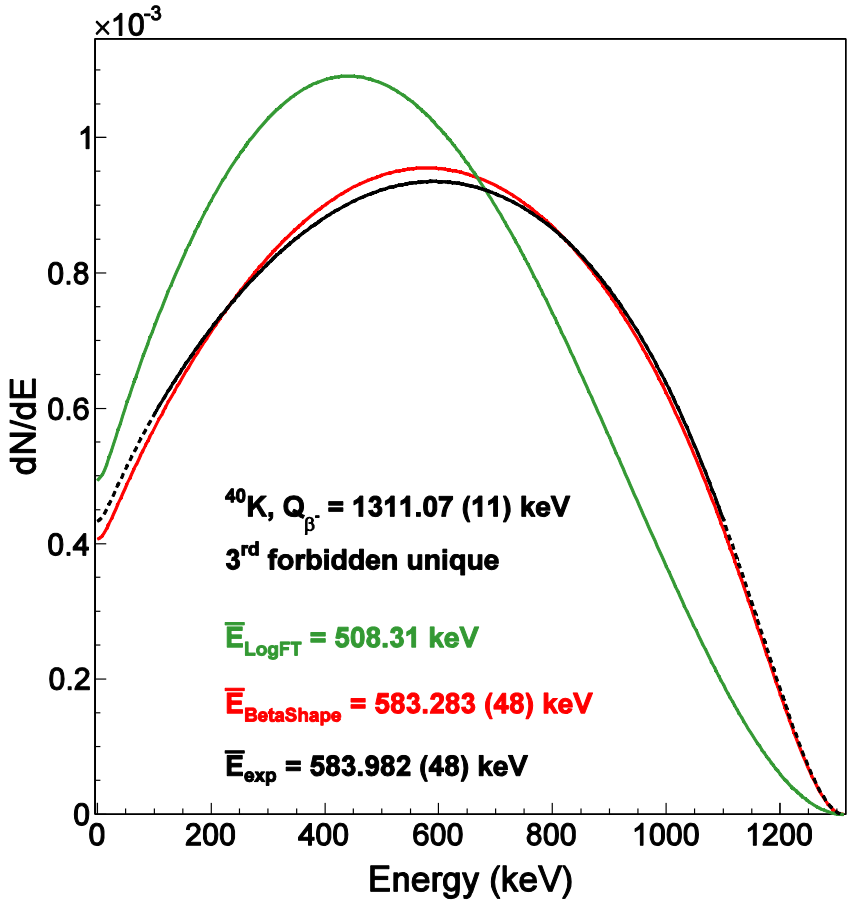
$$\rightarrow \log ft = \log\left(\frac{f_\varepsilon + f_{\beta^+}}{I_\varepsilon + I_{\beta^+}} T_{1/2}\right)$$

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

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

Examples of improved calculations

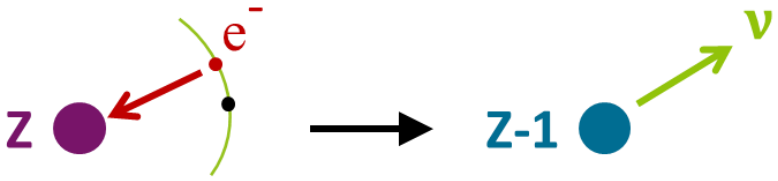




These two transitions are calculated as allowed by the LogFT program.

Electron capture decays

Modelling of electron capture



- Allowed and forbidden unique transitions without nuclear structure
- If transition energy $\geq 2m_e$ → competition with a β^+ transition
- Information provided for each subshell

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
- $\beta^2_{\kappa_x}$: Coulomb amplitude
- $\left(1 + \sum_{m,\kappa} P_{m\kappa}\right)$: shaking effects
- κ_x: shell quantum number
- C_{κ_x}: "shape" factor similar to $C(W)$ in β decay
- B_{κ_x}: overlap and exchange corrections
- $1 + \sum_{m,\kappa} P_{m\kappa}$: + hole effect and radiative corrections

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

Atomic wave functions

Relativistic electron wave functions for the atomic bound states are needed.

The method used was initially developed for the atomic exchange effect in β^- decay calculations.

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

Dirac equation is solved numerically

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

- **Coulomb potential** = **extended nucleus** (uniformly charged sphere)
  + **screened potential** (Coulomb influence of electrons)
  + **exchange potential** (indistinguishability of fermions)

- Iterative procedure to reach atomic energies from relativistic DFT approach with electron correlations
  → Extrapolation from U to Z=120
  → Tabulation of parameters for fast calculation

S. Kotochigova, Phys. Rev. A 56, 5191 (1997)

Overlap and exchange corrections

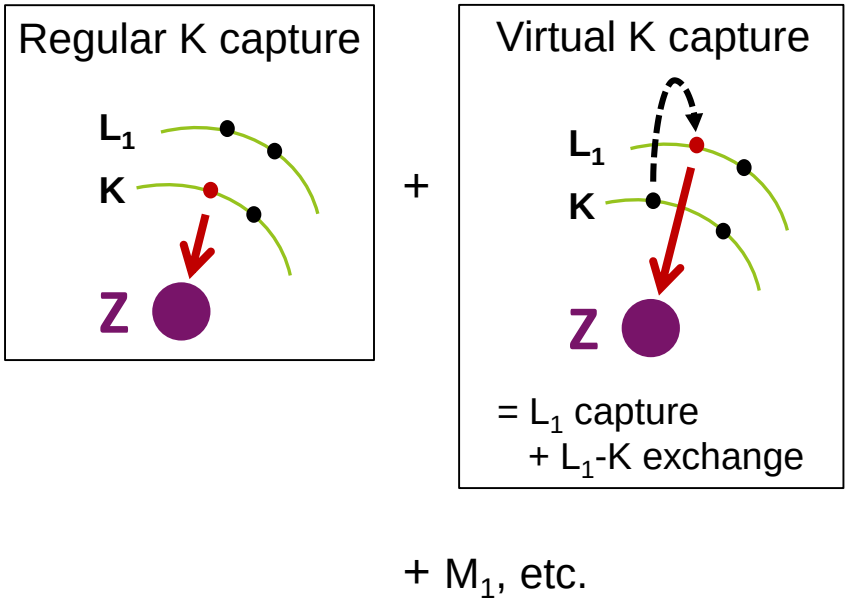
Overlap effect

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?



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
- Best results with Vatai's approach, Bahcall's used to assess uncertainties

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 $(\mathcal{H}_0 + \mathcal{H}')|(i,\kappa)'\rangle = (E_0 + E')|(i,\kappa)'\rangle$

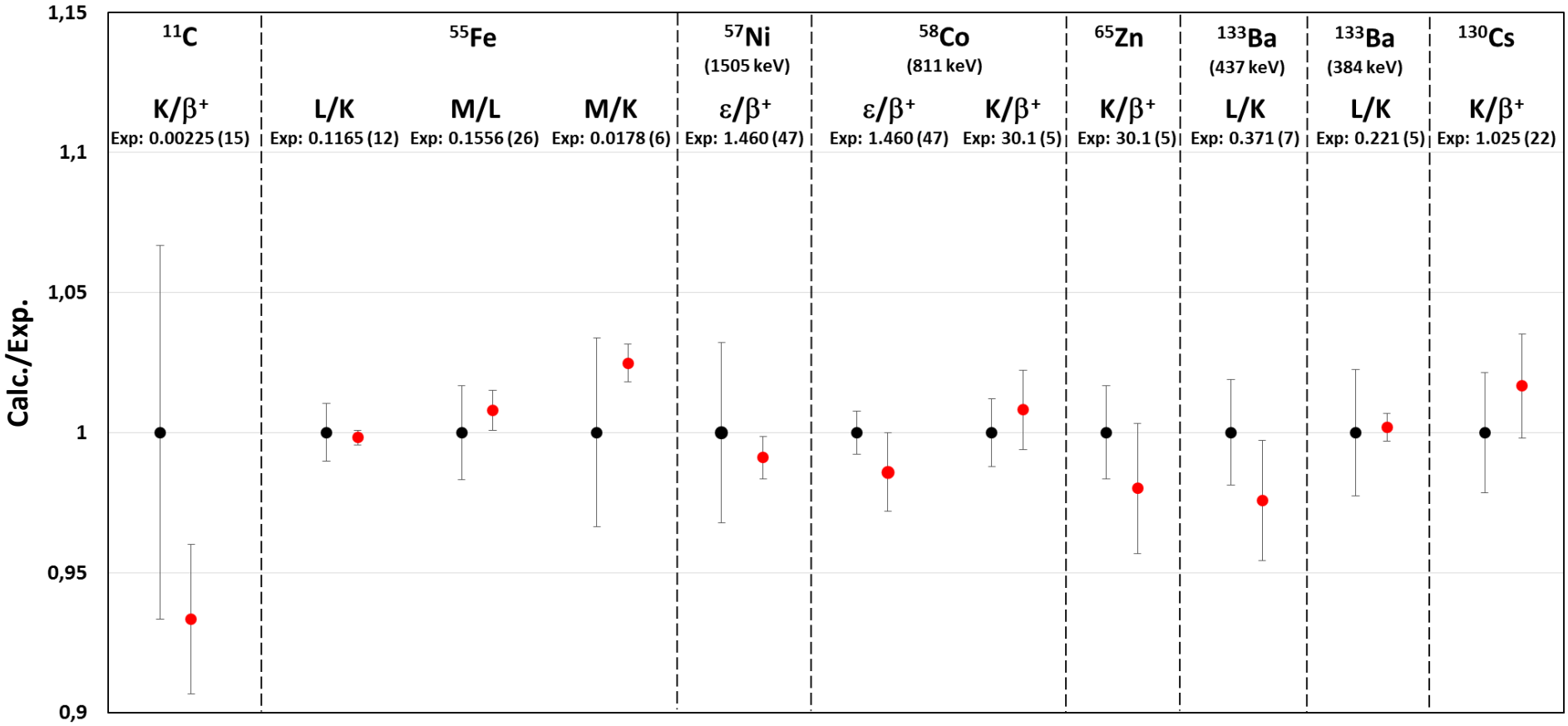
Initial: parent atom **Perturbation**: the electron (n,κ) is captured

$$\mathcal{H}' = \frac{\alpha}{r} - \langle(n,\kappa)|\frac{\alpha}{|\overrightarrow{r_{n\kappa}} - \vec{r}|}|(n,\kappa)\rangle \quad \rightarrow \quad |(i,\kappa)'\rangle = |(i,\kappa)\rangle - \sum_{j\neq i}\frac{\langle(j,\kappa)|\mathcal{H}'|(i,\kappa)\rangle}{W_j - W_i}|(j,\kappa)\rangle$$

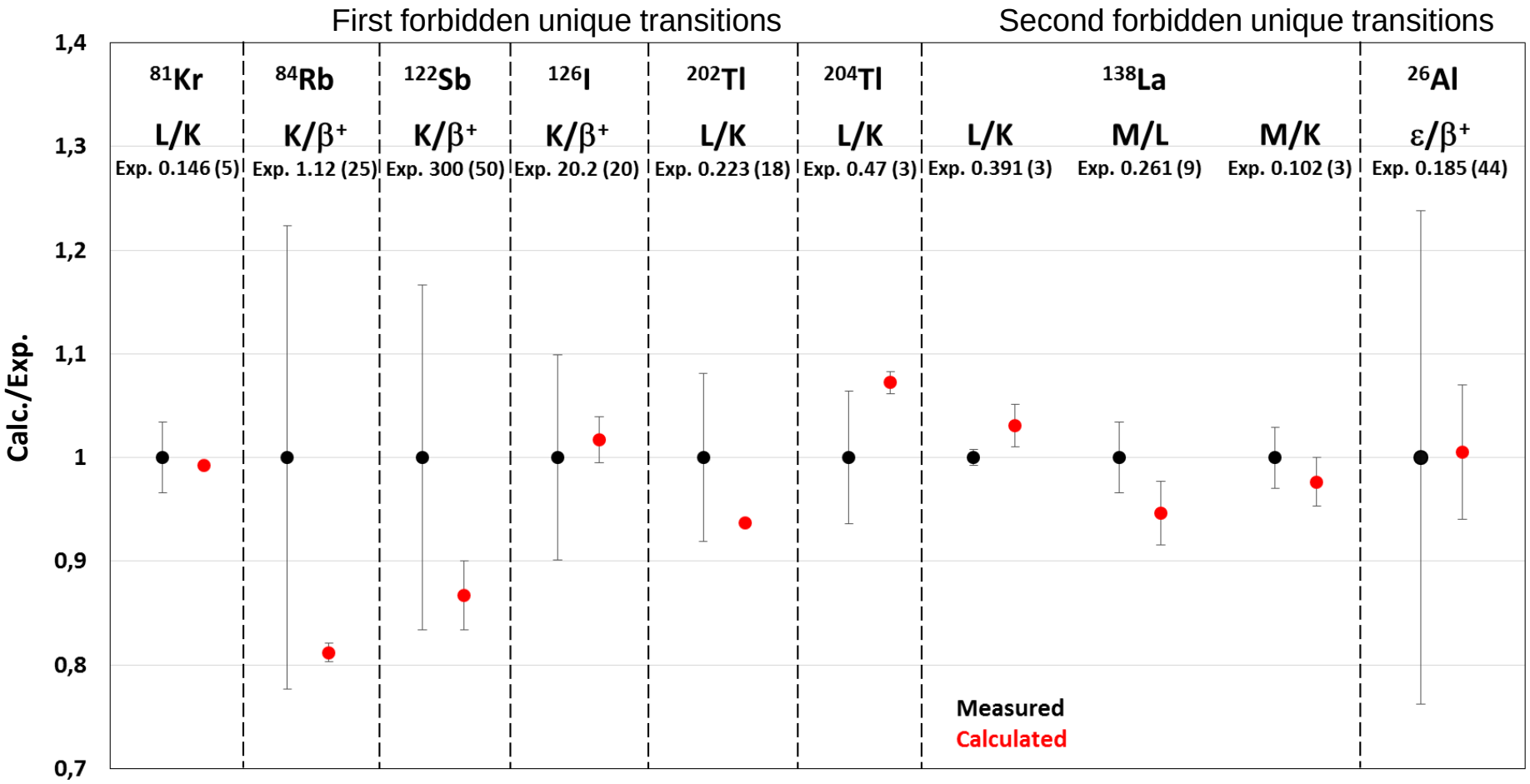
The correction of the hole effect is thus only applied through the **asymmetric overlaps**

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

Allowed transitions

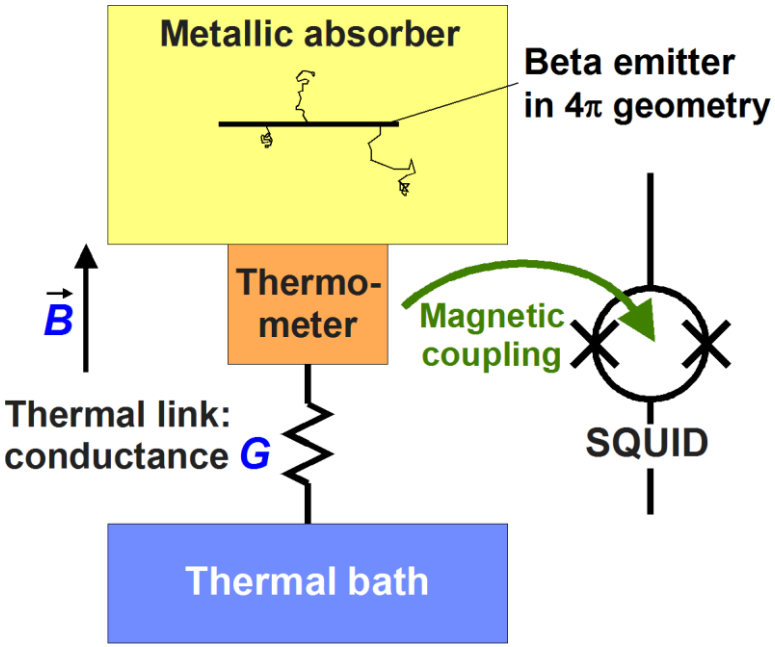


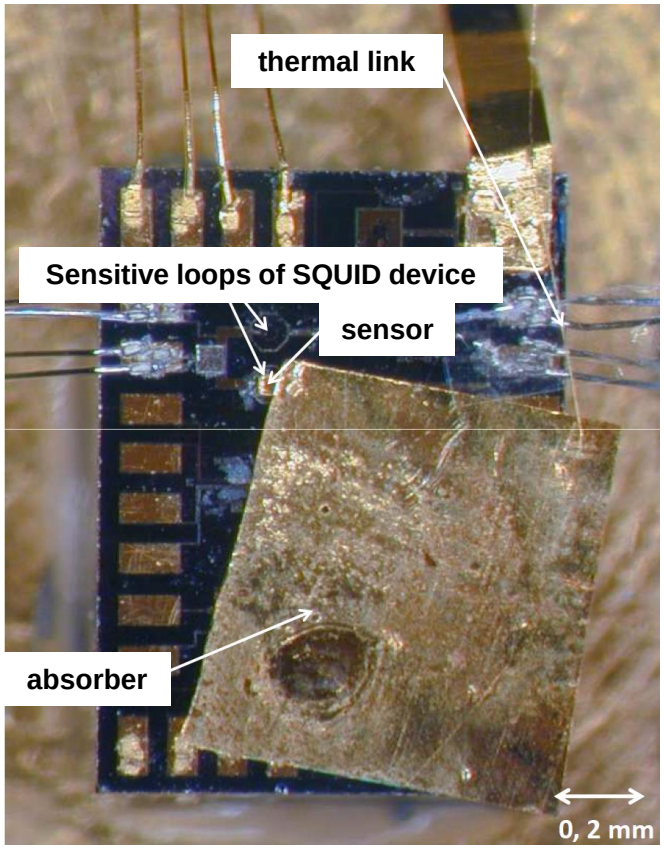
Forbidden unique transitions

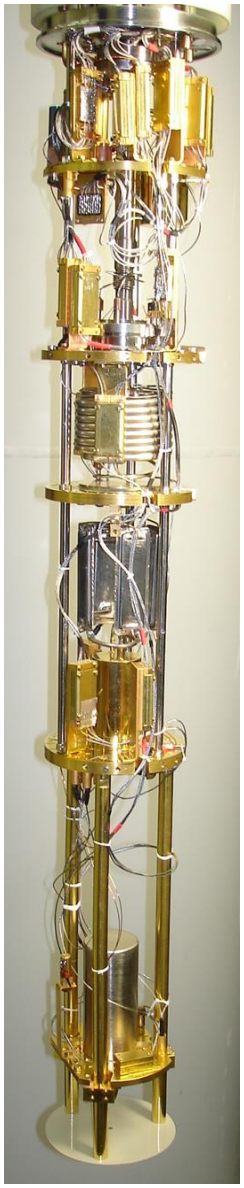


Atomic effects in beta decays

Metallic magnetic calorimetry

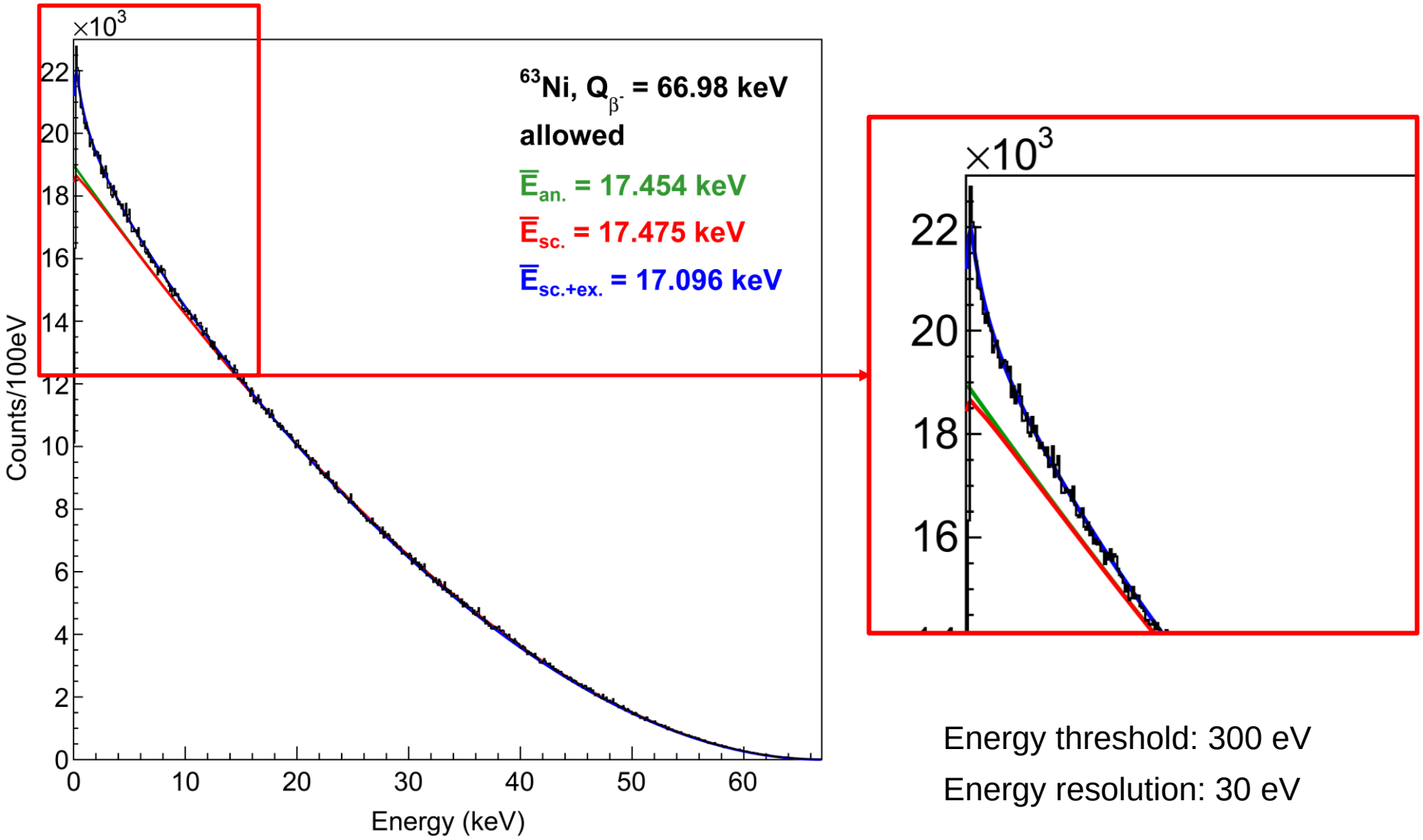






System cooled down to 10 mK

Atomic effects: ^{63}Ni



Energy threshold: 300 eV

Energy resolution: 30 eV

Inclusion of nuclear structure

Beta transition probability per beta particle energy

Phase space

$$P(W_e)\mathrm{d}W_e = \frac{G_\beta^2}{2\pi^3} F_0 L_0 C(W_e) p_e W_e (W_0 - W_e)^2 \mathrm{d}W_e$$

Fermi function

Shape factor

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

Theoretical shape factor

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

This formulation allows the calculation of **beta transition of every nature** (allowed, forbidden unique and forbidden non-unique).

Decay constants, partial half-lives, branching ratios and log *ft* values are integrated quantities of the beta spectrum.

Description of the weak decay process

(V-A) weak interaction

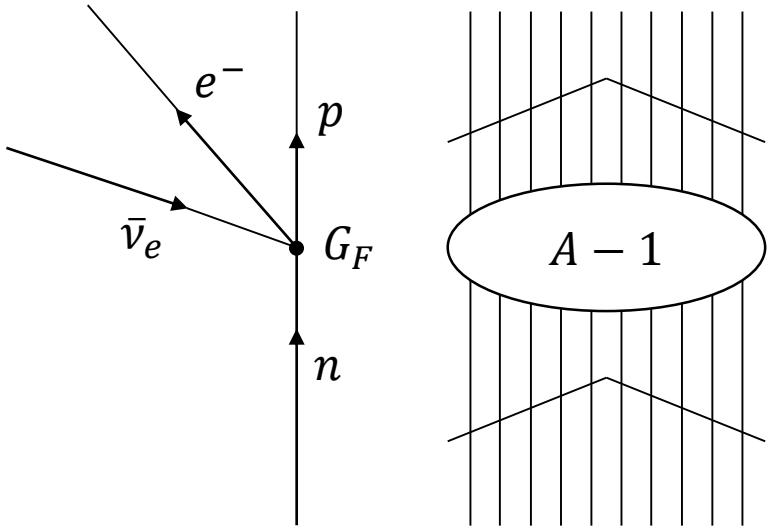
- Current-current interaction.
- Multipole expansions of both nuclear and lepton currents.

Impulse approximation

- At the moment of the decay, the nucleon is assumed to feel only the weak interaction.
- Other nucleons are assumed to be spectators with respect to the weak decay process.

Fermi theory

- Vertex of the weak interaction is assumed to be pointlike.
- No $W^{\pm}$ boson propagation.
- The effective coupling constant G_F is used.



Nuclear matrix elements

Nuclear matrix elements are embedded within M_K quantities.

In the case of single-particle matrix elements, an analytical integration over the transferred momentum q in the M_K quantities can be conducted.

$$^{V}\mathcal{M}_{KK0}(q^2) = \frac{\sqrt{2}}{\sqrt{2J_i+1}} \cdot \frac{(2K+1)!!}{(qR)^K}$$

Geometrical coefficients

$$\times \Big[G_{KK0}(\kappa_f, \kappa_i) \int_0^\infty g_f(r,\kappa_f) j_K(qr) g_i(r,\kappa_i) r^2 \mathrm{d}r$$

$$+ S_{\kappa_f} S_{\kappa_i} G_{KK0}(-\kappa_f, -\kappa_i) \int_0^\infty f_f(r,\kappa_f) j_K(qr) f_i(r,\kappa_i) r^2 \mathrm{d}r \Big]$$

Relativistic single-particle wave functions of the nucleons in their bound states.

→ Input from a nuclear structure model is necessary

Optimization

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

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

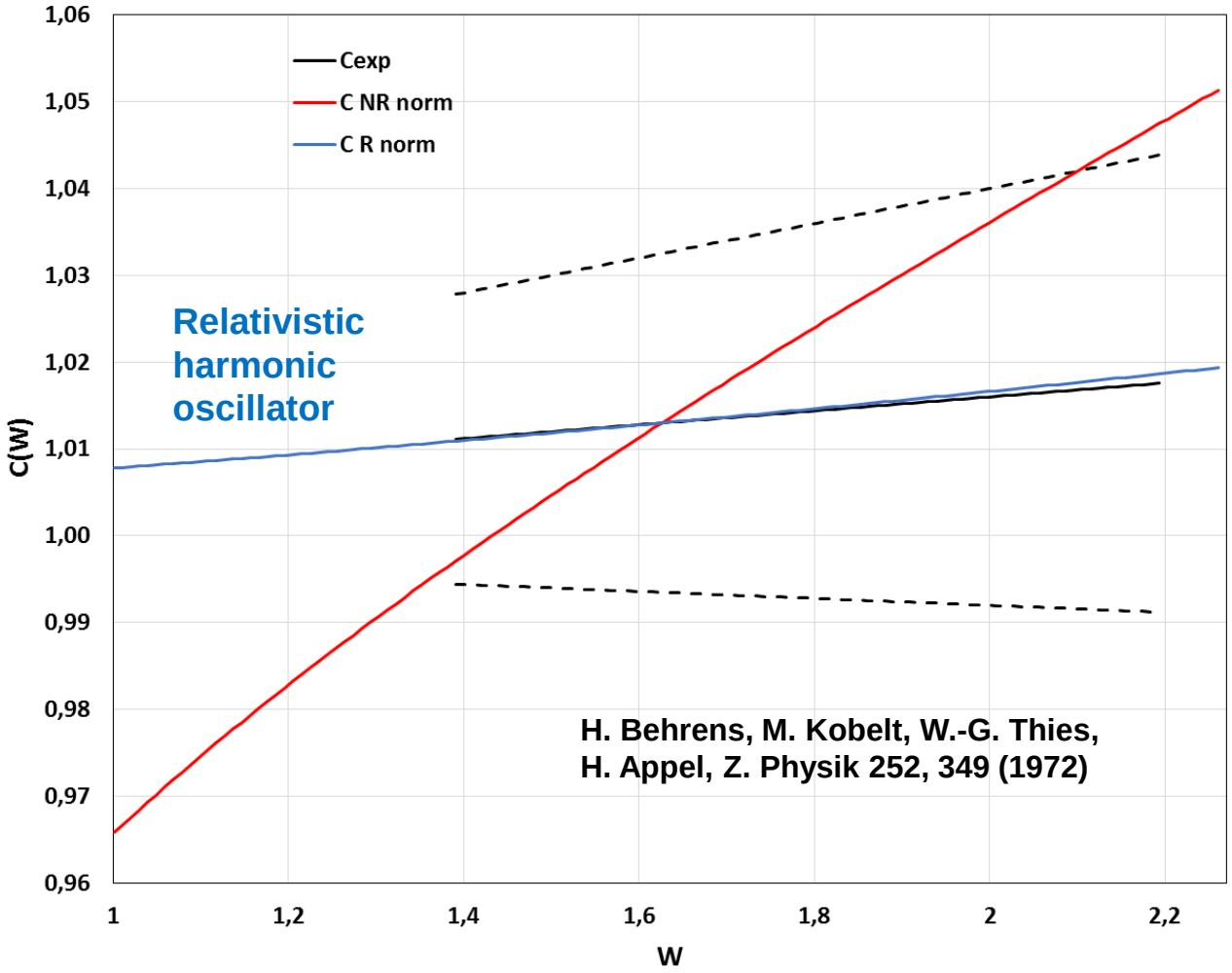
A specific algorithm has thus been developed in order to control the precision of the calculation. A pre-analysis is performed at $W_0/2$ and many possibilities are tested into nested loops:

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

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

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

First forbidden non-unique transition of ^{209}Pb



Non-relativistic harmonic oscillator

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

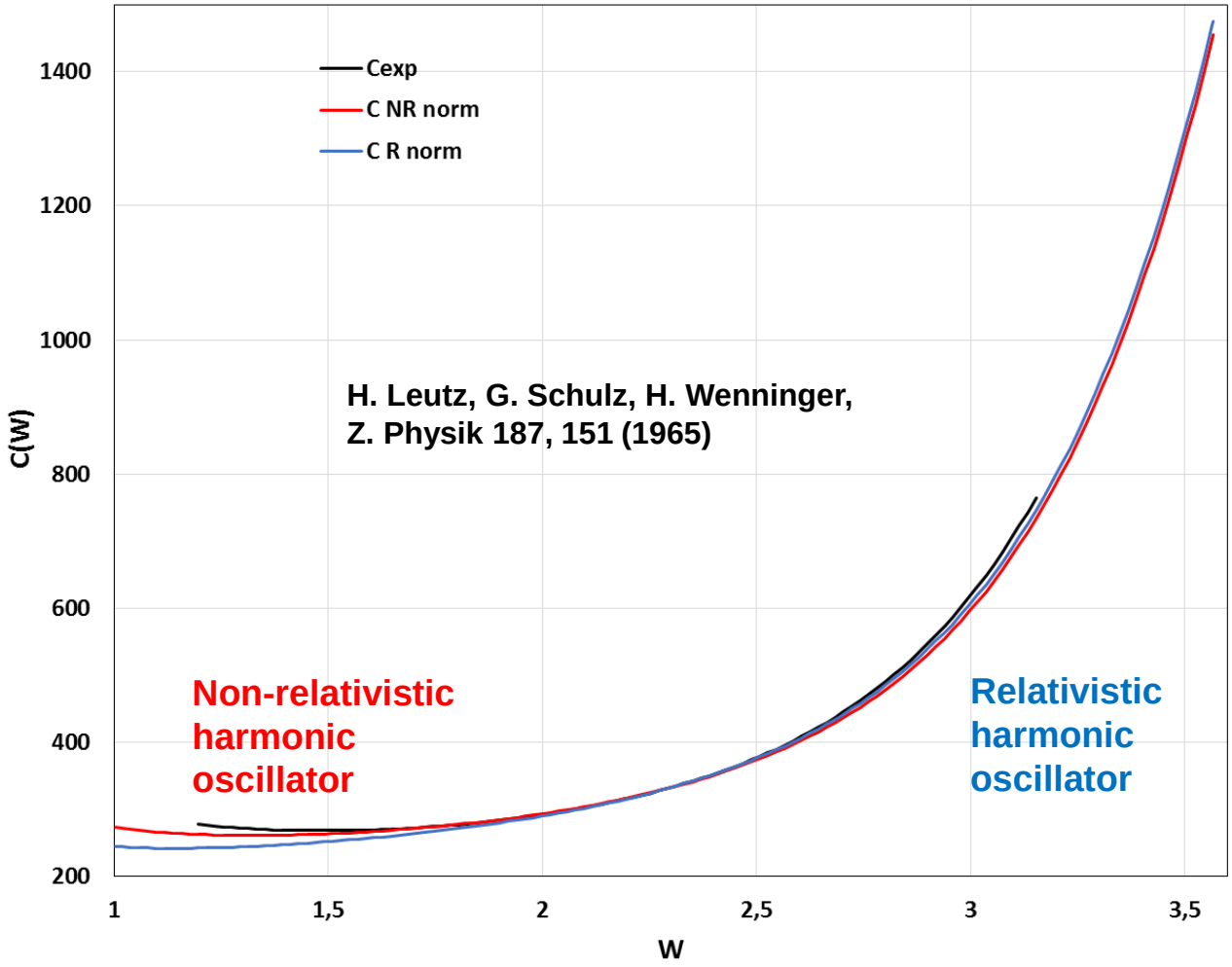
E_0 = 644,0(11) keV

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

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

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

Third forbidden unique transition of ^{40}K decay



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

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

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

$$C(4) = 3$$

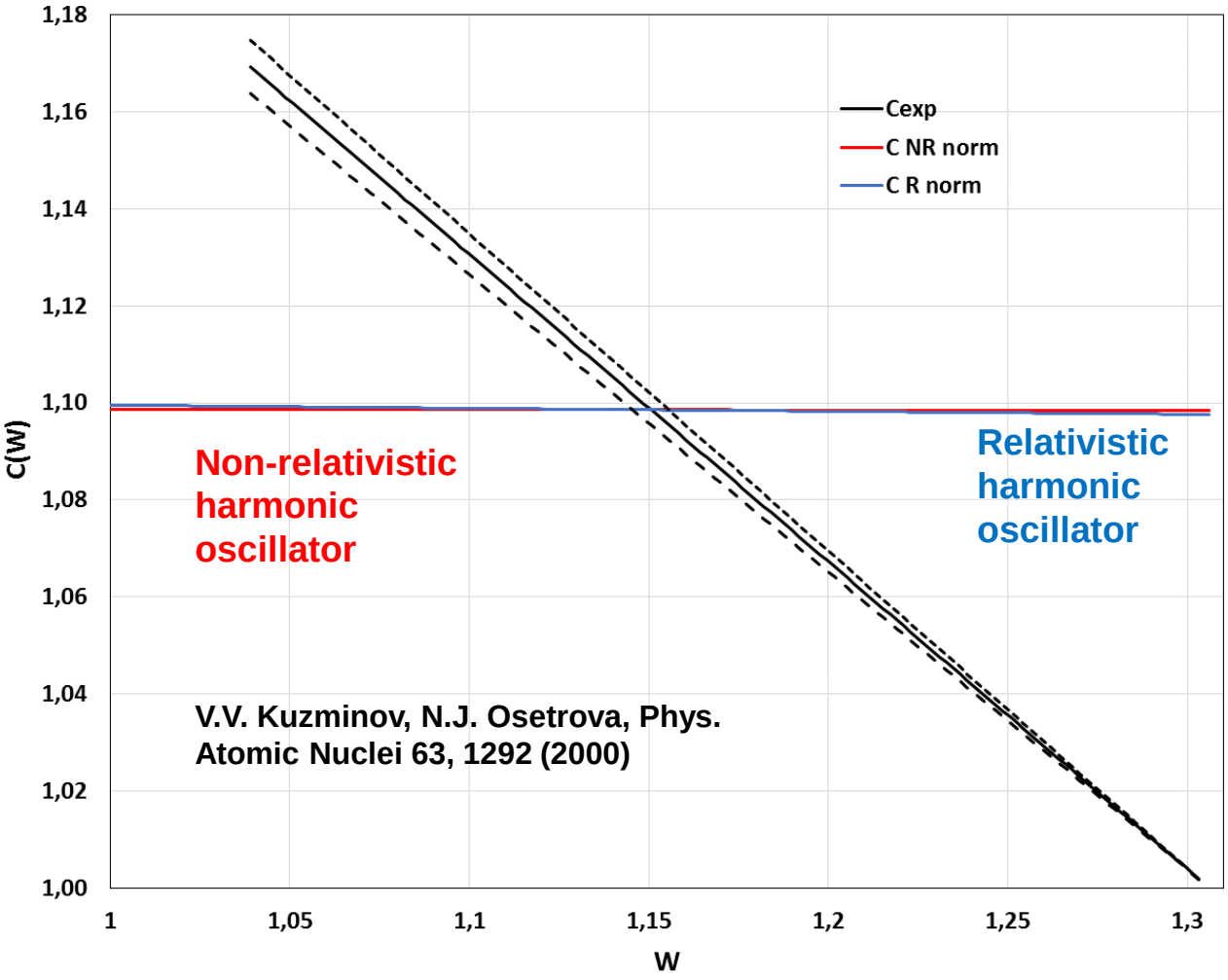
E_0 = 1310,89(6) keV

$t_{1/2}$ exp. = 1,4010(43)·10^9 a

$t_{1/2}$ NR = 5,491·10^8 a

$t_{1/2}$ R = 1,057·10^9 a

Allowed transition of ^{14}C decay



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

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

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

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

E_0 = 156,476(4) keV

$t_{1/2}$ exp. = 5700(30) a

$t_{1/2}$ NR = 0,009 a

$t_{1/2}$ R = 0,012 a

Perspectives

European projects

Theoretical shape factors

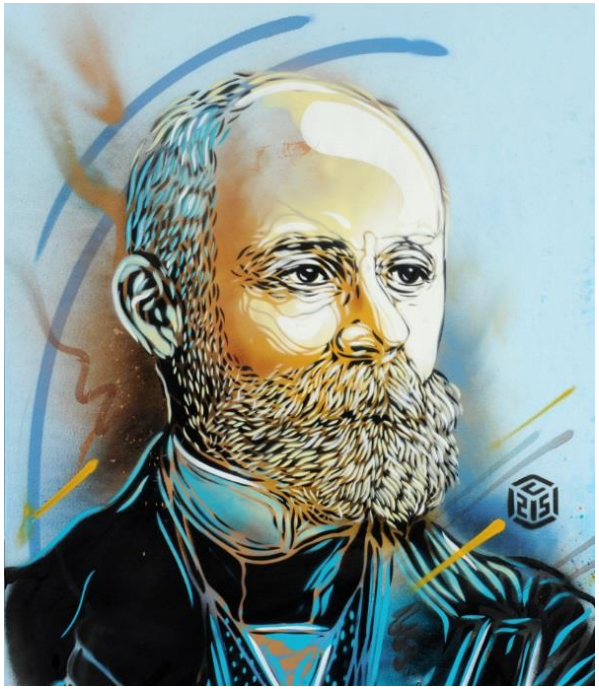
European EMPIR project MetroBeta (2016-2019): improved beta decay calculations. Inclusion of more precise nucleon wave functions from a semi-phenomenological nuclear mean-field approach, still in spherical symmetry. Applied also to electron captures.

Electron captures

European EMPIR project MetroMMC (2018-2021): improved electron capture calculations. Development of an atomic code for high precision wave functions. Will be used afterwards for atomic effects in beta decays.

Future

- Nuclear component: introduction of nuclear deformation and pairing correlations, which is expected to inherently account for configuration mixing.
- Atomic component: extension of exchange effect to forbidden beta decays.
- Uncertainties: estimate of theoretical components and propagation via a Monte Carlo method.



Thank you for your attention

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