Challenges in beta decay calculations

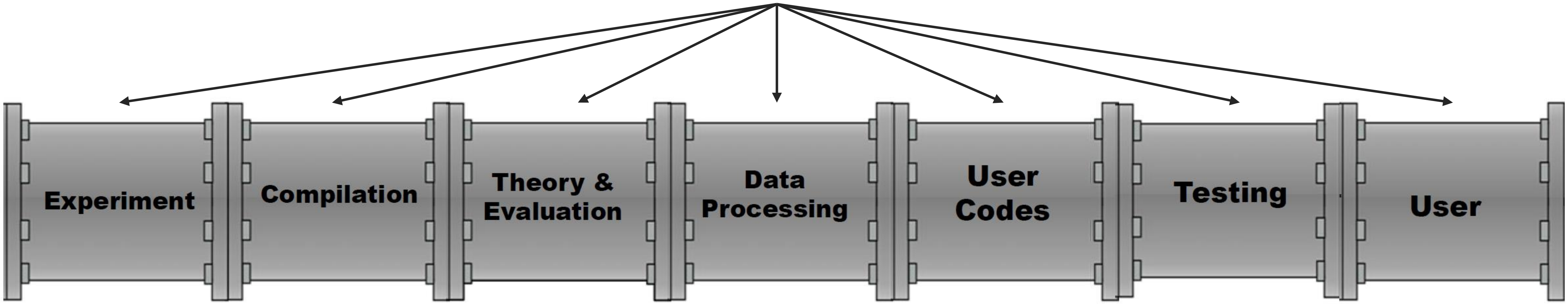
X. Mougeot, CEA-LNHB (France)

Radionuclide metrology

LNHB (National Laboratory Henri Becquerel) is the French Designated Institute for primary standards in ionizing radiation metrology. **We are present at every stage of the nuclear data pipeline, mostly interested in decay data** and around the valley of stability.

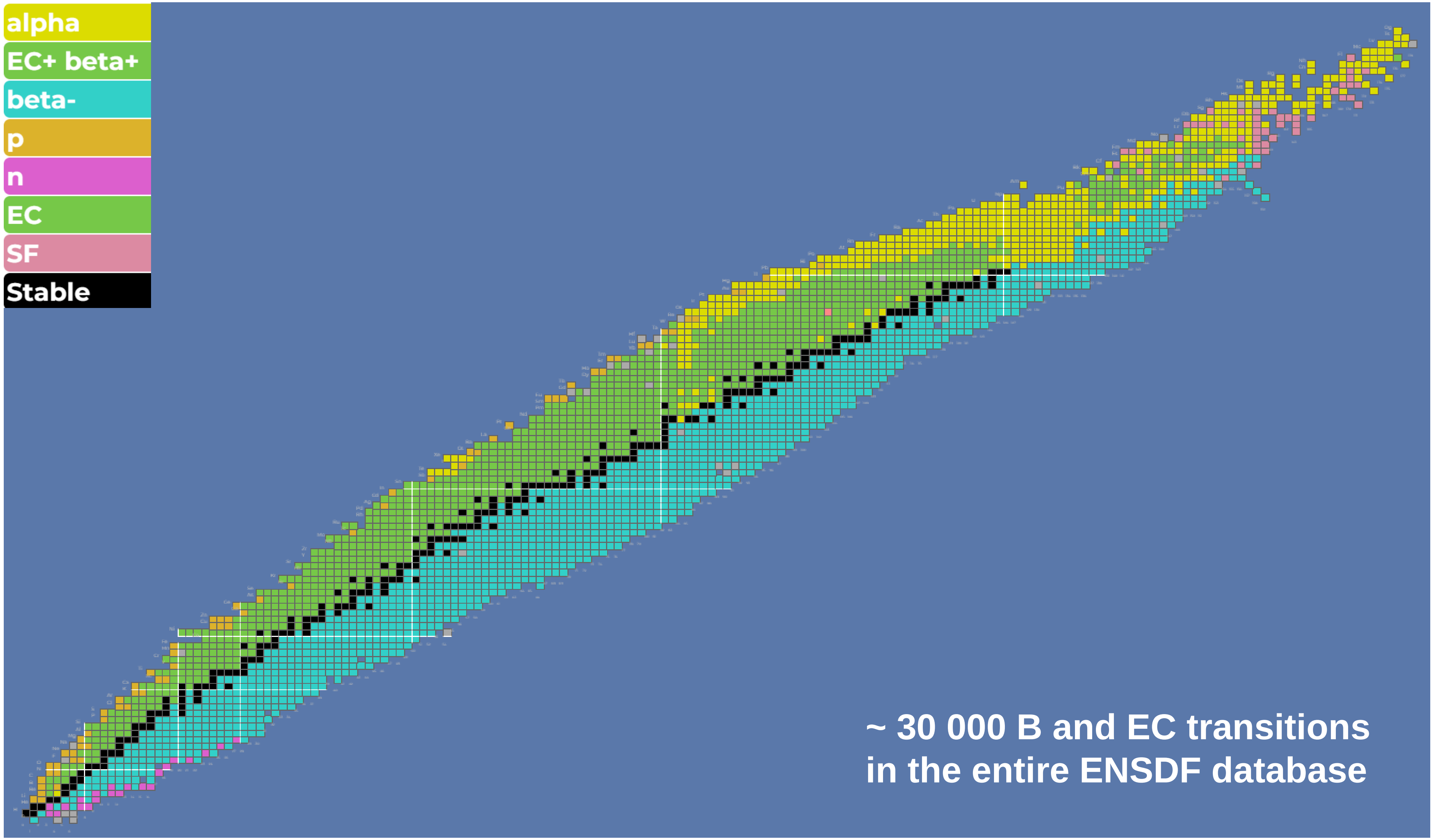
The diversity of radioactive processes makes necessary a certain pre-knowledge to establish primary and secondary standards: decay schemes, atomic and nuclear data. → **Evaluation of atomic and nuclear decay data.**

- ✓ Coordination of the DDEP (Decay Data Evaluation Project) international collaboration. Link with ENSDF community.
- ✓ **Decay data officially recommended by the BIPM. LNHB is also in charge of the JEFF decay data library.**



Courtesys D. Brown

The main radioactive decay mode



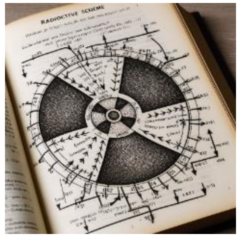
Importance of beta decays

Metrology

Activity measurements
(Liquid scintillation,
Ionization chambers)

Better knowledge → **Improvement of accuracy and uncertainties**

Nuclear decay data



ENSDF, **DDEP**, **JEFF** databases

Properties calculated with the LogFT legacy code (Gove and Martin, 1971)

log-*ft* for Jπ assignment, **no beta spectrum**

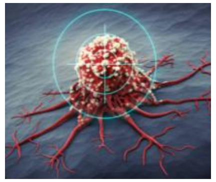
Fundamental research

Nuclear astrophysics (*r*-process)

Neutrino physics (reactor anomaly, reactor monitoring, non-proliferation)

Standard Model (CKM matrix unitarity, weak magnetism)

New physics (Fierz interference, sterile neutrino, dark matter)

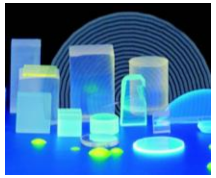


Medical applications

Micro-dosimetry, internal radiotherapy, contamination

Nuclear fuel cycle

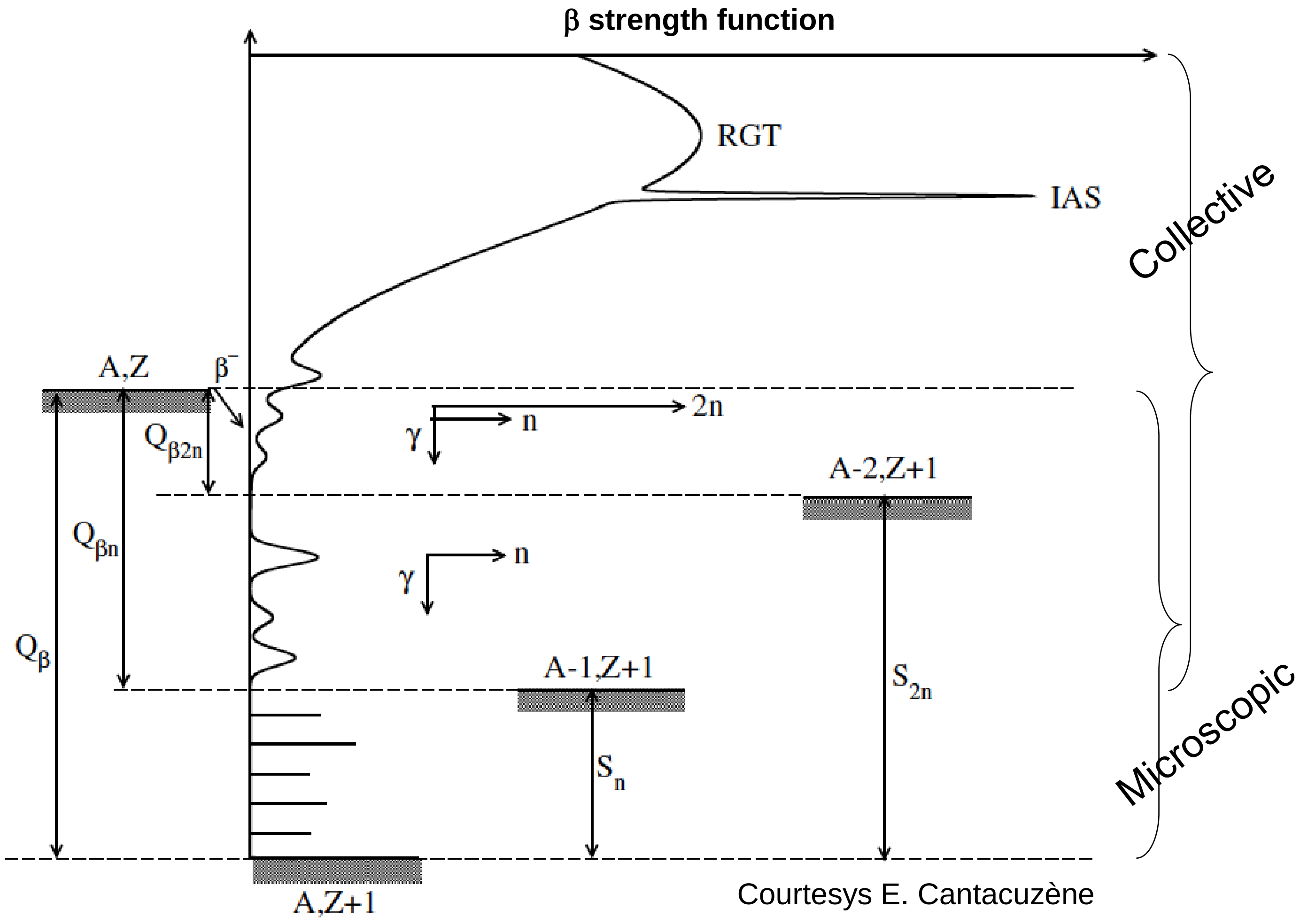
Decay heat, nuclear waste



Developments

Beta-voltaic batteries, new detectors (e.g. $LaBr_3$)

Different physics at different energies



Courtesys E. Cantacuzène

$$S_\beta(E) = \frac{I_\beta(E)}{f(Z, Q_\beta - E) \cdot T_{1/2}}$$

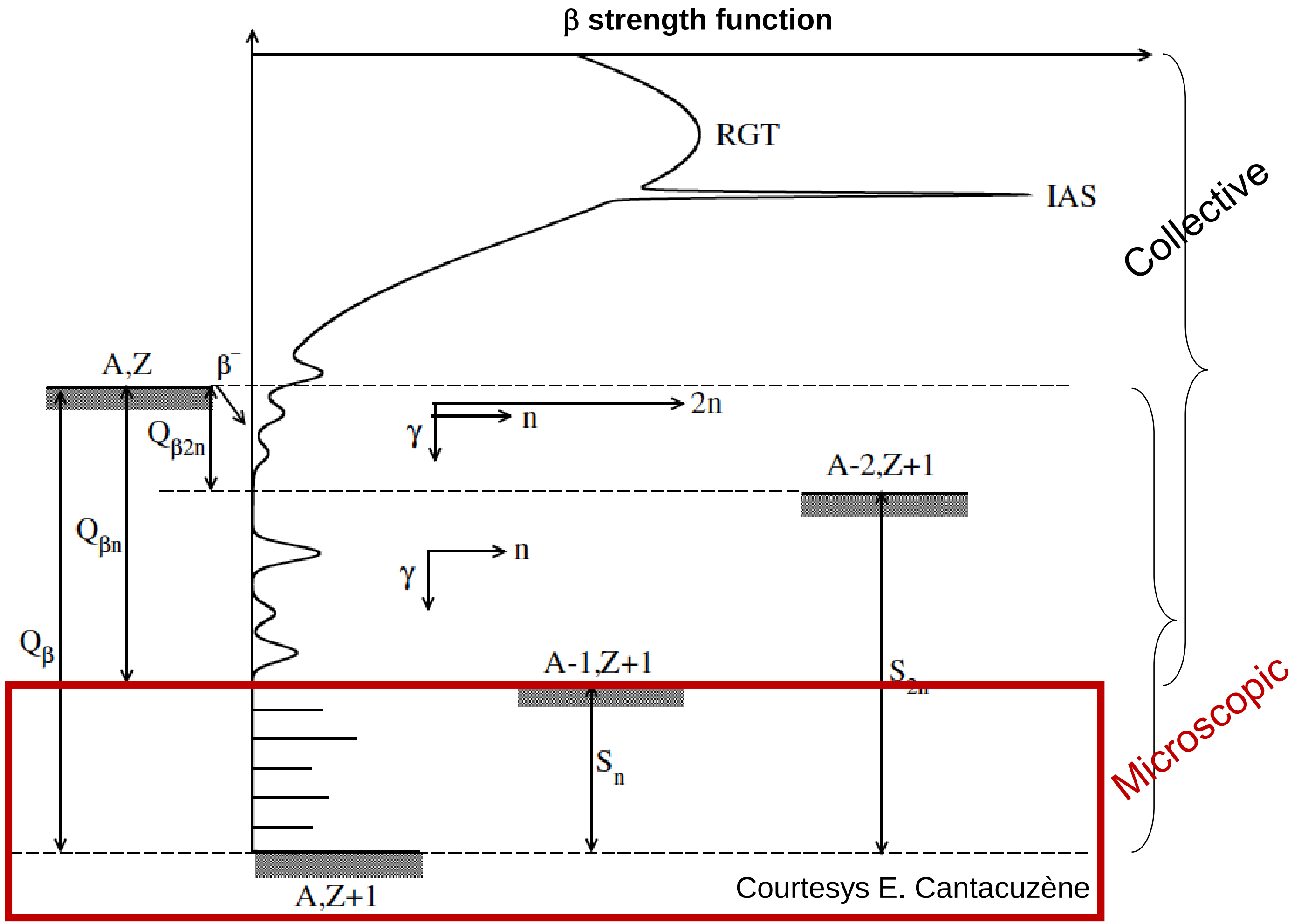
Microscopic
- Independent-particle models + Residual interactions.
- Structure quantum numbers meaningful.
- Strong selection rules.

Collective
- Decaying particles strongly affected by their interaction with other nucleons.
- Statistical models (Hauser-Feshbach).
- Structure quantum numbers meaningless.

Renormalization of weak interaction coupling constants.

Analogous to renormalization of electromagnetic nuclear moments (core polarization, effective charges).

Different physics at different energies



$$S_\beta(E) = \frac{I_\beta(E)}{f(Z, Q_\beta - E) \cdot T_{1/2}}$$

Microscopic

- Independent-particle models + Residual interactions.
- Structure quantum numbers meaningful.
- Strong selection rules.

Collective

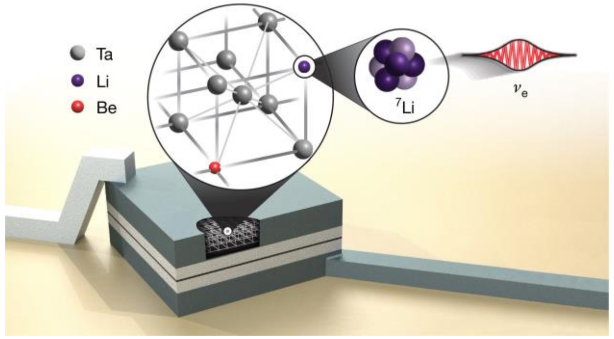
- Decaying particles strongly affected by their interaction with other nucleons.
- Statistical models (Hauser-Feshbach).
- Structure quantum numbers meaningless.

Renormalization of weak interaction coupling constants.

Analogous to renormalization of electromagnetic nuclear moments (core polarization, effective charges).

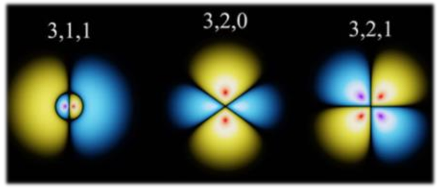
Overview of an ideal modelling

J. Smolsky et al., Nature 638, 640 (2025)

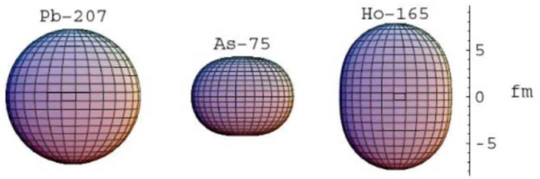


Additional effects

Environmental influence



Atomic modelling



Nuclear modelling

Screening
Exchange

Realistic nuclear structure
Nucleus deformation

Z (J_i, π_i) → Z+1 (J_f, π_f) β^- $\bar{\nu}$

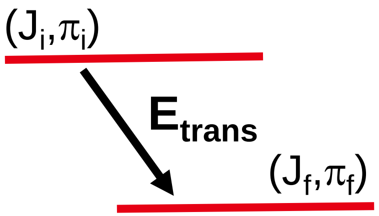
Beta decay modelling

QED, Internal bremsstrahlung

Material, temperature

Coupling lepton and hadron currents
Coupling different formalisms
Specific forbidden non-unique treatment

Selection rules



	Type of transition	Forbiddenness degree	ΔJ	$\pi_i\pi_f$
Energy spectrum of β particles				
Independent of nuclear structure (approx. $\lesssim$1%)	Allowed		0, $\pm$1	+1
	Forbidden unique	1st	$\pm$2	$-$1
		2nd	$\pm$3	+1
		$(\Delta J\text{-}1)^{th}$	>1	$(-1)^{(\Delta J-1)}$
Sensitive to nuclear structure →	Forbidden non-unique	1st	0, $\pm$1	$-$1
		2nd	$\pm$2	+1
		3rd	$\pm$3	$-$1
		$(\Delta J)^{th}$	>1	$(-1)^{(\Delta J)}$

The wavelength of emitted leptons is much larger than the nuclear radius.

→ Double multipole expansion of nuclear and lepton currents, rapidly converging.

→ Transition matrix elements grouped into "allowed", "forbidden unique" or "forbidden non-unique", "first-forbidden", "second-forbidden", etc.

Transition rates obviously depend on nuclear structure.

However, the spectrum shape of the emitted particles can be considered independent for some types of transition.

Current situation in decay libraries

- (J,π) not firmly established
- Forbidden non-unique

→ Transition classified as allowed.

Weak interaction properties in nuclear decay data are incomplete and come from calculation: mean energies, capture probabilities, log-*ft* values.

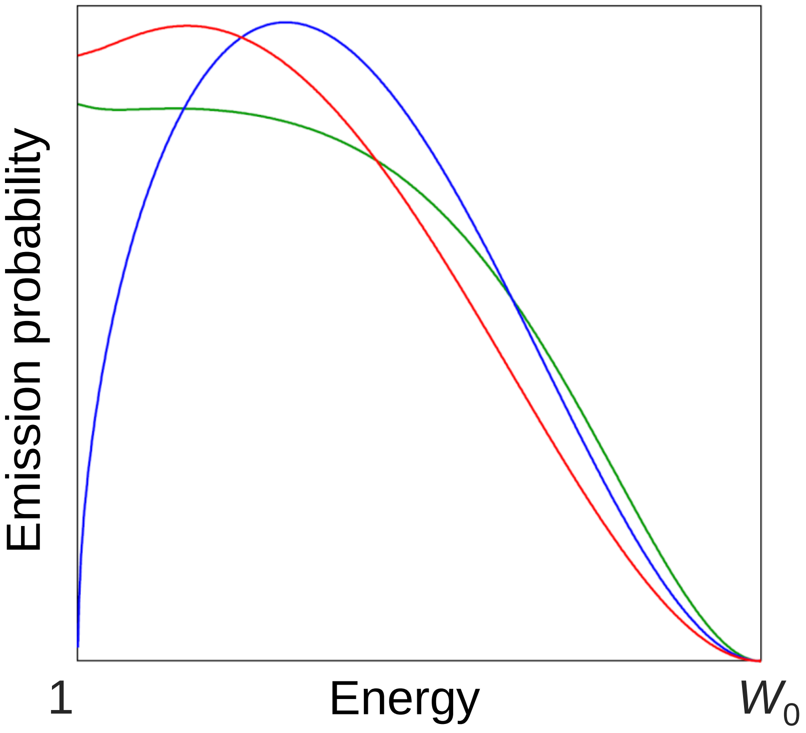
They have been determined for the last 50 years with the LogFT code, developed in the late 1960's.

Quite simple analytical models of beta transitions and electron captures. Limited in forbiddenness degree. No beta spectra, no capture subshells.

The BetaShape code

Phase space Fermi function Shape factor

$$\frac{\mathrm{d}P}{\mathrm{d}W} \propto \boxed{pWq^2} \cdot \boxed{F(Z,W)} \cdot \boxed{C(W)}$$



W electron energy, W_0 transition energy

p electron momentum, q neutrino momentum

Allowed	$C(W) = 1$
First forbidden unique	$C(W) = q^2 + \lambda_2 p^2$
Second forbidden unique	$C(W) = q^4 + \lambda_2 q^2 p^2 + \lambda_3 p^4$
Third forbidden unique	$C(W) = q^6 + \lambda_2 q^4 p^2 + \lambda_3 q^2 p^4 + \lambda_4 p^6$
	Etc.

- ✓ The BetaShape program (version 2.4) now replaces the LogFT code for the new ENSDF evaluations. Electron captures also treated.

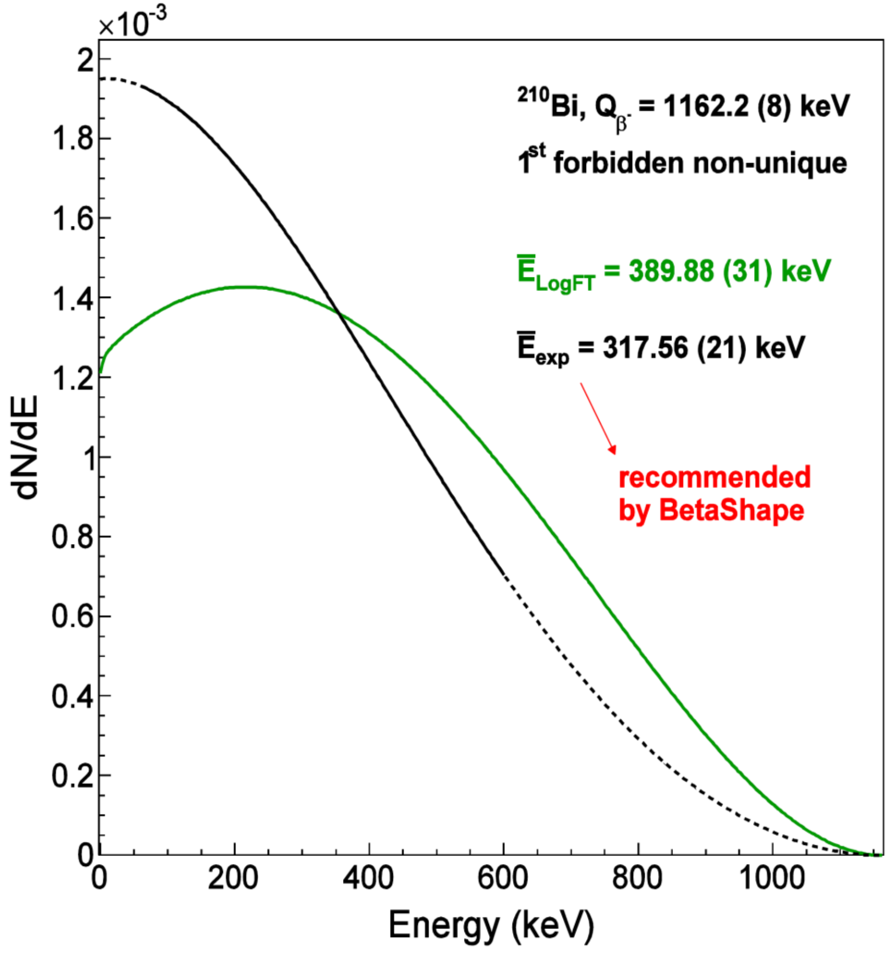
  → Available on IAEA-NSDD GitHub: https://github.com/IAEA-NSDDNetwork

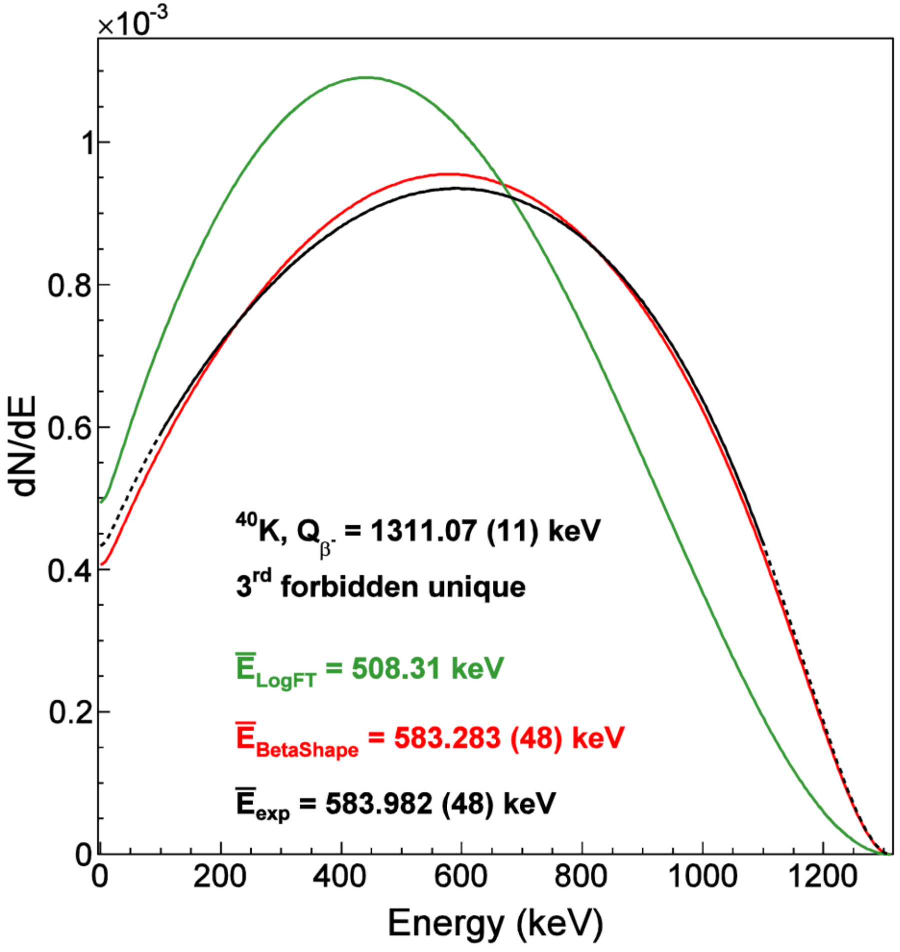
- ✓ $F(Z,W)$ and λ_k parameters determined from the relativistic electron wave functions, obtained by numerical solving of the Dirac equation.
- ✓ Included: extended nucleus; atomic exchange, overlap and screening; radiative corrections; database of experimental shape factors.

For forbidden non-unique transitions, coupling with nuclear structure is necessary.

→ ξ-approximation possible but accuracy is questionable.

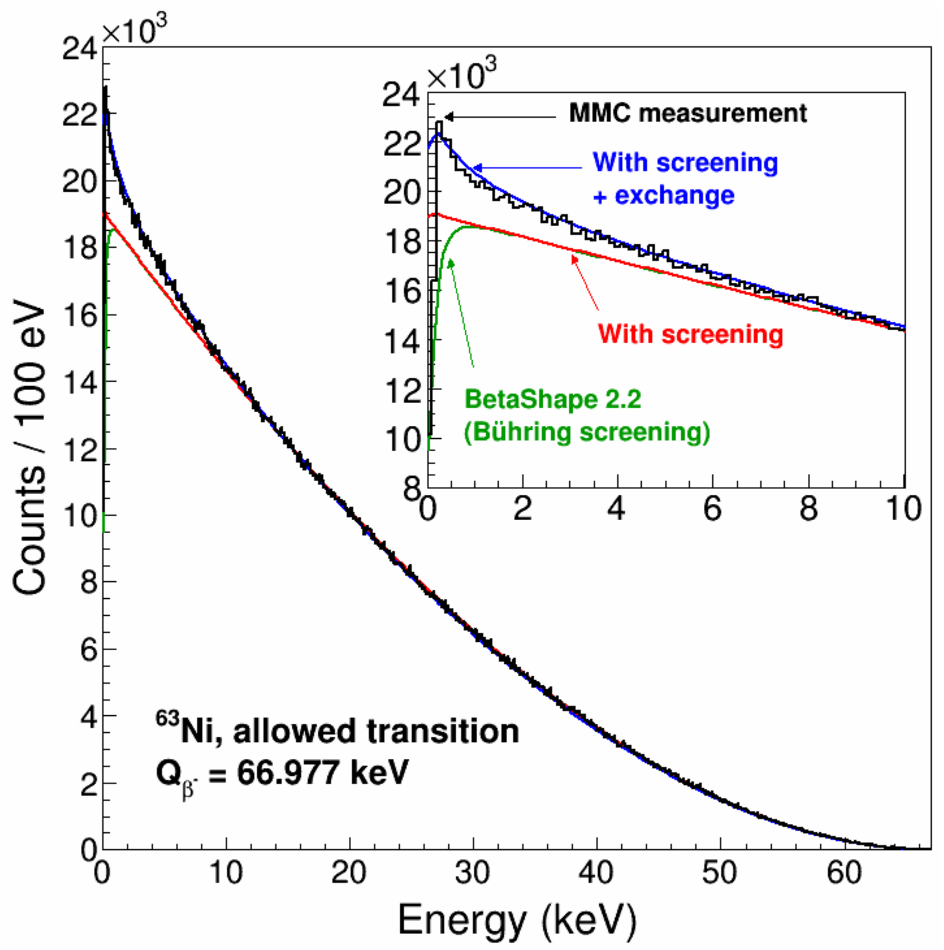
Examples of improved calculations

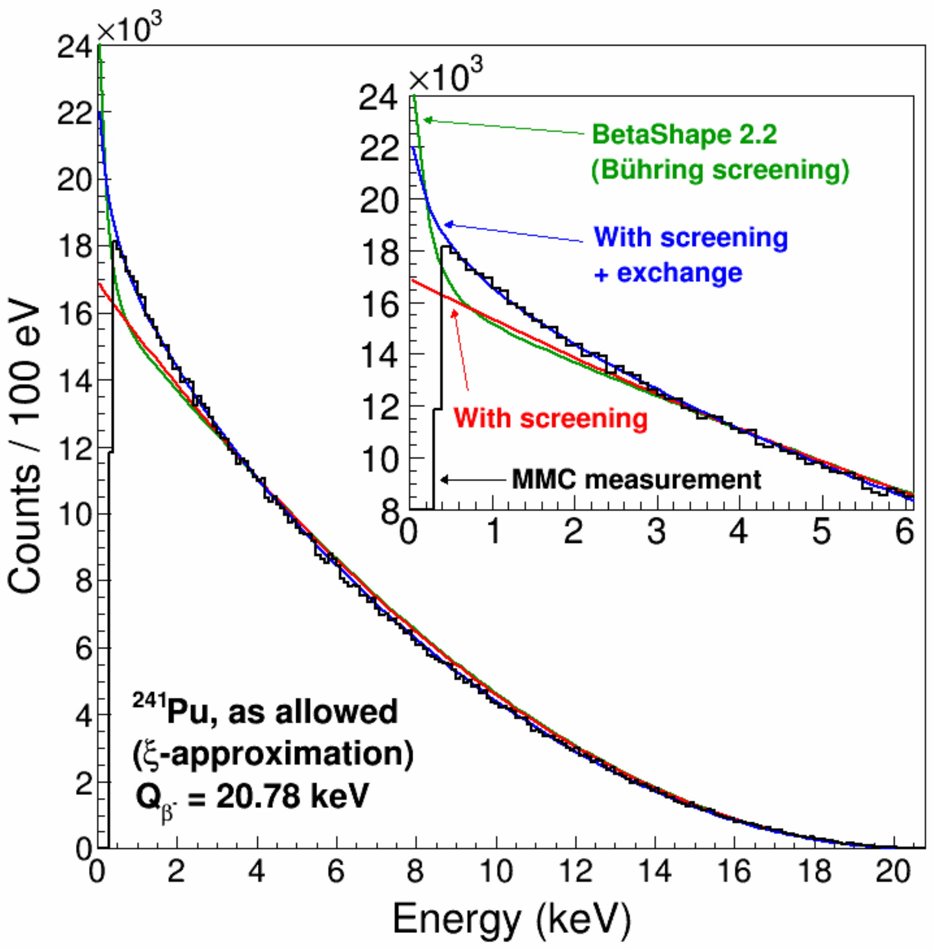




These two transitions are calculated as allowed by the LogFT program, which does not provide any beta spectrum.

Atomic effects





Recent extension of atomic exchange effect to forbidden transitions

X. Mougeot, Appl. Radiat. Isot. 201, 111018 (2023)

New review of log-*ft* values

Former review of log-*ft* values, calculated with the LogFT code: *B. Singh et al., Nuclear Data Sheets 84, 487 (1998)*

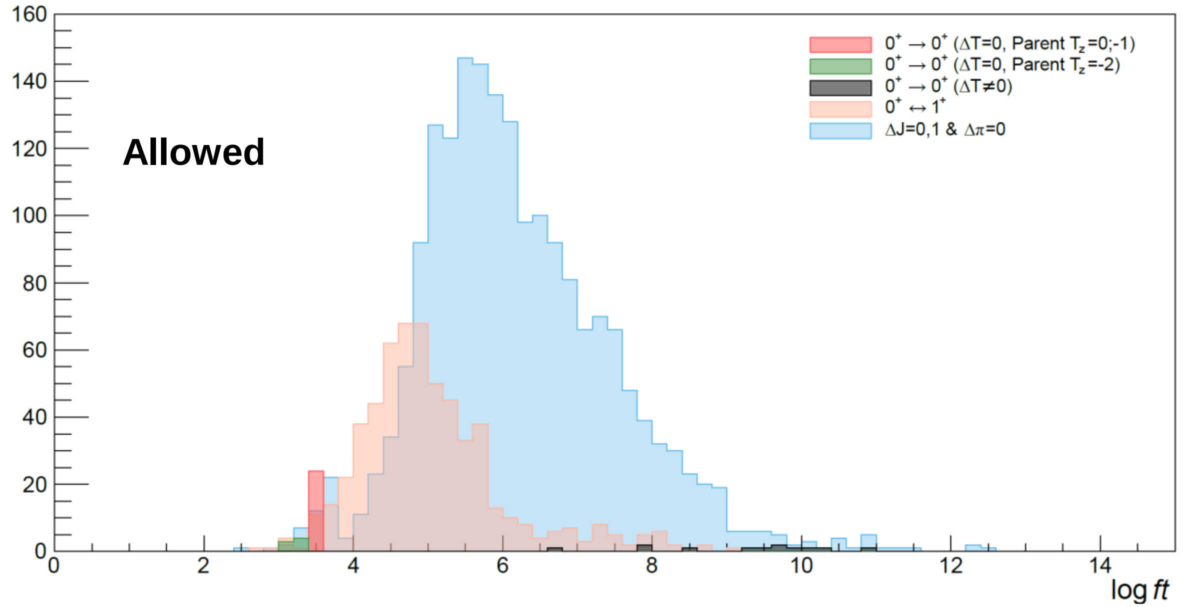
These values are used in nuclear structure studies, e.g. to assign spin and parity to a level.

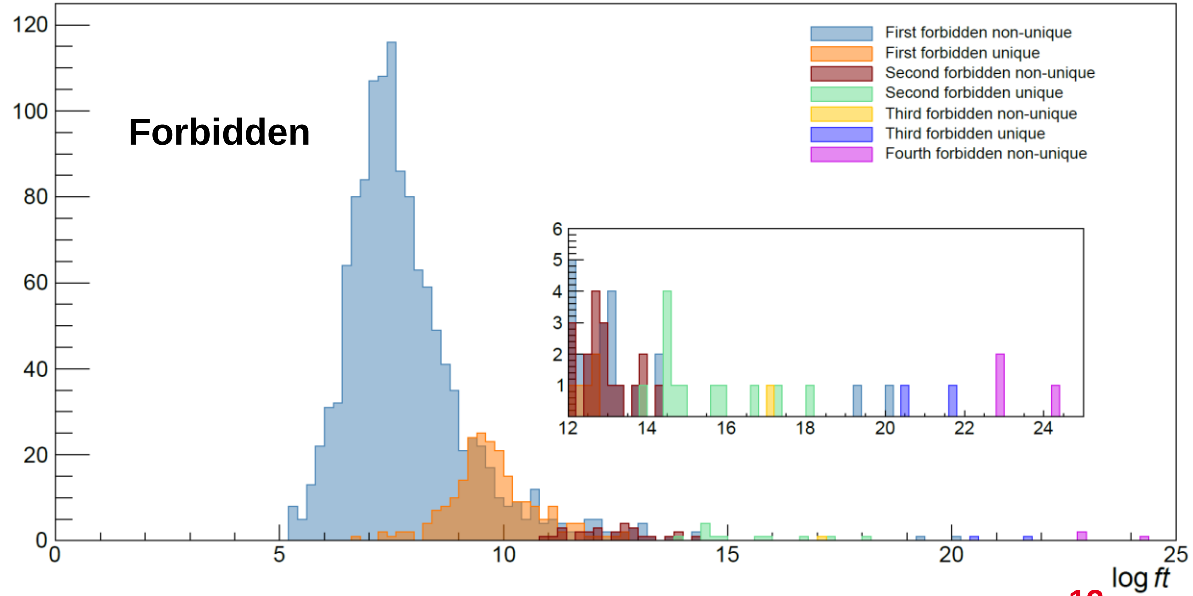
Collaborative work: B. Singh† (McMaster University), S. Turkat and K. Zuber (TU Dresden), X. Mougeot (CEA-LNHB)

- ✓ Update of B and EC decays present in ENSDF database (as of mid-April 2023).
- ✓ Use of BetaShape to calculate the log-*ft* values.
- ✓ In total, 26 318 transitions calculated. Selection of well-defined transitions. Possible pandemonium nuclei flagged.
- ✓ 4 038 transitions survived this filtering. All distributions re-established. Specific transitions are discussed.

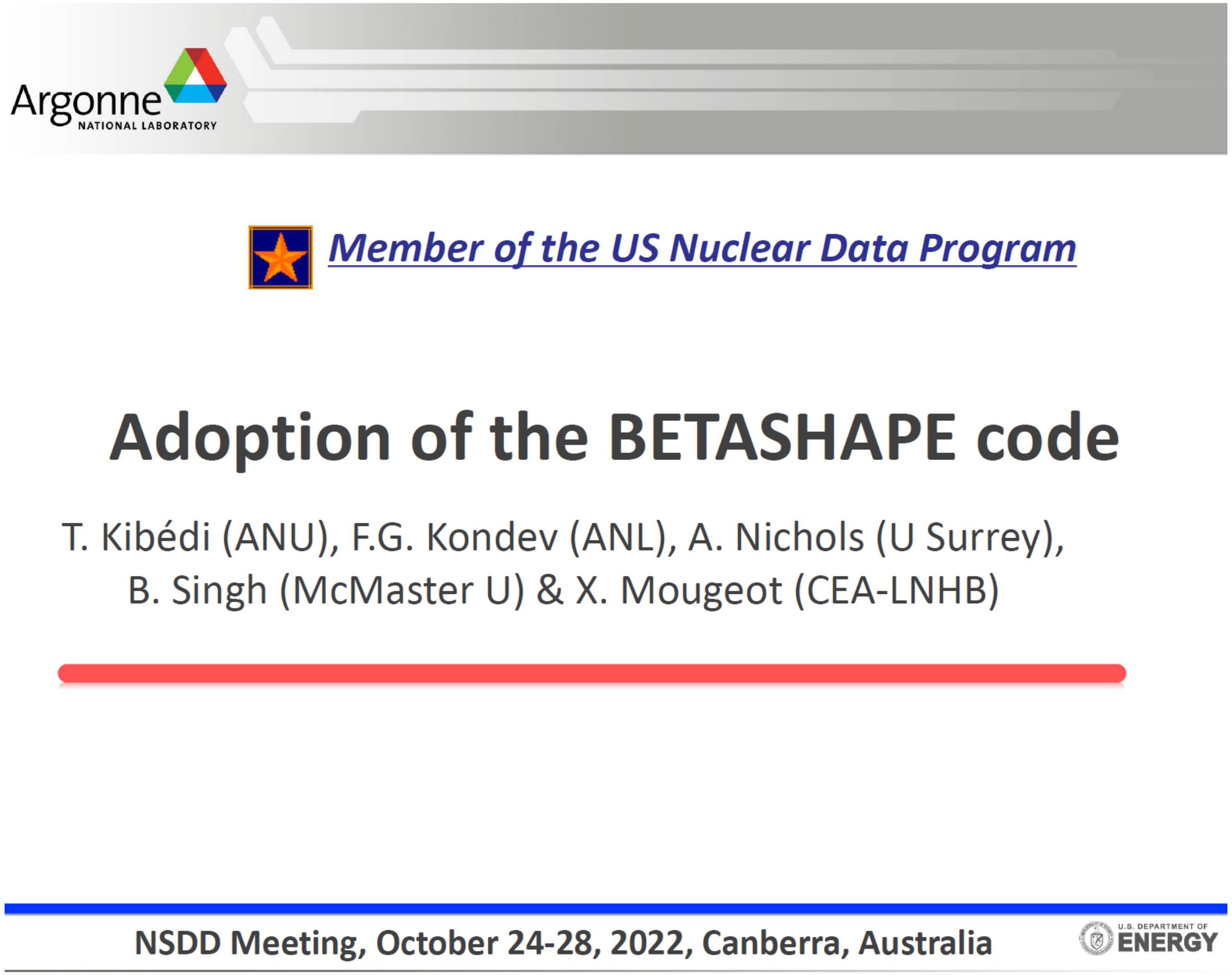
S. Turkat et al., Atomic Data and Nuclear Data Tables 152, 101584 (2023)

† Deceased





Evaluated nuclear decay data



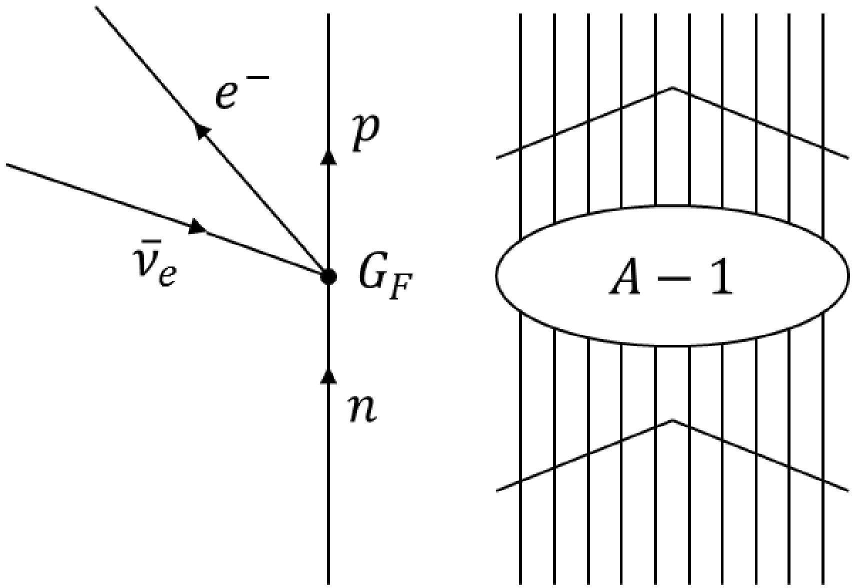
- ✓ The BetaShape code was already adopted several years ago by the DDEP collaboration for their decay data evaluations.
- ✓ Specific requests were formulated by the NSDD evaluators to match ENSDF policies. They were implemented in version 2.3 of the code (current version is 2.4).
- ✓ BetaShape has been adopted in 2023 by the NSDD network for the future ENSDF evaluations.

Theoretical shape factor

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

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

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



Fermi theory

- Vertex of the weak interaction is assumed to be point-like. No propagation of $W^\pm$ boson.
- Effective coupling constant G_F.
- Relativistic lepton and nuclear wave functions.
- Non-relativistic or relativistic, vector or axial-vector matrix elements.

Impulse approximation

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

Realistic nuclear structure

Nuclear state described as a **superposition of nucleon states**.

One-body transition densities must be given by a nuclear structure model → **NushellX (shell model)**.

$$\langle \xi_f J_f || T_\lambda || \xi_i J_i \rangle = \frac{1}{\sqrt{2K+1}} \sum_{a,b} \langle a || T_K || b \rangle \left\langle \xi_f J_f \left\| \left[c_a^\dagger \tilde{c}_b \right]_K \right\| \xi_i J_i \right\rangle$$

transition matrix element

tensor rank

single particle matrix element

one-body transition density (OBTD)

Transition described as a sum of transformations of single nucleons.

Example: Nonrelativistic vector matrix element

$${}^V\mathcal{M}_{KK0}(q^2) = \frac{\sqrt{2}}{\sqrt{2J_i+1}} \cdot \frac{(2K+1)!!}{(qR)^K}$$
$$\times \left[\boxed{G_{KK0}(\kappa_f,\kappa_i)} \int_0^\infty \boxed{g_f(r,\kappa_f)}\, j_K(qr) \boxed{g_i(r,\kappa_i)}\, r^2 \mathrm{d}r + S_{\kappa_f} S_{\kappa_i} \boxed{G_{KK0}(-\kappa_f,-\kappa_i)} \int_0^\infty \boxed{f_f(r,\kappa_f)}\, j_K(qr) \boxed{f_i(r,\kappa_i)}\, r^2 \mathrm{d}r \right]$$

Components of the relativistic bound wave function of the nucleon

Geometrical coefficients

Forbidden non-unique transitions

Relativistic matrix element

Non-relativistic matrix elements

$$M_K(k_e,k_\nu) = C_K (pR)^{k_e-1}(qR)^{k_\nu-1}\left\{-\sqrt{\frac{2K+1}{K}}\,\underline{{}^VF^{(0)}_{K,K-1,1}} - \frac{\alpha Z}{2k_e+1}\,\underline{{}^VF^{(0)}_{K,K,0}(k_e,1,1,1)}\right.$$
$$\left. - \left[\frac{WR}{2k_e+1}+\frac{qR}{2k_\nu+1}\right]\underline{{}^VF^{(0)}_{K,K,0}} - \frac{\alpha Z}{2k_e+1}\sqrt{\frac{K+1}{K}}\,\underline{{}^AF^{(0)}_{K,K,1}(k_e,1,1,1)} - \left[\frac{WR}{2k_e+1}-\frac{qR}{2k_\nu+1}\right]\sqrt{\frac{K+1}{K}}\,\underline{{}^AF^{(0)}_{K,K,1}}\right\}$$

Nuclear structure models are non-relativistic, but forbidden non-unique transitions are sensitive to $^{V}F_{K,K-1,1}$

→ Conserved Vector Current (CVC) hypothesis

- Derived from the gauge invariance of the weak interaction.
- Provides relationships between non-relativistic and relativistic vector matrix elements.
- Depends on the Coulomb displacement energy ΔE_C.

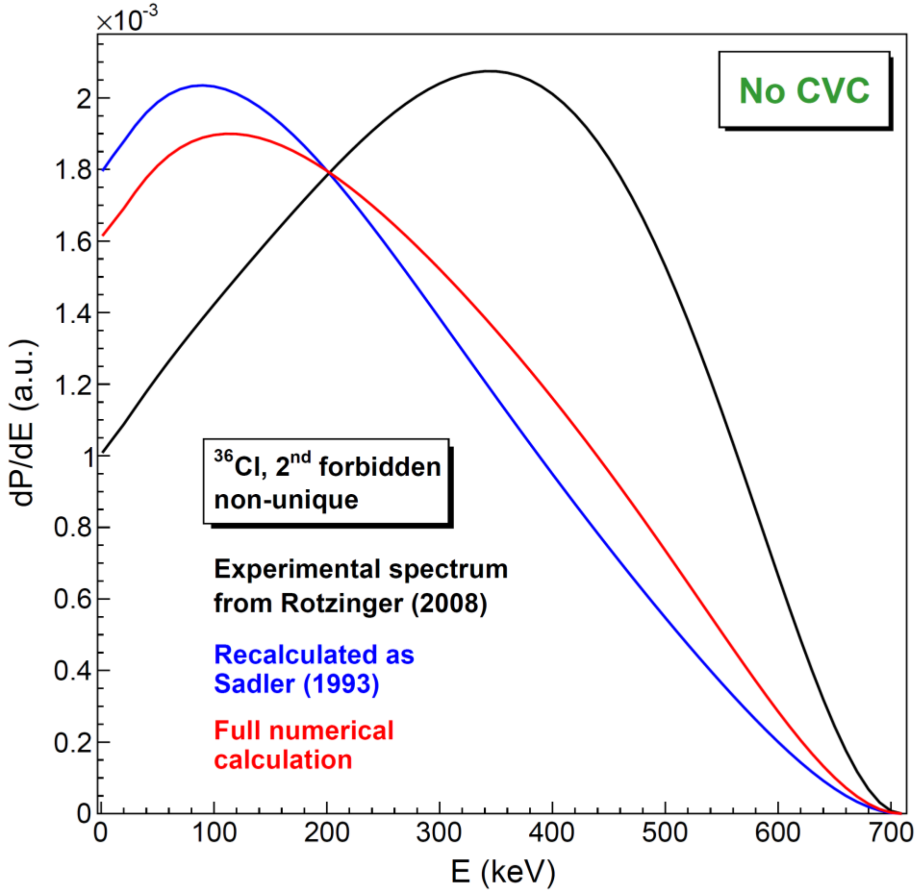
Influence of lepton current treatment: usually approximated only to dominant terms (formula here).

→ Full numerical treatment is also possible, avoiding approximations and next-to-leading-order terms.

^{36}Cl 2nd forbidden non-unique decay

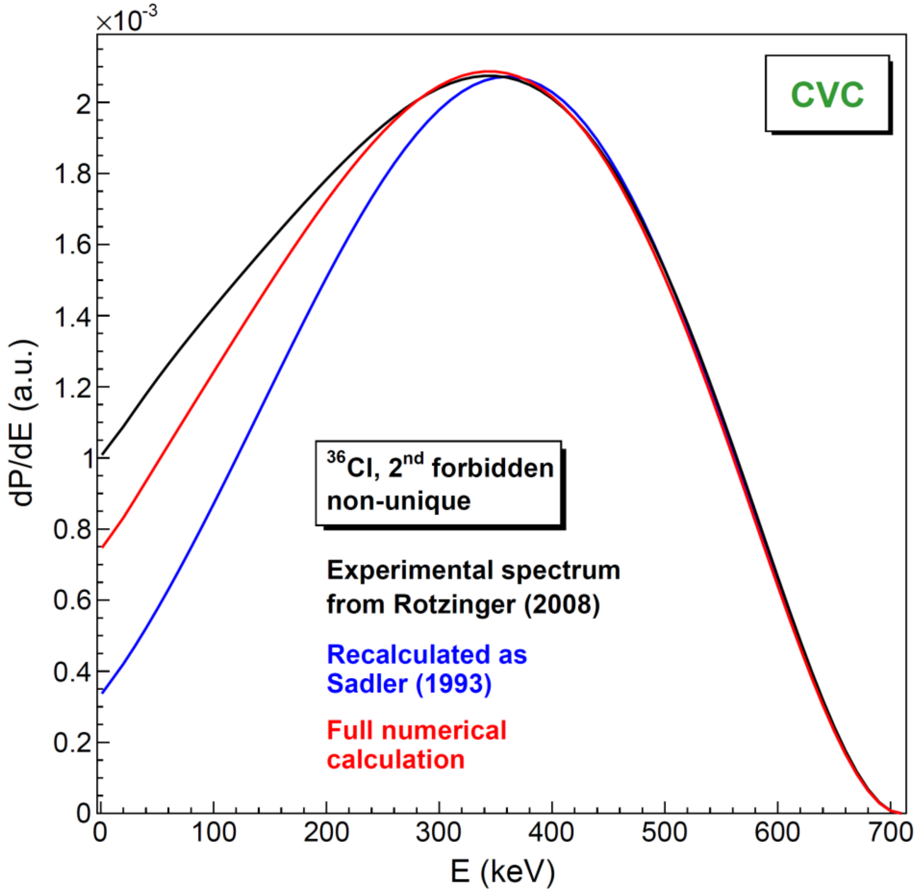
Precise measurement exists

Rotzinger et al., J. Low Temp. Phys. 151, 1087 (2008)



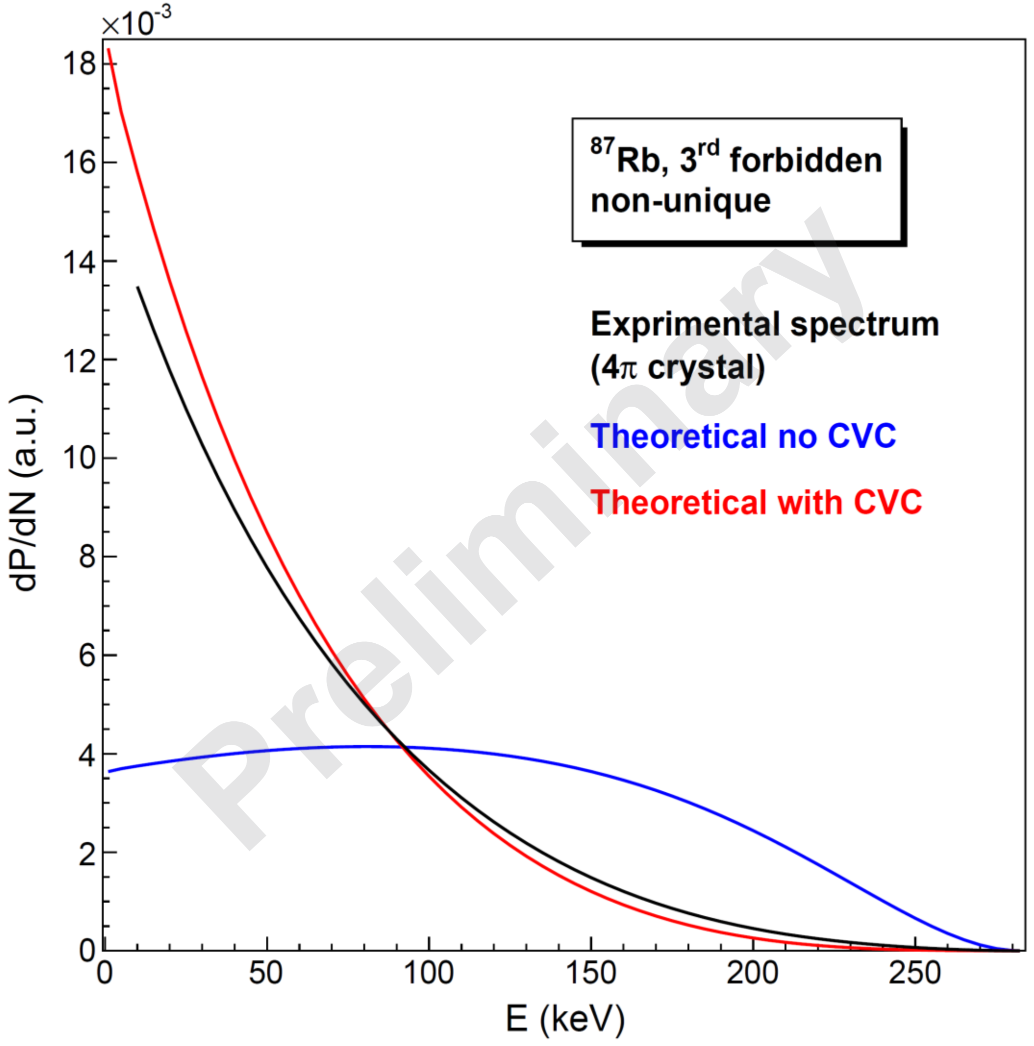
Detailed theoretical study (simplified lepton current)

Sadler, Behrens, Z. Phys. A 346, 25 (1993)



→ CVC hypothesis mandatory + Influence of lepton current treatment

^{87}Rb 3rd forbidden non-unique decay

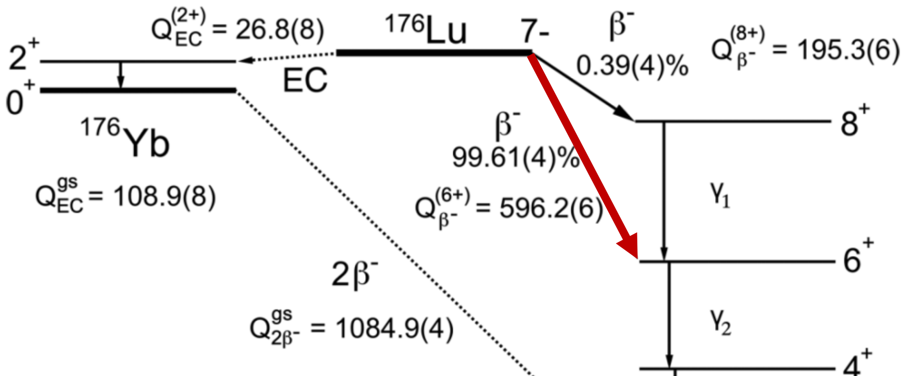


$^{87}\mathrm{Rb}\,(\mathrm{gs}, 3/2^-) \rightarrow {}^{87}\mathrm{Sr}\,(\mathrm{gs}, 9/2^+)$

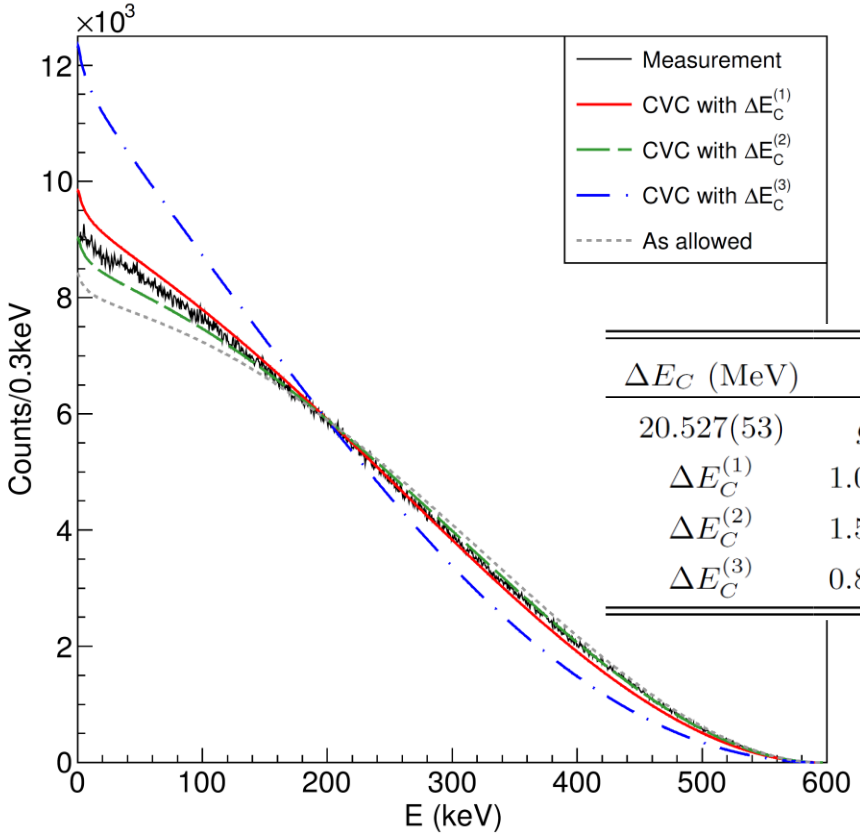
- Third forbidden non-unique transition
- NushellX ^{56}Ni doubly magic core, jj44 model space, jj44b interaction
- Preliminary measurement from the European MetroBeta project (4π $RbGd_2Br_7$ crystal)

→ **CVC hypothesis mandatory to describe the spectrum correctly**

^{176}Lu decay



	E(γ)	I(γ)
γ_1	400.99(4)	0.37(4) %
γ_2	306.78(4)	93.6(1.7) %
γ_3	201.83(3)	78.0(2.5) %
γ_4	88.34(3)	14.5(6) %



ΔE_C (MeV)	g_A
20.527(53)	g_A^{free}
$\Delta E_C^{(1)}$	1.057(5)
$\Delta E_C^{(2)}$	1.560(6)
$\Delta E_C^{(3)}$	0.834(4)

First forbidden non-unique transition

- ✓ First high-precision spectrum measurement from self-scintillation of a LuAG:Pr crystal at TU Delft.
- ✓ New Q-values: Q_β = 1193.0 (6) keV and Q_ε = 108.9 (8) keV. From AME2020: Q_β = 1194.1 (9) keV and Q_ε = 109.0 (12) keV.
- ✓ Spectrum shape retrieved adjusting the Coulomb displacement energy ΔE_C or the axial-vector coupling constant g_A.
- ✗ Calculated half-life shorter by 13 orders of magnitude!

  → **Detailed analysis would require accurate modelling with nuclear deformation: hindered transition ($\Delta K = 7$).**
- ✓ F.G.A. Quarati et al., Phys. Rev. C 107, 024313 (2023).

Effective coupling constants

- Free-nucleon value g_V = 1 according to CVC
- Free-nucleon value g_A = 1.2754 (13) [PDG 2020]

Review of J. Suhonen in Front. Phys. 5, 55 (2017)

→ Coupling constants g_V and g_A of the weak interaction can be affected by nuclear medium effects and nuclear many-body effects.

→ Spectral shapes can help for a better quantification of the effective values.

1st forbidden non-unique

g_V^{eff} ~ 0.3 – 0.7 and g_A^{eff} ~ 0.46 – 0.56

Higher non-unique

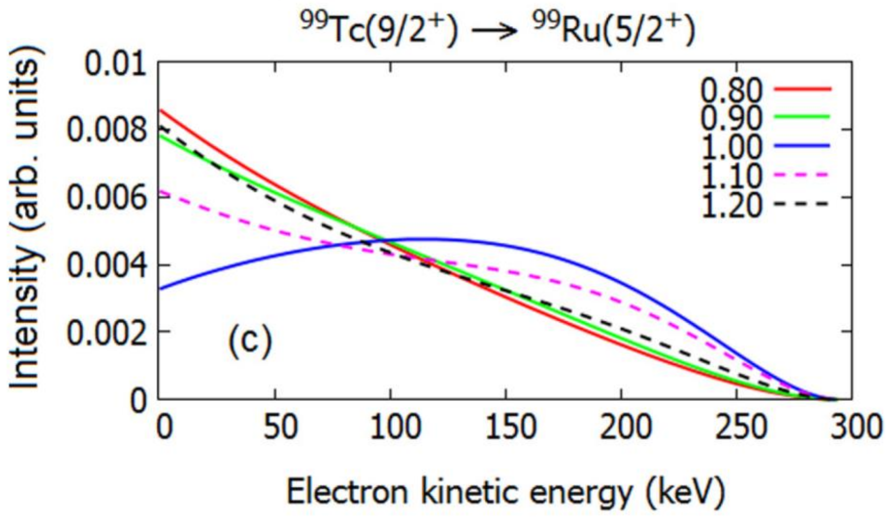
Lack of high-quality measurements

Suggests g_V = 1 and g_A^{eff} ~ 0.4

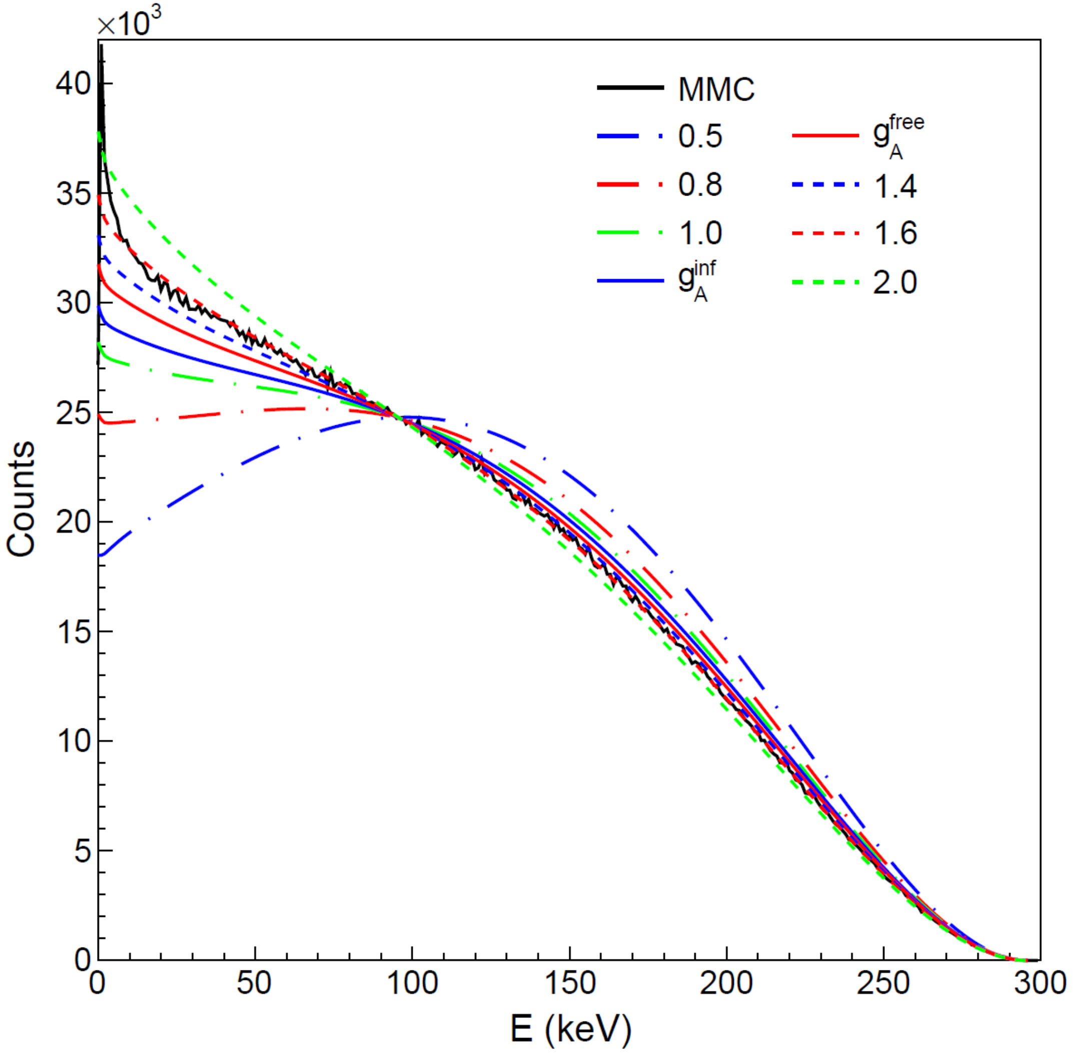
^{99}Tc beta spectrum

- Second forbidden non-unique.
- Predicted to be very sensitive to g_A.

J. Kostensalo, J. Suhonen, PRC 96, 024317 (2017)



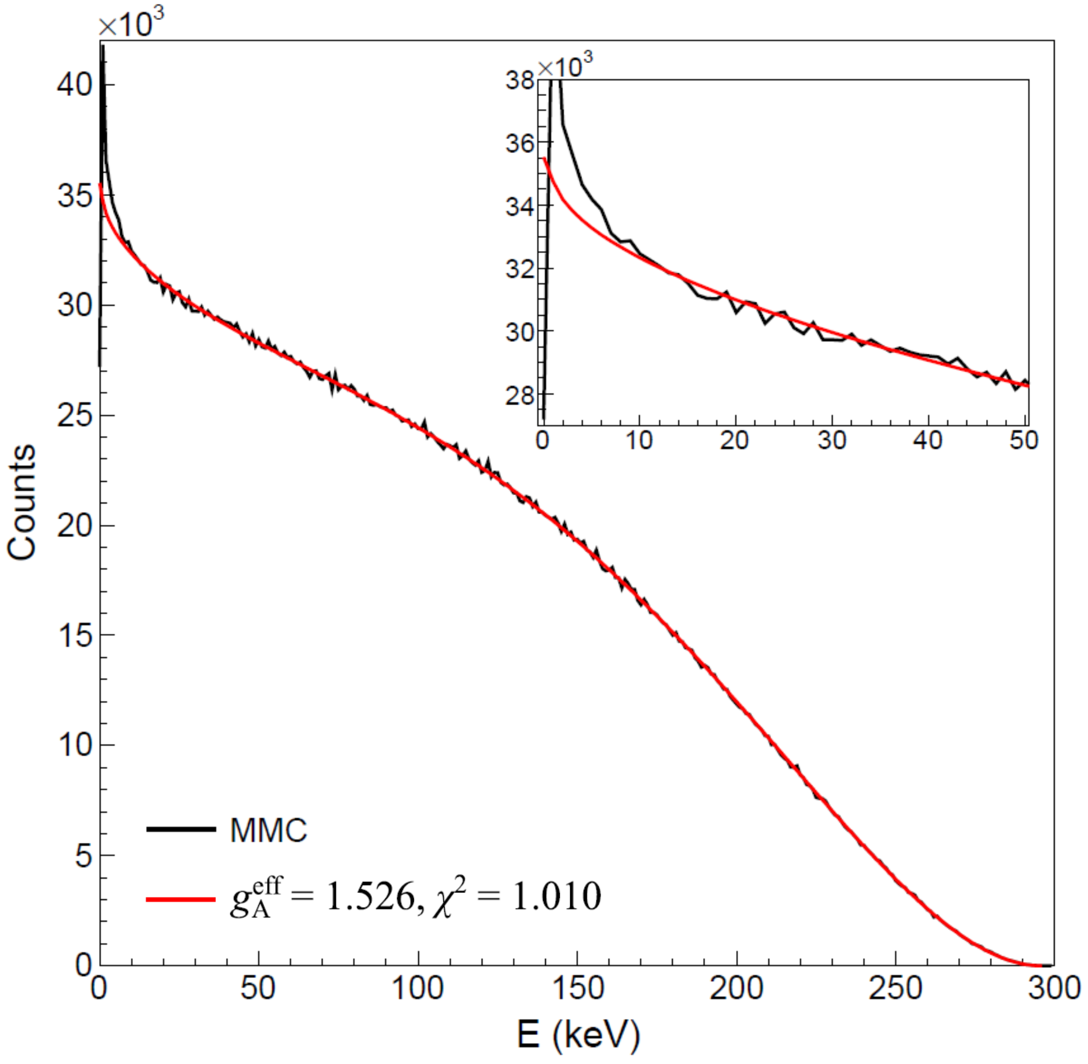
^{99}Tc 2nd forbidden non-unique decay



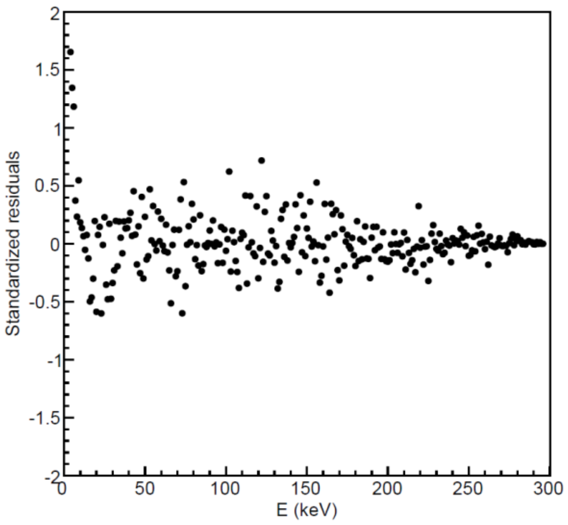
Within the European project PrimA-LTD

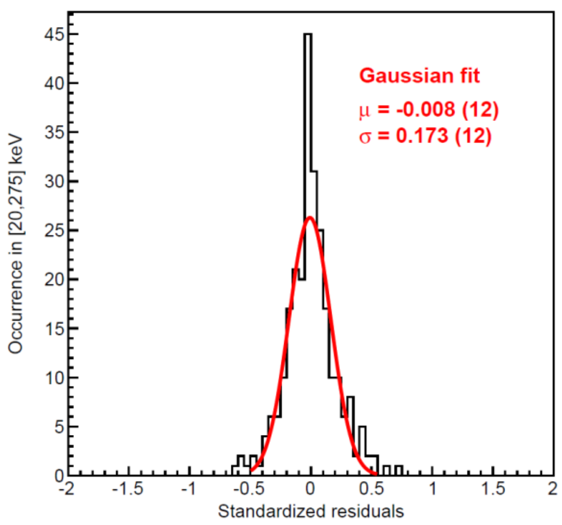
- ✓ High-precision measurements of ^{99}Tc spectrum with MMC at CEA-LNHB and PTB, and with Silicon detectors at CEA-LNHB.
- ✓ Excellent agreement of all the three spectra.
- ✓ **New Q-value = 295.82 (16) keV** not consistent with AME2020 value of 297.5 (9) keV.
- ✓ **High sensitivity to the effective value of g_A confirmed.**

^{99}Tc 2nd forbidden non-unique decay



- ✓ Three different model spaces used with NushellX (GL, GLEKPN, jj45pn) to quantify the influence of nuclear structure.
- ✓ Theoretical calculations with nuclear structure, CVC and complete lepton current.
- ✓ Best adjustment gives an effective axial-vector coupling constant g_A^{eff} = 1.526 (92), far from g_A^{eff} ~ 0.4.
- ✓ Excellent residuals, without any trend down to 6 keV.





^{99}Tc 2nd forbidden non-unique decay

‼ Effective g_A value is **enhanced** while should be **quenched**. What happens?

- Calculated half-life is about one order of magnitude too low.
- From DDEP: $T_{1/2}$ = 211.5 (11) · 10^3 y → Additional experimental constraint
- We can use it to renormalize the calculation and obtain a consistent picture: accurate shape, accurate half-life.

First possibility: **renormalization of the OBTD**

Example: GLEKPN

Multipole	Transition	Original	Corrected
K = 2	n $1g_{7/2}$ → p $1g_{9/2}$	0.00994	0.00362
	n $2d_{5/2}$ → p $1g_{9/2}$	0.47752	0.17383
K = 3	n $1g_{7/2}$ → p $1g_{9/2}$	-0.01709	-0.00622
	n $2d_{5/2}$ → p $1g_{9/2}$	-0.43403	-0.15800
	n $2d_{3/2}$ → p $1g_{9/2}$	0.03143	0.01144

Second possibility: **renormalization of g_V and g_A**

→ g_V^{eff} = 0.376 (5) and g_A^{eff} = 0.574 (36)

Consistent with 1st forbidden non-unique results

g_V^{eff} ~ 0.3 – 0.7 and g_A^{eff} ~ 0.46 – 0.56

✓ Study published in M. Paulsen et al., Phys. Rev. C 110, 055503 (2024).

^{99}Tc decay – Decay heat calculations

Eur. Phys. J. Plus (2022) 137:665
https://doi.org/10.1140/epjp/s13360-022-02865-7

THE EUROPEAN PHYSICAL JOURNAL PLUS

Regular Article

Check for updates

Nuclear data evaluation for decay heat analysis of spent nuclear fuel over 1–100 k year timescale

Hannah R. Doran[1,2,a], **Alan J. Cresswell**[2], **David C. W. Sanderson**[2], **Gioia Falcone**[1]

[1] James Watt School of Engineering, University of Glasgow, Glasgow G12 8QQ, UK
[2] Scottish Universities Environmental Research Centre, East Kilbride G75 0QF, UK

Table 3 Mean beta energies from different evaluated libraries (keV)

Nuclide	Evaluated library					
	JEF2.2	JEFF3.1.1	JEFF3.3	ENDF/B-VIII.0	ENSDF	DDEP
99Tc	**85.0**	**85.4 ± 0.6**	**95.3 ± 0.4**	**55.2 ± 0.3**	**84.6 ± 0.5**	**94.6 ± 1.7**

→ $\overline{E_\beta}$ = 98.51 (23) keV

✓ Value updated in JEFF4.0 (release in May 2025)

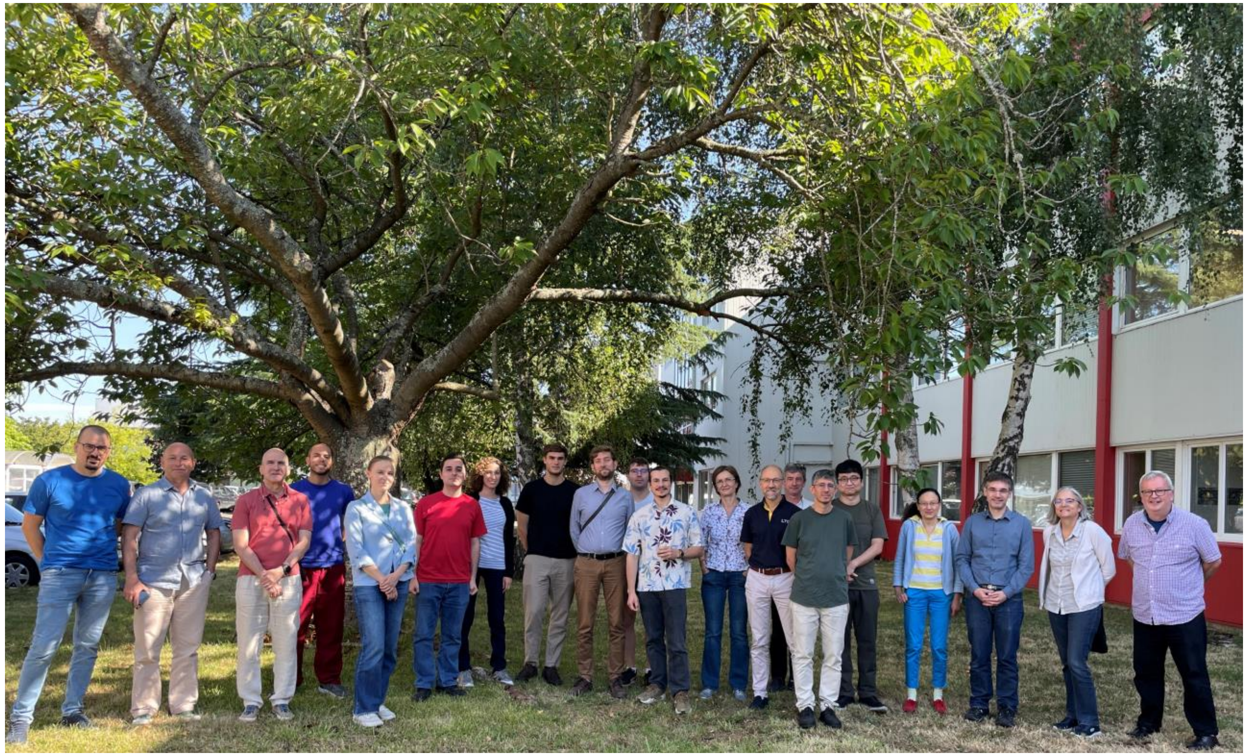
ESNT Workshop

Organization of workshop within the Theoretical Nuclear Structure and reaction framework of CEA/Irfu (Fundamental Research Division).

Probing nuclear structure with beta-decay energy spectra

CEA Saclay, 7-10 July 2025

- ✓ Scientific organization with B.C. Rasco from ORNL.
- ✓ 21 participants from Canada, Germany, Italy, Spain, UK, USA, and France (Metrology, Strasbourg University, IJCLab, CEA/Irfu, CEA/DAM).
- ✓ Half theorists, half experimentalists.
- ✓ **Second edition is scheduled on 21-25 September 2026. Feel free to contact us if you are interested.**



Program and presentations available on the ESNT website:

https://esnt.cea.fr/Phocea/Page/index.php?id=129

For the next decade

Over the last 15 years, there has been a resurgence of interest in beta decays, both experimentally and theoretically. **We have entered the era of high precision. The topic is mature for improving decay data.**

- ✓ High-precision measurements can be used to probe nuclear models.
- ✓ Beta spectra provide complementary information to that provided by half-lives.
- ✗ **Non-unique forbidden transitions are not predictable**: adjustment on experimental spectra is needed. This is a strong limitation.
- ➢ Effective values of weak interaction coupling constants are still an open subject. In-depth discussions between experimentalists and theorists will be necessary.

→ **There is a strong need for coupling beta decay formalism with a reliable structure model** that incorporates operator/coupling constant renormalization.

→ Coupling is a highly technical exercise that requires time to be done correctly.

Collaboration with CEA-DAM and CEA-DES is underway regarding QRPA.

- ✓ QRPA will allow for greater accuracy with deformed nuclei.
- ➢ Computing power will be a real challenge.

Another suggestion for JEFF

Over 3852 nuclei present in the JEFF decay data library, 2295 have properties only from NUBASE 2003 (60%).

NUBASE provides only the main decay modes

→ No information on intensity breakdown to the various levels of the daughter nucleus.

→ When isomers present in NUBASE, adopted rule was equal distribution

Ground-state + One isomer: 50% - 50%

Ground-state + Two isomers: 33% - 33% - 33%

etc.

➢ **A more realistic estimate could be obtained from reliable microscopic calculations.**

That would improve the accuracy of the decay data.

Thank you for attention