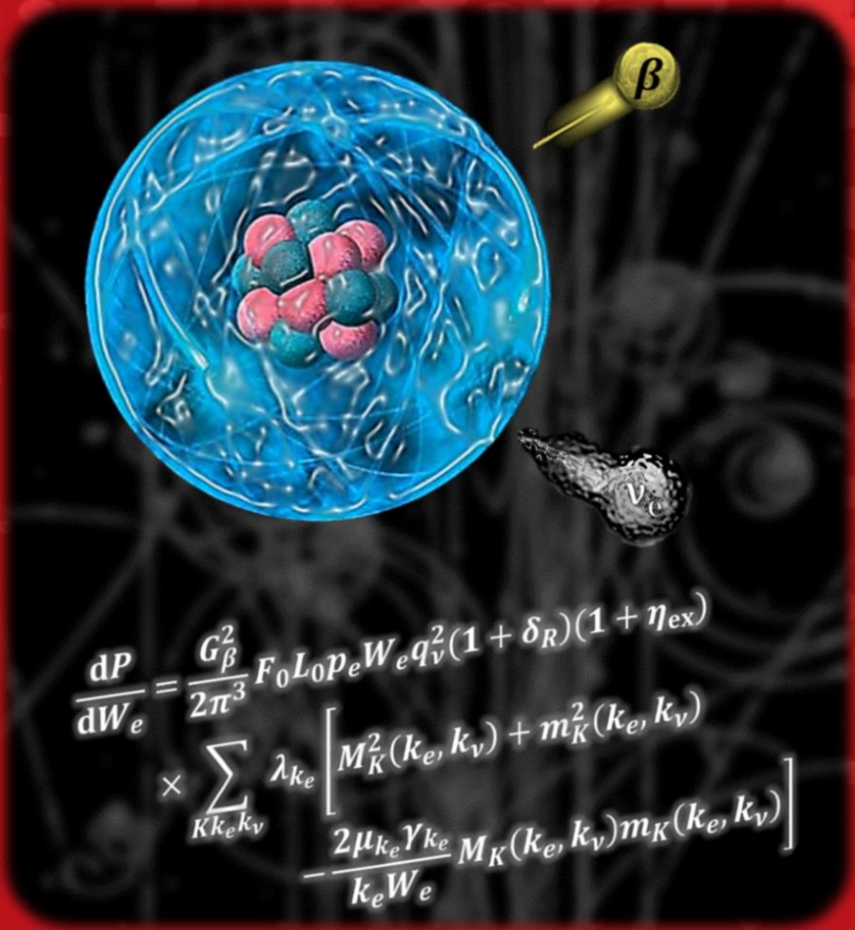
DE LA RECHERCHE
À L'INDUSTRIE

Latest developments in BetaShape



NSDD Spring Meeting – April 4-7, 2022

X. Mougeot

LNE LABORATOIRE NATIONAL DE MÉTROLOGIE ET D'ESSAIS

LNHB Laboratoire National Henri Becquerel

Current version

BetaShape v2.2 has been released in June 2021

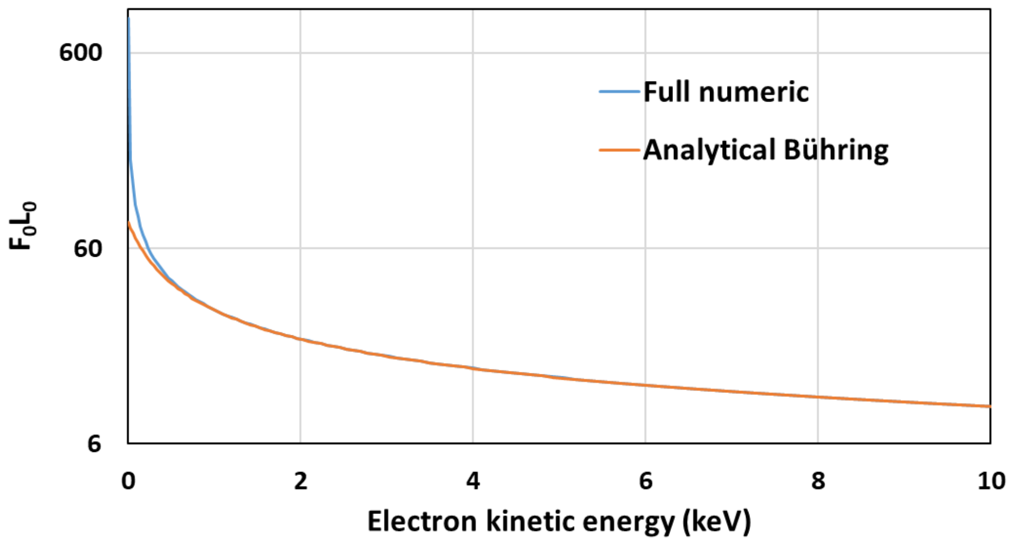
- ✓ Treatment of beta transitions and electron captures with improved theoretical models.
- ✓ Allowed and forbidden unique transitions (no limitation).
- ✓ Provision of :
  - ✓ Beta and neutrino spectra for each transition, and total spectrum of the decay.
  - ✓ Capture probabilities, capture probability ratios and capture-to-beta-plus ratios, for each subshell and gathered by shell; splitting of the branch when competition between capture and beta plus processes.
  - ✓ Mean energies of continuum spectra, log-*f*, log-*t* and log-*ft* values.
  - ✓ Experimental beta shape factors (database included).
- ✓ Reads and updates of ENSDF files. Uncertainty propagation of input parameters. Report files.
- ✓ Various options such as: switching on/off the corrections; fixing energy step in continuum spectra; automatic update of Q-values from AME2020; creation of CSV files; coupling with the Saisinuc software for DDEP evaluations.
- ✓ Executables are available for various platforms: Windows 10, macOS Big Sur (Intel and M1), Scientific Linux 6.7, Ubuntu 20.04 and Centos 8.

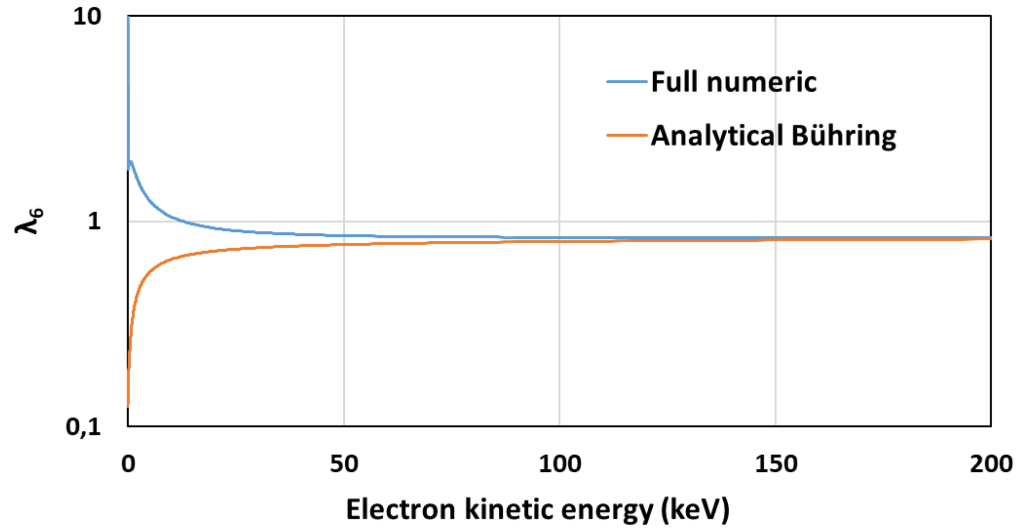
http://www.lnhb.fr/rd-activities/spectrum-processing-software/

Next version – Improved screening correction

Problem: Full numerical, precise calculations of relativistic electron wave functions including atomic screening is very time-consuming, especially at high kinetic energies where the effect is negligible.

- ✘ Theoretical work to establish a fast and precise computation of screening. Unfortunately, no method could be set.
- ➢ Hybrid method? Full numerical calculation at low energy, analytical when a given precision is reached.
- ➢ Comparison of analytical screening correction from Bühring (default one in current released version of BetaShape) with full numerical calculation.
- ➢ Example: Z = 28. Precision of 0.01 % reached by Bühring correction à 3.1 MeV for Fermi function F_0L_0 and at 13.4 MeV for λ_6!
- ✓ **Solution**: extensive tabulation of parameters sensitive to screening up to 30 MeV, Z = 120 and 6th forbidden unique $\beta^{\pm}$ transitions (λ_7).
- → Interpolation in tables. Exponential energy grid for better accuracy at low energy. Covers more than the currently known transitions.





Next version – Including atomic exchange effect

Problems: Atomic exchange effect can have a strong impact on the beta spectrum at very low energy. Full numerical, precise calculations is much more time-consuming than for screening (several minutes per spectrum). Model only available for allowed decays.

✓ Theoretical work: extension of the formalism to forbidden unique transitions.

✓ Our numerical code for the calculation of the exchange effect in allowed transitions has been adapted:

→ Treatment of the forbidden unique transitions.

→ Use of the same atomic wave functions as for electron captures: identical for all isotopes of same atomic number.

✓ Extensive tabulation of the exchange correction factors:

→ All atomic orbital included, up to Z = 120.

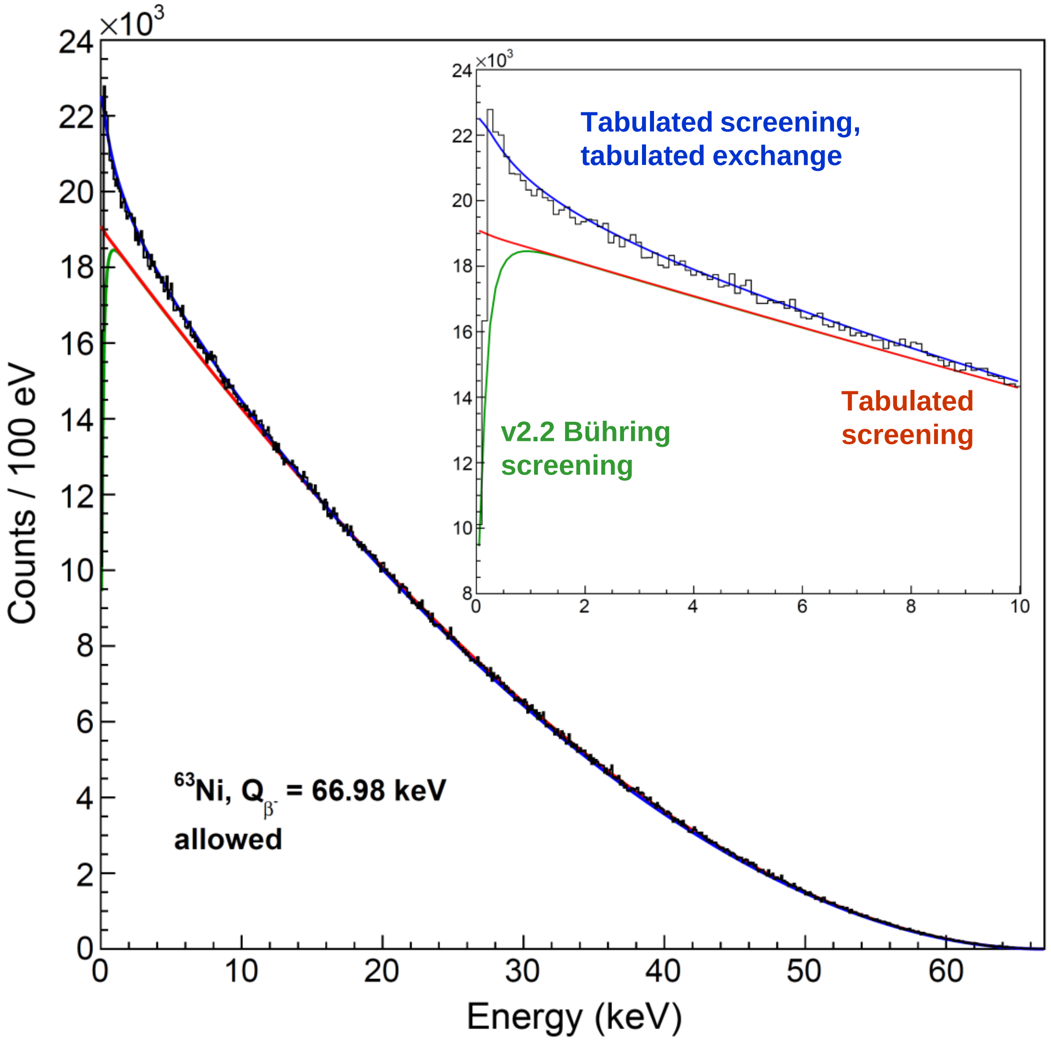
→ Exponential energy grid for better accuracy at low energy.

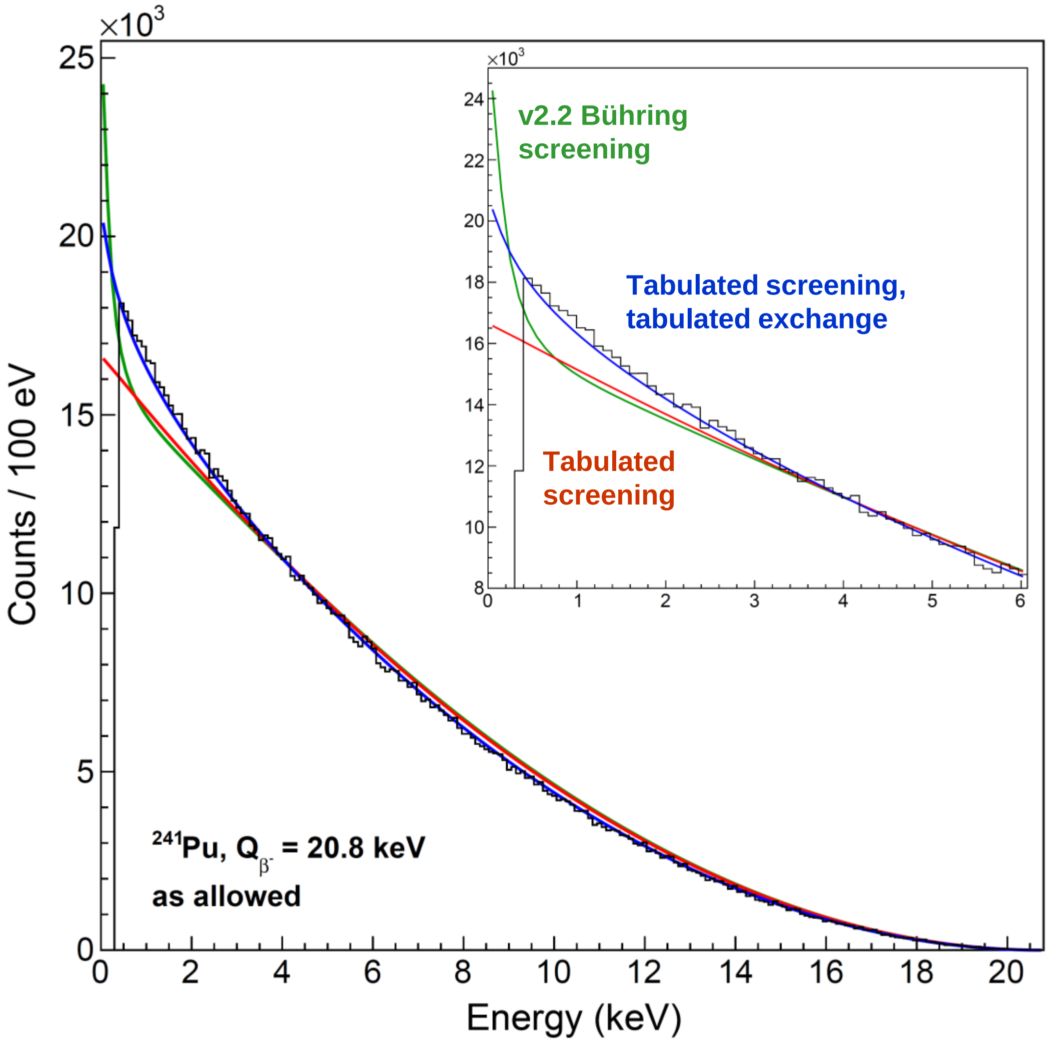
→ Correction factors converge to unity: tabulation up to a precision < 0.001 %.

⚠ This correction may be not accurate enough in the case of ultra-low end-point energies. Further studies (experimental and theoretical) are needed.

Next version – Results for ^{63}Ni and ^{241}Pu decays

High-precision measured spectra available from metallic magnetic calorimetry (MMC).





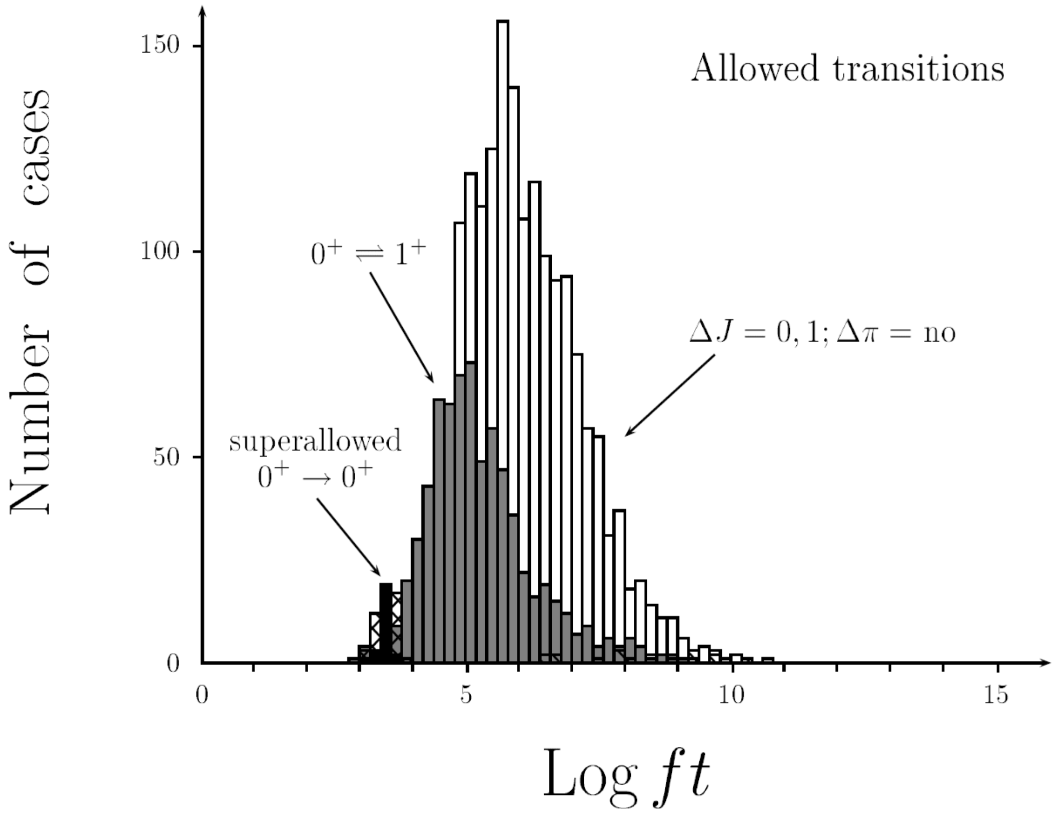
Next version – Others

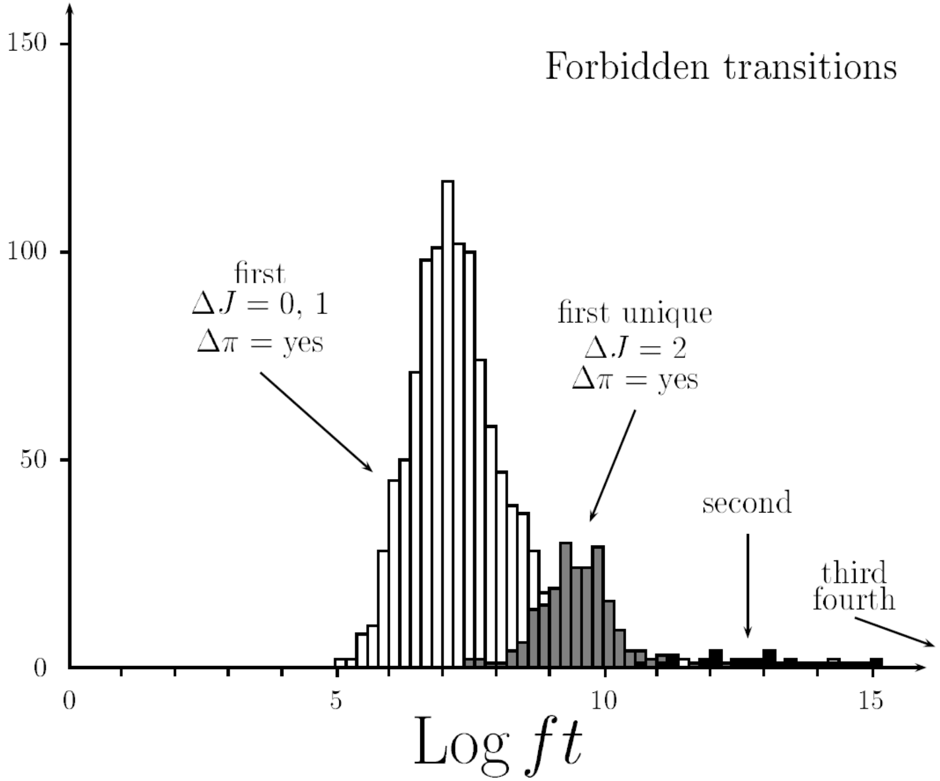
- ✓ Inclusion of the atomic overlap correction in beta decays. Negligible influence except close to the end-point energy, which can appear lower by hundreds of eV.
- ✓ A few bugs have been fixed in output format in very specific cases.
- ✓ Negative Q-values are now possible: decay of isomeric state with stable ground state (^{87m}Sr).
- ✓ ^{129}I experimental shape factor has been updated.
- ✓ Some security checks have been added to deal with ENSDF files that are not following the format, making code crashing.
- ➢ Unknown uncertainties (AP, SY, GT, etc.) are treated as null. Implementation is ongoing to treat them correctly for intensities and log-*ft* values.

Former review of log-*ft* values

Latest review done in 1998 for a selection of well-known beta transitions and electron captures.

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

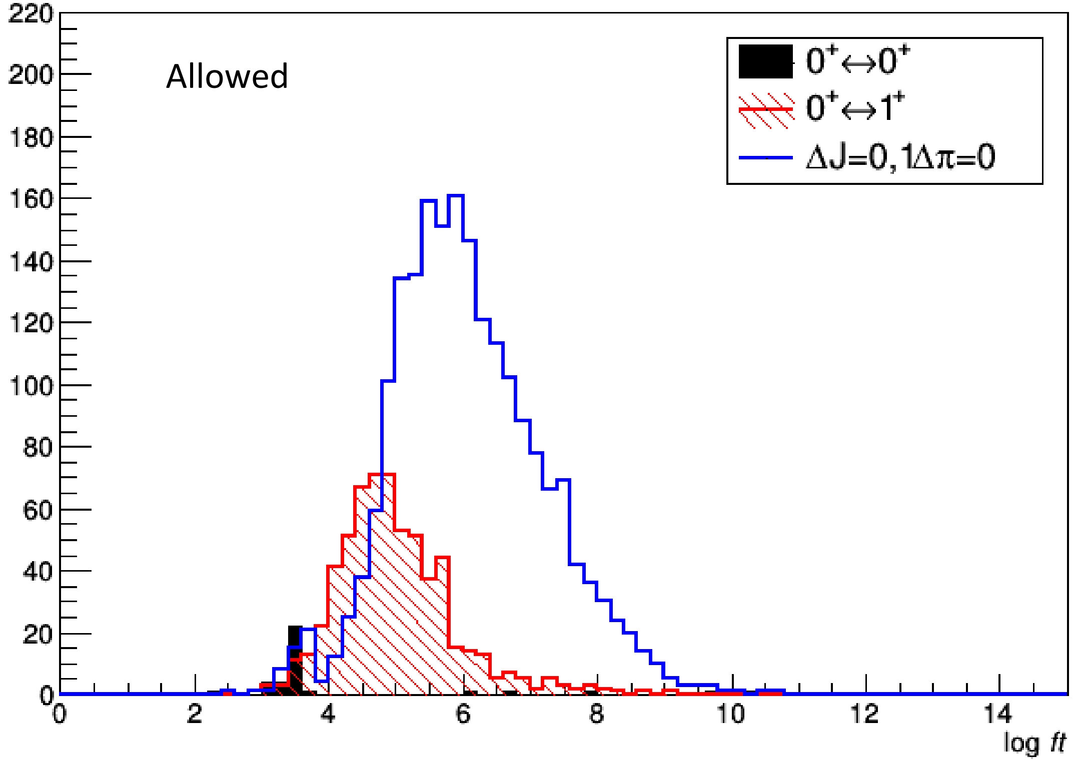


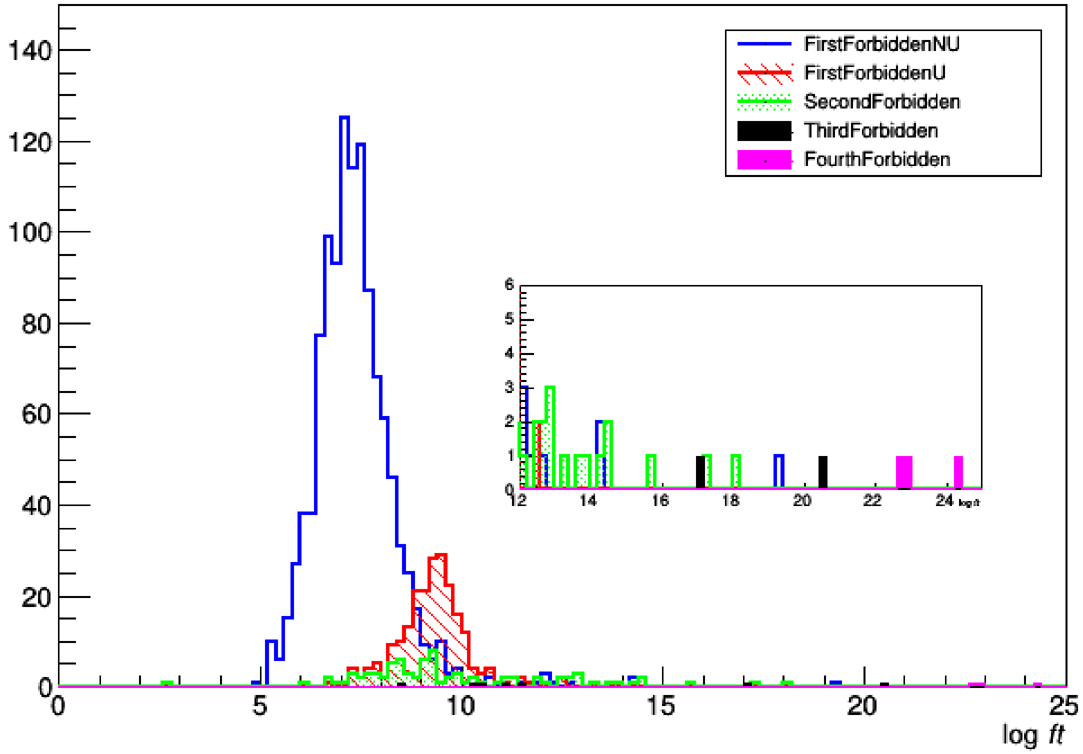


Updated review of log-*ft* values

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

- ✓ Update of beta and electron capture decays present in ENSDF database (as of March 2022).
- ✓ Use of BetaShape to calculate the log-*ft* values (with the developments since v2.2).
- ➢ Preliminary results (December 2021):





Forbidden non-unique transitions

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

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

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

Leading term for these transitions, simplifying the lepton current:

Relativistic matrix element: couples small and large components of nucleons wave functions

$$M_n(k_e, k_\nu) = K_n (pR)^{k_e - 1} (qR)^{k_\nu - 1} \left\{ -\sqrt{\frac{2n+1}{n}}\, {}^V F_{n,n-1,1}^{(0)} - \frac{\alpha Z}{2k_e+1}\, {}^V F_{n,n,0}^{(0)}(k_e, 1,1,1) - \left[\frac{WR}{2k_e+1} + \frac{qR}{2k_\nu+1}\right] {}^V F_{n,n,0}^{(0)} - \frac{\alpha Z}{2k_e+1}\sqrt{\frac{n+1}{n}}\, {}^A F_{n,n,1}^{(0)}(k_e,1,1,1) - \left[\frac{WR}{2k_e+1} - \frac{qR}{2k_\nu+1}\right]\sqrt{\frac{n+1}{n}}\, {}^A F_{n,n,1}^{(0)} \right\}$$

Nuclear structure models are non-relativistic. I'm using NushellX@MSU, spherical shell model with fitted Hamiltonians.

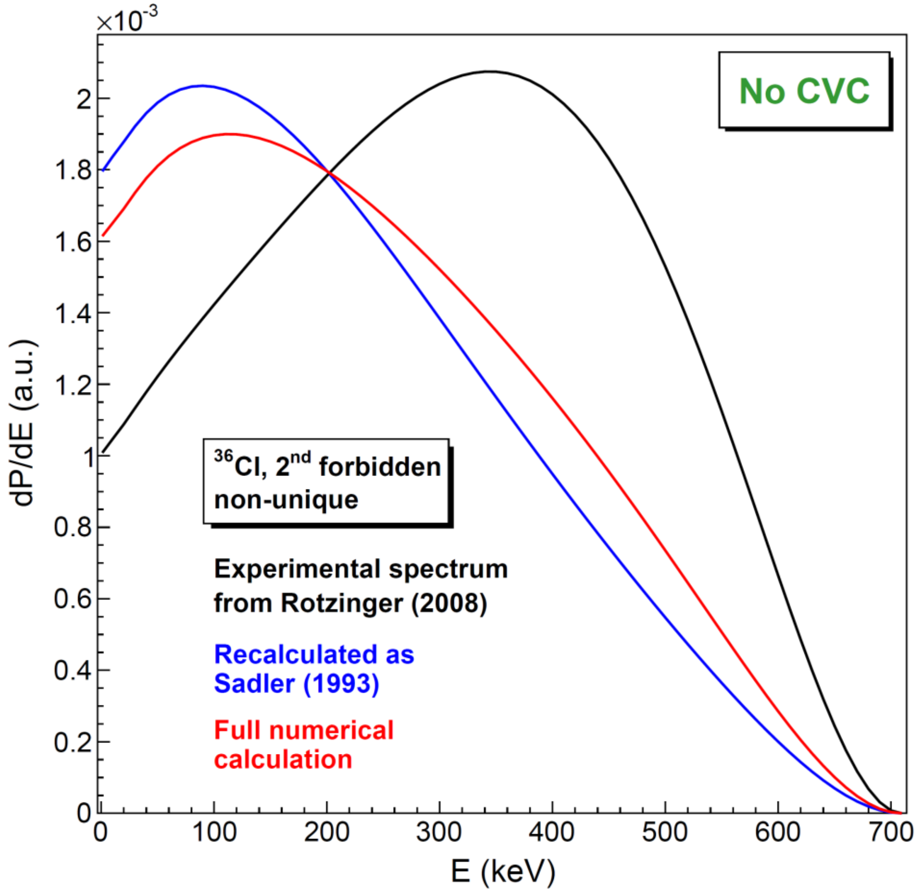
→ **Conserved Vector Current (CVC) hypothesis**

- Comes from gauge invariance of the weak interaction.
- Relationships between **non-relativistic** and **relativistic** vector matrix elements.

^{36}Cl decay

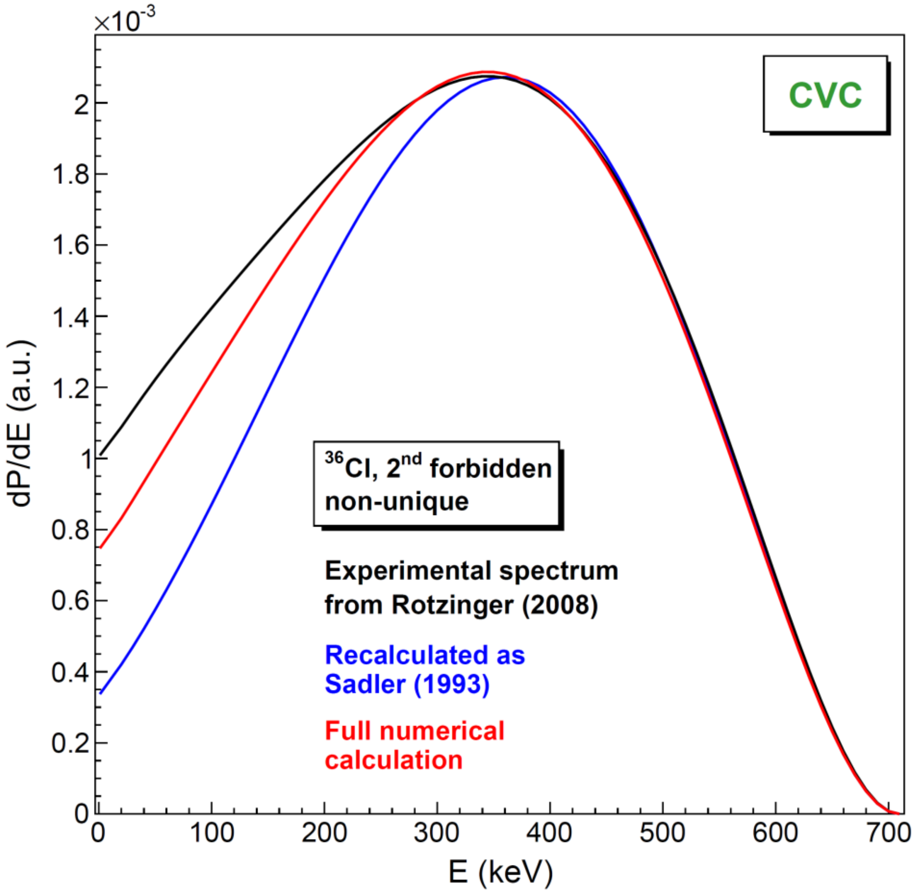
Precise measurement exists

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



Detailed theoretical study (with approximations)
→ Matrix elements are correctly recalculated

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

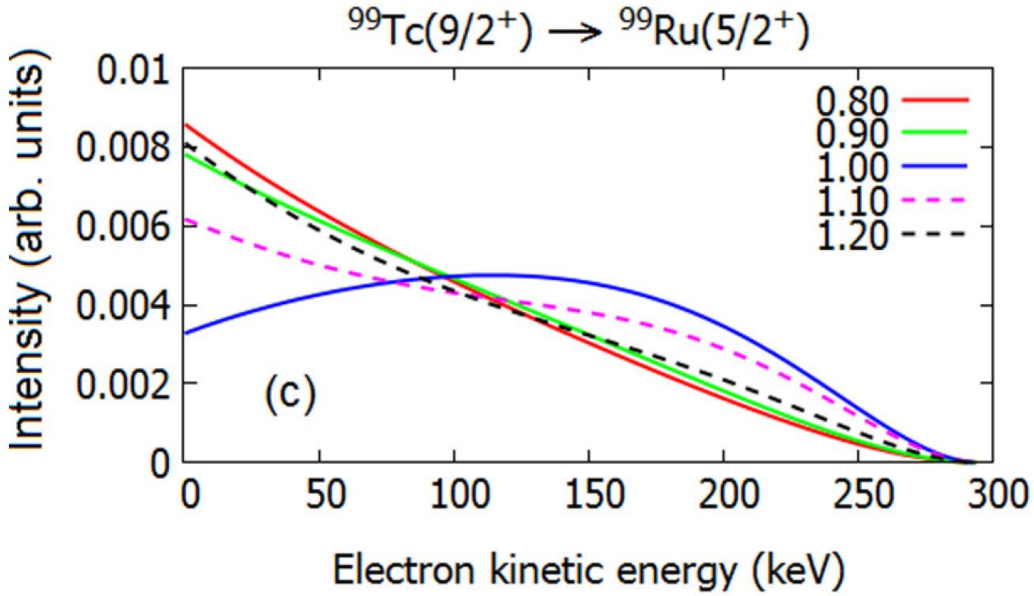


→ CVC hypothesis mandatory + Influence of lepton current treatment

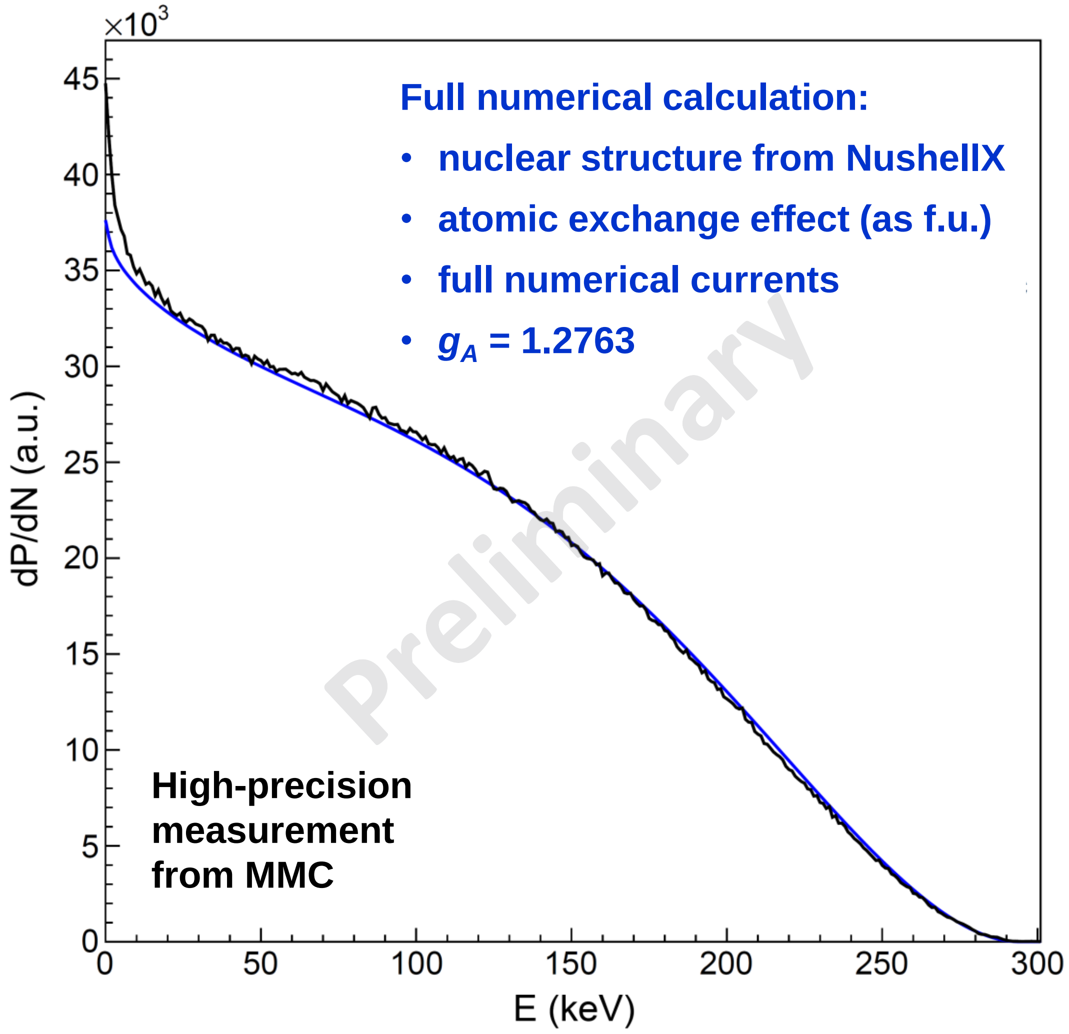
^{99}Tc decay – Preliminary results

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

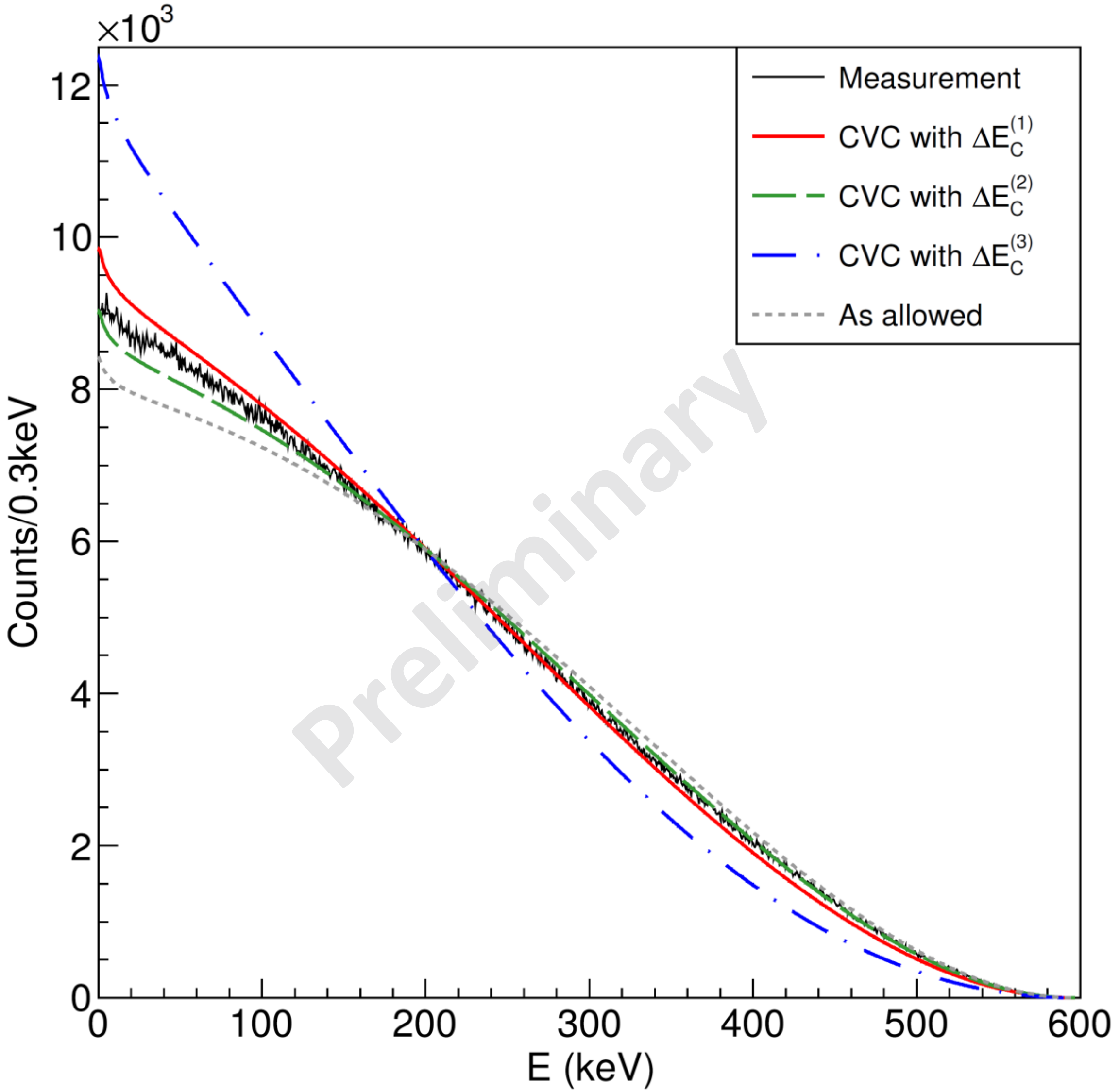
g_A-driven shapes of electron spectra of forbidden beta decays in the nuclear shell model



- ✓ Shape sensitivity to g_A value well reproduced with partial lepton current.
- ✓ The only way to get the measured spectrum is to apply CVC with a full numerical treatment of the lepton current. Free-nucleon value of g_A seems to be (almost) sufficient.



^{176}Lu decay – Preliminary results



First forbidden non-unique transition

- ✓ First high-precision Q-value
- ✓ First high-precision spectrum measurement (crystals)
- ➢ Calculations with nuclear structure
  - One-body transition densities with NushellX
  - Expansion of the lepton current
  - Screening and exchange included from tables

→ Realistic shape only possible with CVC, which is quite sensitive to the Coulomb displacement energy.

Adjustments lead to similar residuals but very different effective g_A coupling constant and log-f value.

ΔE_C (MeV)	g_A	log f
20.527(53)	g_A^{free}	-0.835(19)
$\Delta E_C^{(1)}$	1.057(5)	-0.975(14)
$\Delta E_C^{(2)}$	1.560(6)	-0.679(12)
$\Delta E_C^{(3)}$	0.834(4)	-1.148(14)

Nucleus deformation: hindered transition ($\Delta K = 7$)

$$t_{1/2}^{\text{exp}} = t_{1/2}^{\text{theo}} / \left[F^{\Delta K - 1}\right]^2 \quad \rightarrow \quad F = 0.0768(20)$$

Conclusion

BetaShape

- ✓ Version 2.1 released in June 2019.
- ✓ Version 2.2 (current) released in June 2021.
- ✓ Executables available for various platforms: Windows, macOS, Scientific Linux, Ubuntu and Centos.

http://www.lnhb.fr/rd-activities/spectrum-processing-software/

→ **Feedback on the results, comments, suggestions and bug reports are very welcome.**

- ➢ Next version with improved model of beta decay with precise atomic effects (screening, exchange and overlap).

Updated review of log-*ft* values: completed, paper to draft.

Forbidden non-unique transitions

- ✓ Inclusion of nuclear structure in the calculations, from NushellX (usable by non-specialists).
- ✓ Study of the influence of the lepton current treatment, CVC hypothesis, Coulomb displacement energy and effective g_A.
- ➢ Ongoing developments in a European project: accurate atomic wave functions with a on-purpose DFT code; nuclear structure of deformed nuclei with (HFB + pnQRPA) large-scale calculations.

Thank you for your attention.