

PrimA-LTD

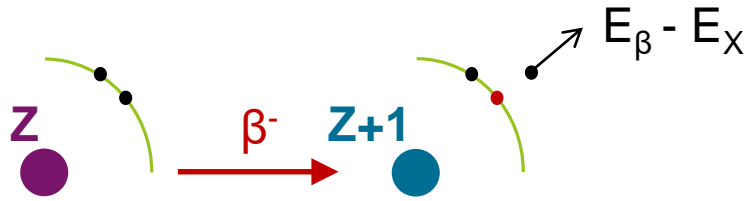
Atomic exchange correction in forbidden unique beta transitions

X. Mougeot

ICRM conference | 27 March 2023



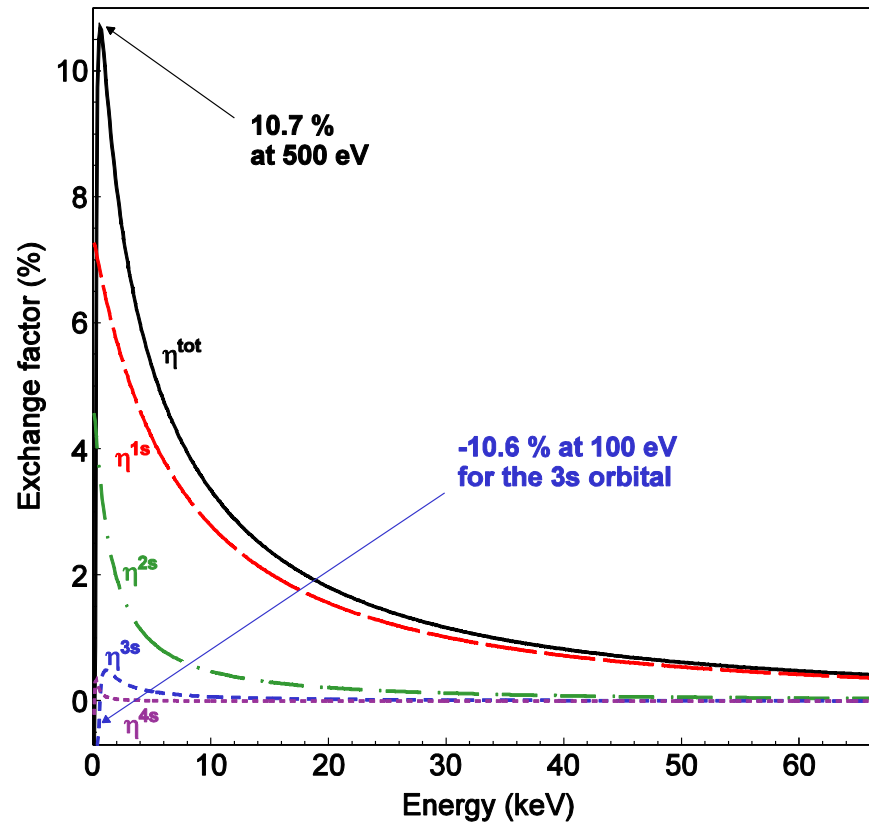
The atomic exchange effect



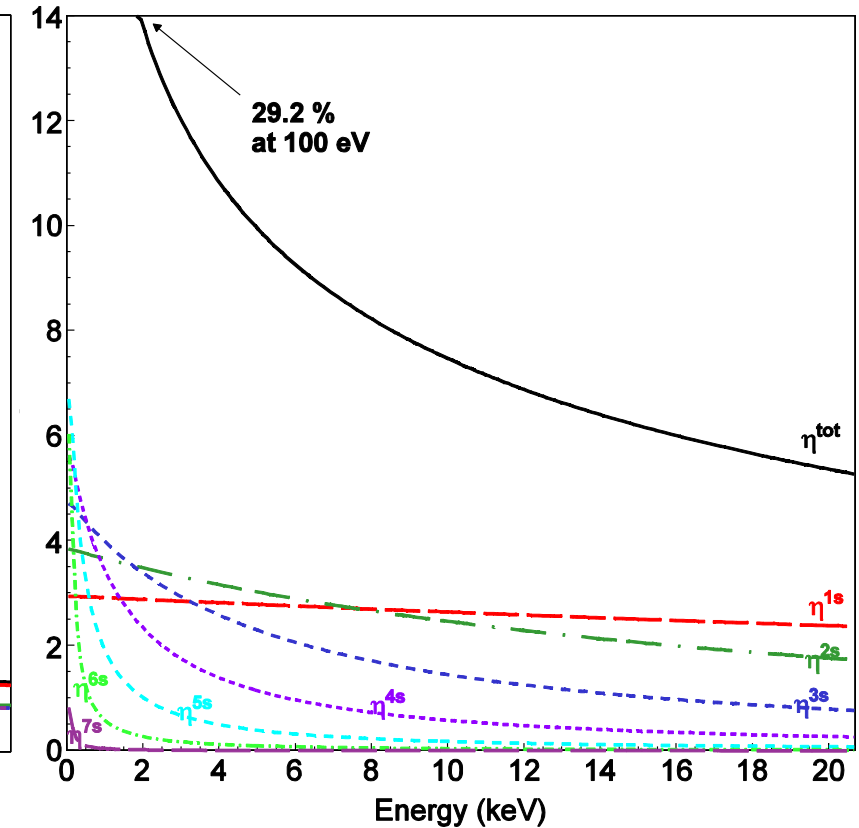
N.C. Pyper, M.R. Harston, Proc. Roy. Soc. Lond. A 420, 277 (1988)

- Indistinguishable from the direct decay to a final continuum state.
- Depends on the overlap of the continuum and bound electron wave functions.
- Allowed transitions: $s_{1/2}$ and $p_{1/2}$ orbitals only.

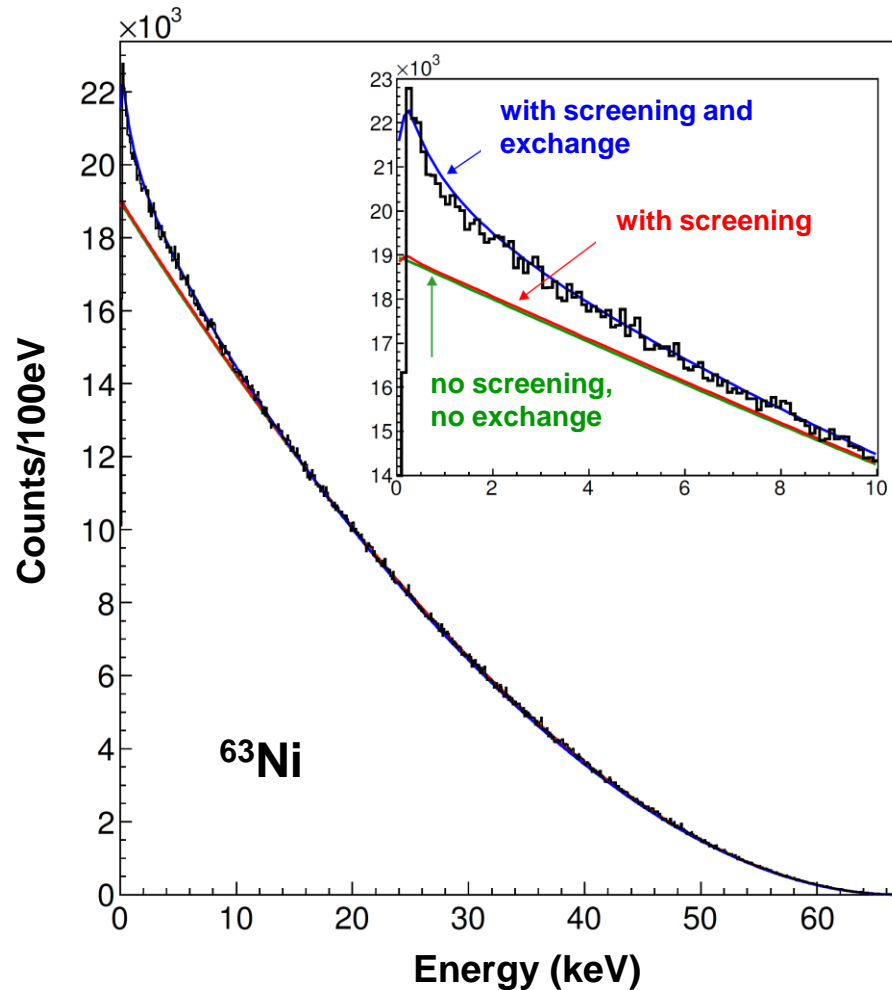
⁶³Ni decay



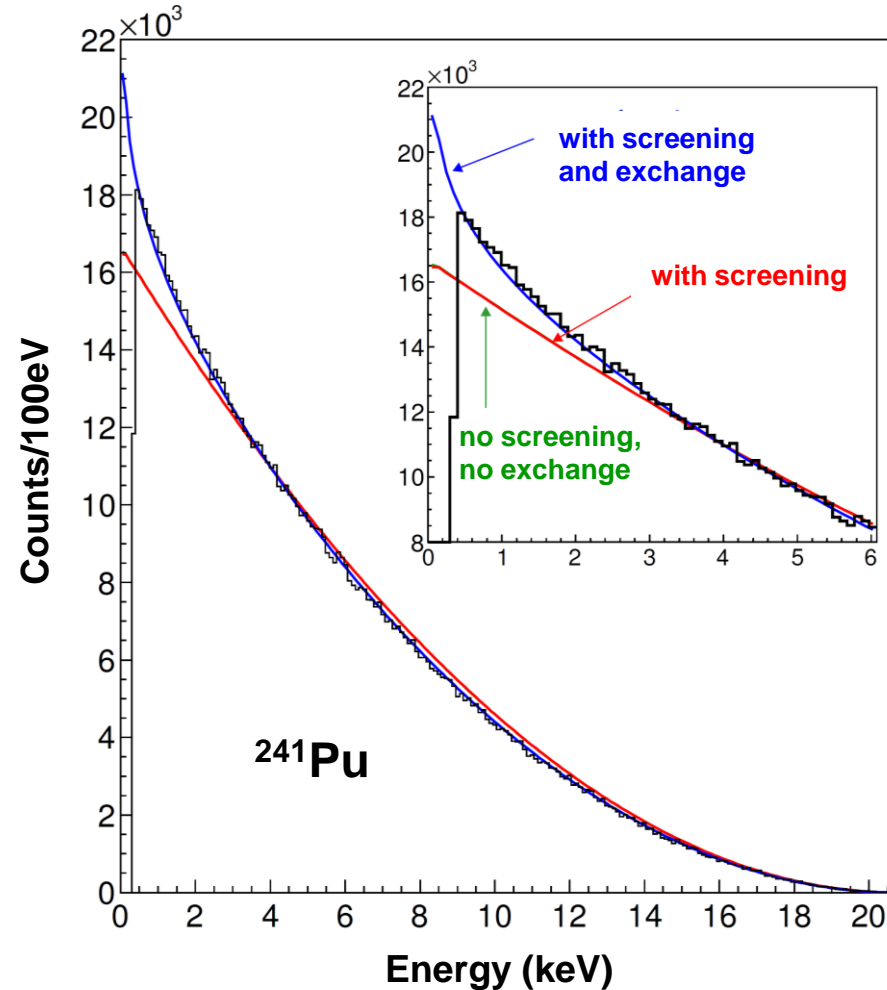
²⁴¹Pu decay



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



Usual calculation: $E_{\text{mean}} = 17.45 \text{ keV}$
 Full calculation: $E_{\text{mean}} = 17.06 \text{ keV}$



Usual calculation: $E_{\text{mean}} = 5.24 \text{ keV}$
 Full calculation: $E_{\text{mean}} = 5.04 \text{ keV}$

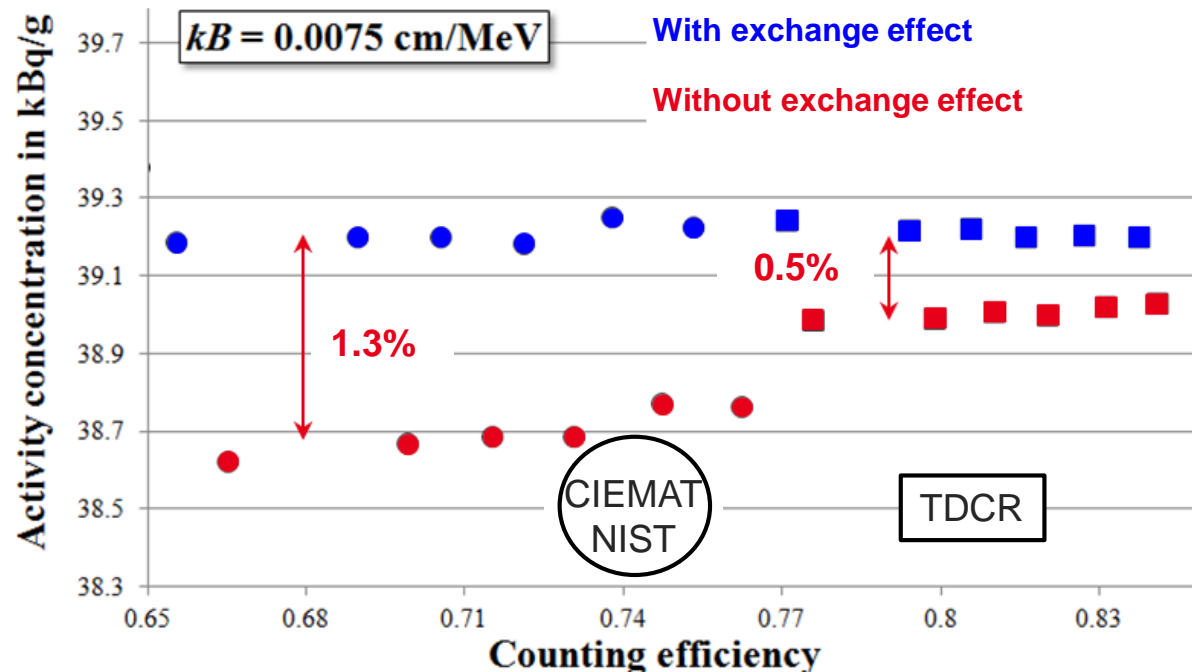
M. Loidl *et al.*, App.
Radiat. Isot. 68,
1454 (2010)

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

Impact in radionuclide metrology

CIEMAT/NIST $\varepsilon = \int_0^{E_{\max}} S(E)(1 - e^{-\eta})^2 dE$

TDCR $\frac{R_T}{R_D} = \frac{\int_0^{E_{\max}} S(E)(1 - e^{-\eta})^3 dE}{\int_0^{E_{\max}} S(E)[3(1 - e^{-\eta})^2 - 2(1 - e^{-\eta})^3] dE}$



Improvement of primary activity determination by Liquid Scintillation Counting

✓ ^{63}Ni : K. Kossert, X. Mougeot, Appl. Radiat. Isot. 101, 40 (2015)

✓ ^{60}Co : K. Kossert et al., Appl. Radiat. Isot. 134, 212 (2018)

➤ See presentation of C. Bobin on Thursday (LSC session) about $^{106}\text{Ru}/^{106}\text{Rh}$

✓ $^{90}\text{Sr}/^{90}\text{Y}$: K. Kossert, X. Mougeot, Appl. Radiat. Isot. 168, 109478 (2021)

First forbidden unique transitions, applying exchange correction as for allowed transitions.

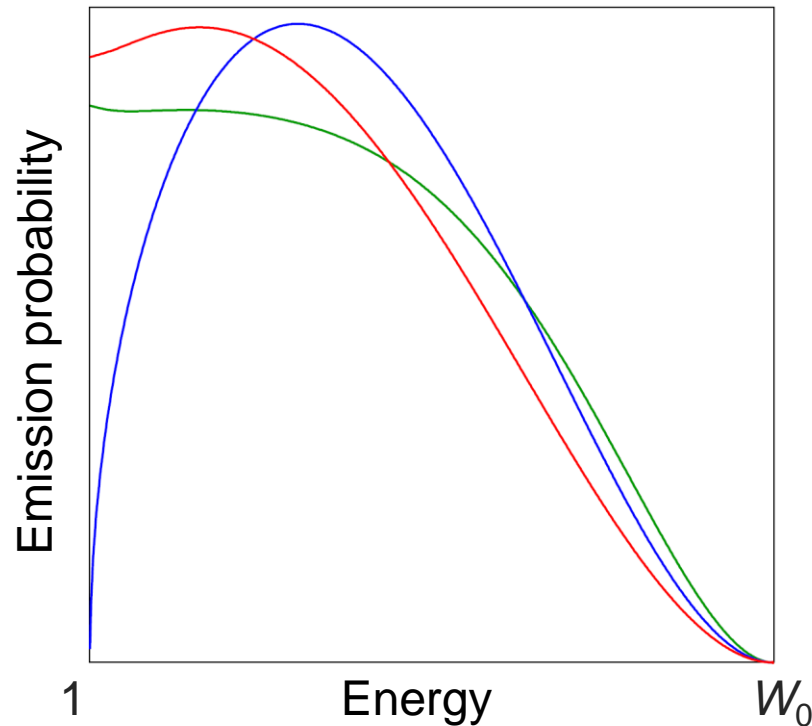
→ Accuracy of this approximation? How to go beyond?

Beta spectrum shape



Phase space Fermi function Shape factor

$$\frac{dP}{dW} \propto pWq^2 \cdot F(Z, W) \cdot C(W)$$



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.

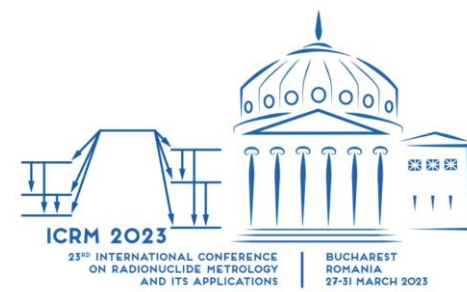
For forbidden non-unique transitions, coupling with nuclear structure is needed.

In Behrens and Bühring formalism, with k the main electron quantum number:

$$F(Z, W) = \frac{\alpha_{-1}^2 + \alpha_{+1}^2}{2p^2} \quad \lambda_k = \frac{\alpha_{-k}^2 + \alpha_{+k}^2}{\alpha_{-1}^2 + \alpha_{+1}^2}$$

Coulomb amplitudes of the relativistic electron wave functions, determined by normalization conditions.

Extension of the formalism 1/2



Allowed transitions

Beta electrons in $k = 1$ states \rightarrow Exchange only with atomic $k = 1$ states, i.e. $s_{1/2}$ and $p_{1/2}$.

$$C(W_e) = 1 \longrightarrow C(W_e) \times (1 + \eta_1)$$

Shape factors of forbidden unique transitions are established considering only the dominant matrix elements.

Derivation was restarted from the beginning, keeping every k state.

\rightarrow In general, atomic, nuclear and lepton matrix elements are coupled altogether.

\rightarrow Forbidden non-unique transitions: there is no possibility to simplify the calculation.

✓ **Forbidden unique transitions: it is still possible to keep the dominant matrix elements and factor out the nuclear component.**

Each term in the shape factor depends on its k value, and has its specific exchange correction.

Example: First forbidden unique transition

$$C(W_e) = q^2 + \lambda_2 p^2$$

$$q^2 \longrightarrow q^2 \times (1 + \eta_1) \quad \text{and} \quad \lambda_2 p^2 \longrightarrow \lambda_2 p^2 \times (1 + \eta_2)$$

Exchange with atomic electrons in $s_{1/2}$ and $p_{1/2}$ states \quad and \quad with atomic electrons in $p_{3/2}$ and $d_{3/2}$ states.

Extension of the formalism 2/2



The exchange correction factor has been established to be:

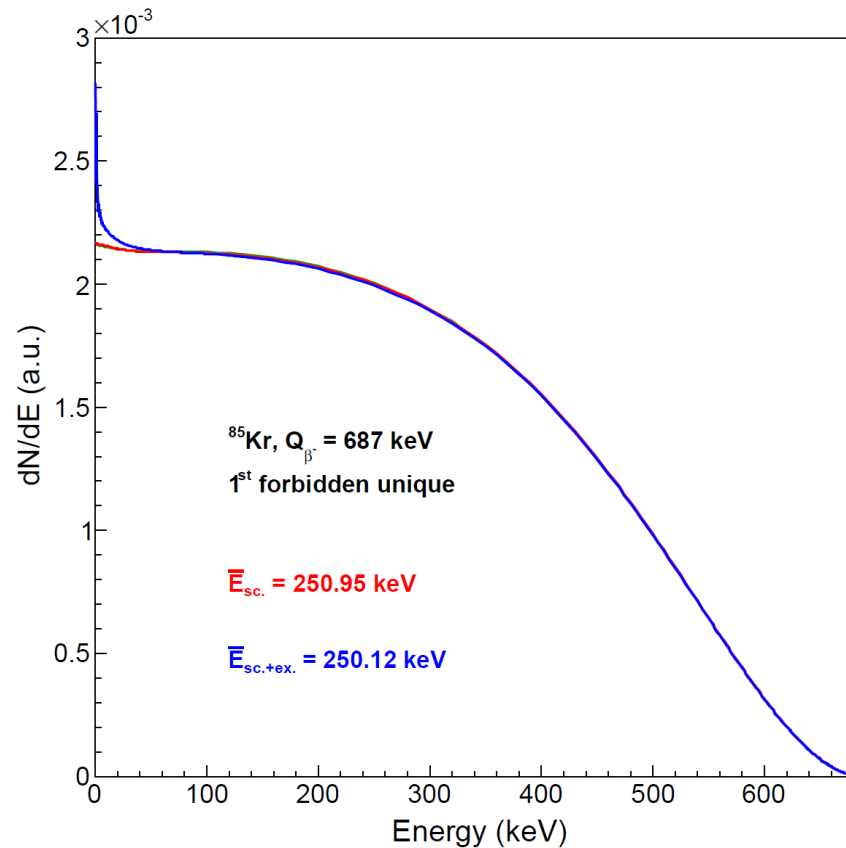
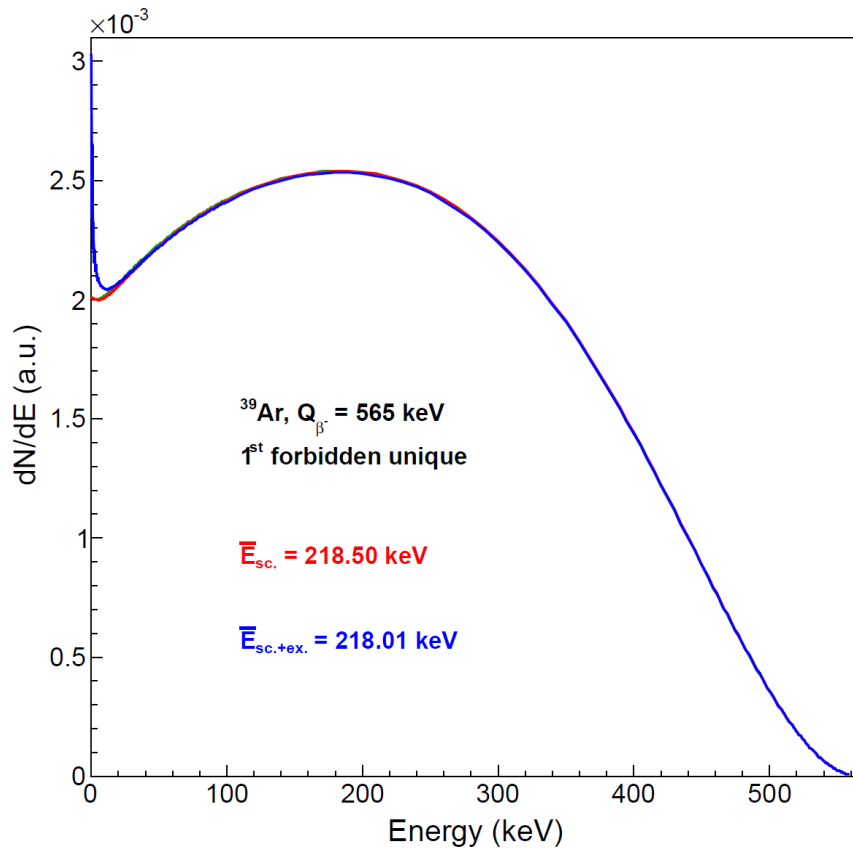
$$\eta_k = \frac{T_{+k}(T_{+k} - 2\alpha_{+k}) + T_{-k}(T_{-k} - 2\alpha_{-k})}{\alpha_{+k}^2 + \alpha_{-k}^2}$$

Assuming full orbitals and no shaking processes (auto-excitation and auto-ionization), one finds:

$$T_k = \sum_n \frac{\langle \phi'_{c,k} | \phi_{b,nk} \rangle}{\langle \phi'_{b,nk} | \phi_{b,nk} \rangle} \beta'_{nk} \left(\frac{p'_{nk}}{p} \right)^{k-1}$$

- Ratio of two overlaps between: initial atomic state and final continuum state; and the same initial and final atomic states. Harston and Pyper assumed $\langle \phi'_{b,nk} | \phi_{b,nk} \rangle = 1$.
 - β'_{nk} is the Coulomb amplitude of the atomic wave function in the final state.
 - Last term is the ratio of electron momenta.
- ✓ **This extended formalism is fully consistent with the allowed formalism.**
- The dominant contribution comes from $k = 1$ (upper overlap, ratio of momenta).
 - In the shape factor, q dominates over p at low energy, where exchange effect is significant.
- **Applying the allowed exchange correction simply to the Fermi function is a good approximation for the forbidden unique transitions.**

Background of DarkSide experiment



Pushing the limits of dark matter detection requires describing the background with high accuracy, especially at low energy.

^{39}Ar and ^{85}Kr decays are of special importance in the background of the DarkSide experiment.

- P. Agnes et al., Physical Review D 107, 063001 (2023)
- P. Agnes et al., Physical Review Letters 130, 101001 (2023)
- P. Agnes et al., Physical Review Letters 130, 101002 (2023)

Inclusion in BetaShape



Problems

- Precise exchange correction requires precise screening correction.
- Full numerical, precise calculations of relativistic electron wave functions including atomic screening are very time-consuming, especially at high kinetic energies where the effect is negligible.
- Full numerical, precise calculations of atomic exchange effect are much more time-consuming than for screening.

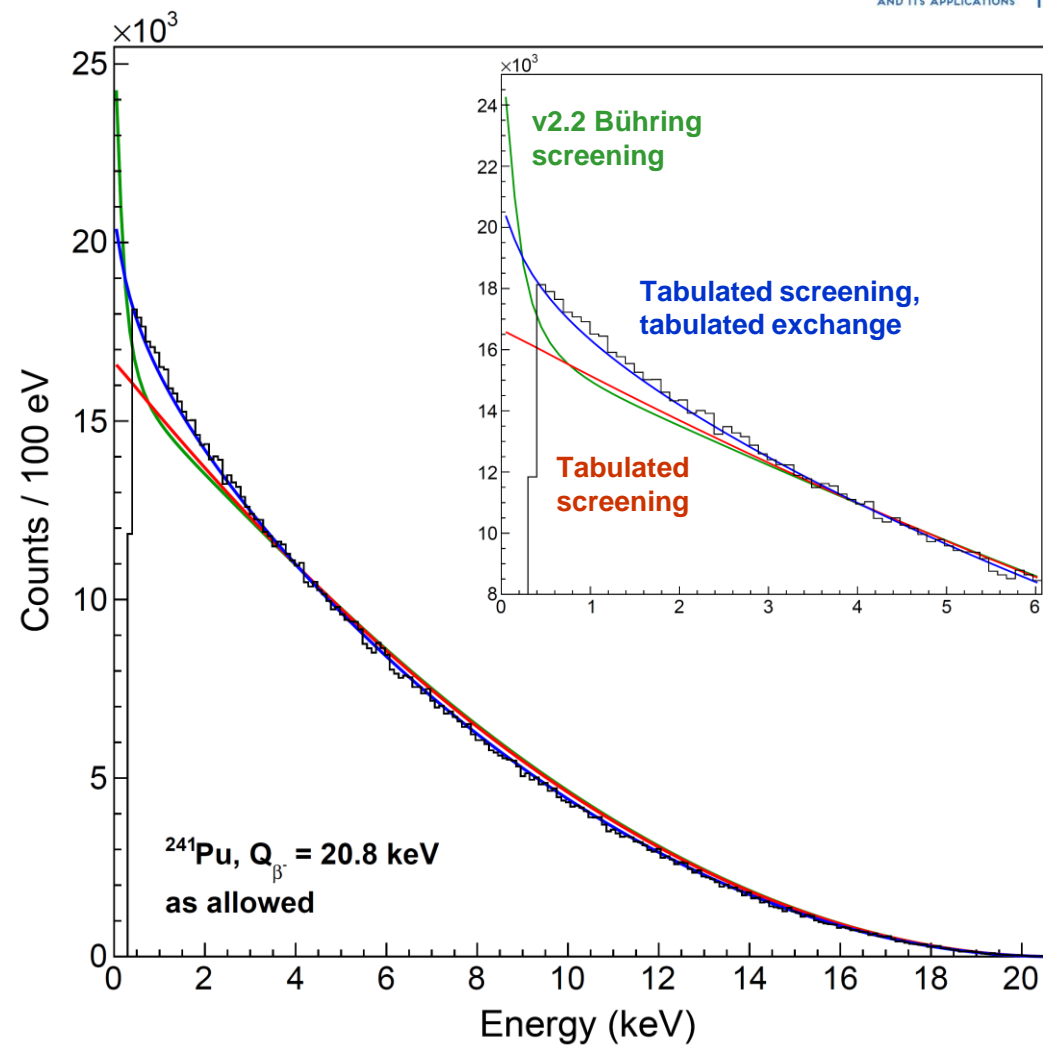
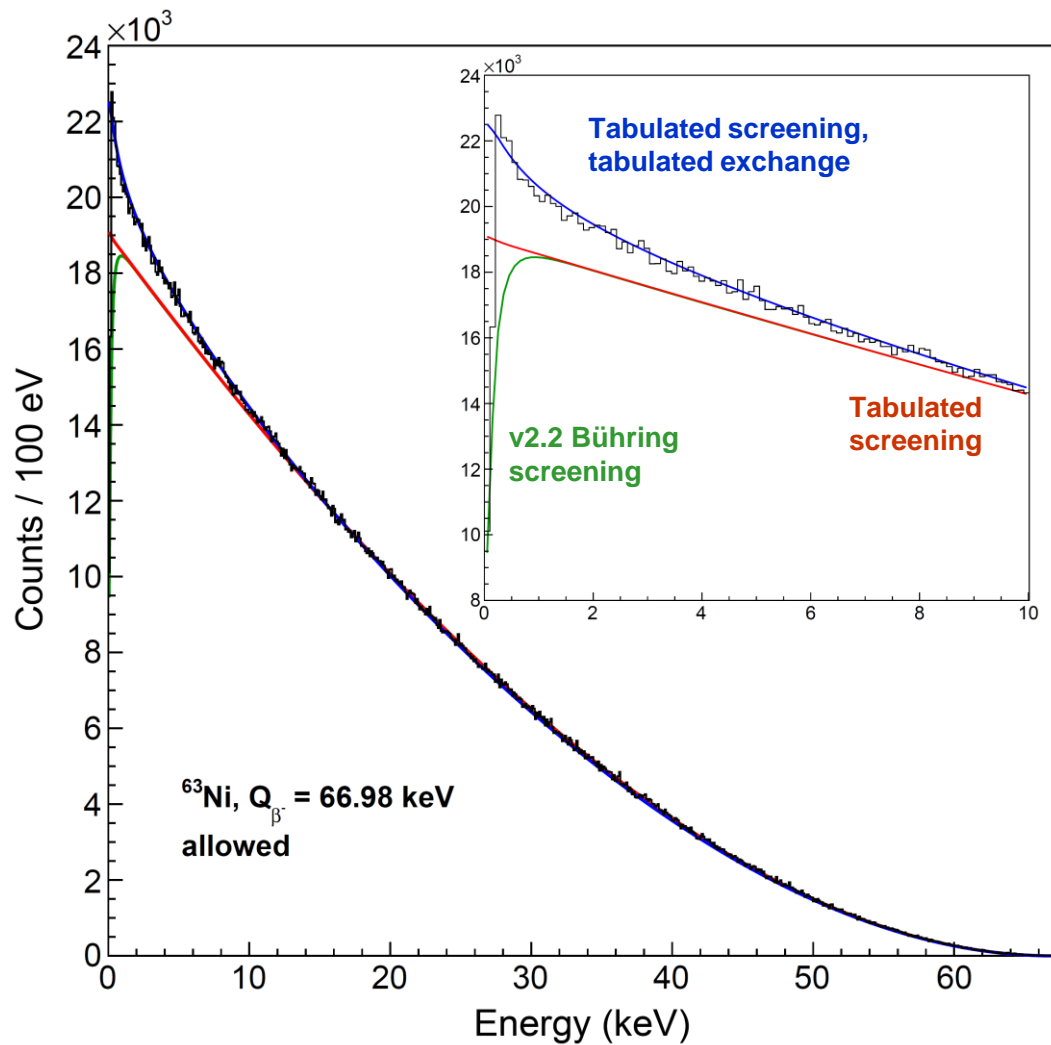
✓ **Solution: Extensive tabulation of both corrections, screening and exchange.**

- Screening: Parameters up to 30 MeV, $Z = 120$ and 6th forbidden unique β^{\pm} transitions (λ_7). Covers more than the currently known transitions.
- Exchange: All atomic orbital included, up to $Z = 120$. Correction factors converge to unity: tabulation up to a precision < 0.001 %.
- Exponential energy grid for better accuracy at low energy.

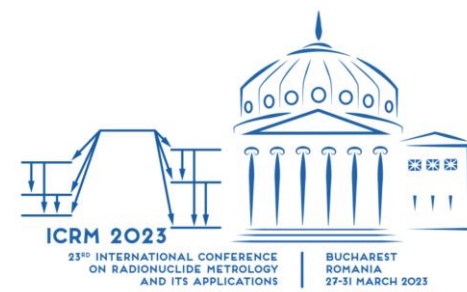


These corrections may be not accurate enough in the case of ultra-low endpoint energies. Further studies (experimental and theoretical) are needed.

Application to ^{63}Ni and ^{241}Pu spectra



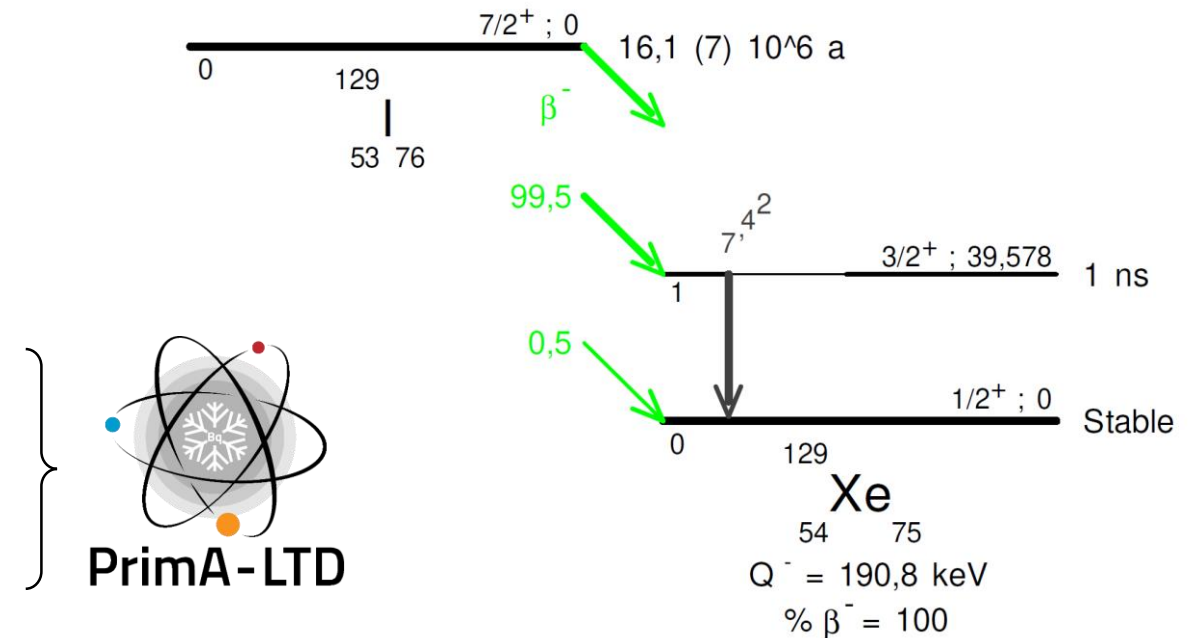
Conclusion



- ✓ Formalism of atomic exchange effect extended to forbidden unique transitions.
- ✓ Precise atomic screening and exchange included in the forthcoming version of BetaShape thanks to extensive tabulations.
- ✓ Can be applied to forbidden non-unique transitions in first approximation, correcting the Fermi function and the λ_k parameters.
 - Done in recent studies: ^{99}Tc , ^{151}Sm , ^{176}Lu (**see BS WG session on Tuesday**).

There is still some work to do:

- Need more high-precision measurements to test the predictions, and to revise them if necessary. ^{107}Pd decay could be a good candidate.
- Use of high-precision atomic wave functions.
- Complete calculations in forbidden non-unique transitions, including realistic nuclear structure.





Thank you for attention

