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Atomic exchange correction in forbidden unique beta transitions

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The extended international reference system (ESIR) is being developed by the international bureau of weights and measures (BIPM) [1]. The objective is to create a specific instrument for comparing primary standards of almost pure alpha and beta emitters and low-energy electron capture decaying radionuclides, for which gamma emission is inexistent or extremely low. The measuring device is based on the liquid scintillation counting technique with the triple-to-double coincidence ratio (TDCR) method and a 0.1% standard uncertainty is aimed at [2]. The CIEMAT/NIST method is also commonly used in radionuclide metrology when carrying out liquid scintillation activity measurements. Both methods necessitate precise knowledge of the beta spectrum to compute the efficiency. Recent studies [3-5] have demonstrated that not using an accurate description of the very low-energy part of the spectrum, where atomic effects play a major role, can lead to an underestimation of the activity of a fraction of a percent and even more in some cases. In addition, observed discrepancies between the activities determined with these two methods are resolved when using such accurate beta spectra.

However, the available modelling of the atomic exchange effect applies only to allowed transitions. In this case, the angular momentum carried away by the beta particles limits the exchange process to atomic electrons in $s_{1/2}$ and $p_{1/2}$ orbitals. In relation to the ESIR, it is necessary to ensure the same level of accuracy for the beta spectra from forbidden transitions. The beta particles can then be emitted with higher angular momenta and exchange becomes possible with atomic electrons in other orbitals. In the present work, the formalism of the exchange effect has been extended to forbidden unique transitions. The correction associated to a specific angular momentum is demonstrated to act on the corresponding component with identical angular momentum in the shape factor. Consequently, overlaps of continuum and bound relativistic electron wave functions have to be calculated for all the possible angular momenta at each beta particle kinetic energy. Theoretical predictions for different transitions of interest are presented.

The computational burden to determine the exchange correction is significant, typically several tens of minutes on a recent 16-processor workstation for a single beta spectrum with fine energy binning. In order to make these predictions available in a simple manner through the BetaShape code, extensive tabulation of the exchange correction factors has been considered. However, the atomic screening correction in BetaShape [6] had also to be revised because the analytical correction in the current version is not as accurate as the exchange correction. Full numerical computation of the screening effect on the Fermi function and on the λ_k parameters that enter in the definition of the shape factors has thus been performed. For both atomic corrections, tables have been generated up to $Z=120$ considering an exponential energy grid in order to ensure sufficient precision at very low energy. For the exchange effect, all atomic orbitals have been considered and a numerical precision of at least 0.001% has been ensured. For the screening effect in beta plus and beta minus transitions, the Fermi function and the λ_k parameters have been tabulated up to 30 MeV and λ_7 , corresponding to a sixth forbidden unique transition. Interpolation within these tables allows the fast and precise inclusion of these atomic effects in the beta spectra provided by the BetaShape code.

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