EPJ Web of Conferences **146**, 12015 (2017) DOI: 10.1051/epjconf/201714612015
ND2016

BetaShape: A new code for improved analytical calculations of beta spectra

Xavier Mougeot[a]

CEA, LIST, Laboratoire National Henri Becquerel (LNE-LNHB), Bât. 602 PC111, CEA-Saclay, 91191 Gif-sur-Yvette Cedex, France

Abstract. The new code BetaShape has been developed in order to improve the nuclear data related to beta decays. An analytical model was considered, except for the relativistic electron wave functions, for ensuring fast calculations. Output quantities are mean energies, log ft values and beta and neutrino spectra for single and multiple transitions. The uncertainties from the input parameters, read from an ENSDF file, are propagated. A database of experimental shape factors is included. A comparison over the entire ENSDF database with the standard code currently used in nuclear data evaluations shows consistent results for the vast majority of the transitions and highlights the improvements that can be expected with the use of BetaShape.

1. Introduction

By its very nature, beta decay is a three-body process, producing a beta electron, a neutrino and a daughter nucleus, all having continuous energy spectra. The beta spectrum shape varies due to the nature of the transition, which can be allowed or forbidden depending on the structure of the nuclei involved, and certain atomic effects.

Beta and electron capture processes govern the vast majority of radionuclide decays and their emission properties are crucial features in nuclear data evaluations for building the decay schemes. Modern evaluations, from either DDEP (Decay Data Evaluation Project [1]) or ENSDF (Evaluated Nuclear Structure Data File [2]) provide spectrally integrated emission quantities determined using the LogFT program [3]. For various applications, users now require lower uncertainties than those present in current nuclear databases, as well as the full beta and neutrino spectra.

Following this renewed interest, a review of the existing codes has been conducted showing their limitation in terms of the nature of the transitions calculated and the analytical formalisms whose restrictive approximations do not allow calculations of high accuracy. The LogFT program is based on the original code from [4] and was developed over a period of more than 30 years. This code handles both beta and electron capture transitions and propagates the uncertainties of the input parameters. Reading and writing standard ENSDF files, it provides mean energies of beta spectra, log ft values, as well as β^+ and electron capture probabilities. However, in order to ensure very fast calculations, this program uses simple analytical models that lead to a lack of accuracy: any lepton or nuclear wave function is calculated; the electron is assumed to interact with the Coulomb field of a point nucleus; inaccurate corrections estimate both the screening effect and the shape factors of first and second forbidden unique transitions.

Improved physical models were implemented when developing the BetaShape program described below. This program includes a database of experimental shape factors and provides mean energies, log ft values and the associated energy spectra for beta transitions. To ensure its ease-of-use, BetaShape handles ENSDF files. Hereafter, the theoretical model is summarized in Sect. 2.1; the calculated quantities are given in Sect. 2.2; the program structure is described in Sect. 3; and the validation of the code through a systematic comparison of the LogFT and BetaShape results over the entire ENSDF database is described in Sect. 4.

2. Calculations

2.1. Theory

The theoretical model has already been described in detail in [5], except Bühring screening. The Behrens and Bühring formalism [6] was followed. Assuming massless neutrinos, the beta spectrum shape is

$$\frac{dN}{dW} \propto pWq^2F(Z,W)C(W)S(Z,W)R(Z,W) \qquad (1)$$

with W and p the total energy and momentum of the beta particle, q the momentum of the correlated neutrino, $F(Z,W)$ the Fermi function, $C(W)$ the shape factor, $S(Z,W)$ the screening correction and $R(Z,W)$ the radiative corrections. In order to ensure fast calculations, the atomic exchange effect was not included as its evaluation is time-consuming [7].

In this formalism, the Fermi function includes the finite nuclear size effect as it is defined by the product of the usual Fermi function F_0 and a factor L_0 which accounts for the distortion of the electron wave function by a non-point-like nuclear charge

$$F(Z,W) = F_0L_0 = \left(\alpha_{-1}^2 + \alpha_{+1}^2\right) \Big/ 2p^2 \qquad (2)$$

The Fermi function is determined from the Coulomb amplitudes α_k of the relativistic electron wave functions.

[a] e-mail: xavier.mougeot@cea.fr

These wave functions are calculated for the Coulomb potential of a uniform spherical charge by numerically solving the Dirac radial equations according to *the fast but complicated method* from [6] (see [5] for more details).

The forbiddenness of a transition is determined by the spin change $\Delta J = |J_i - J_f|$ and the parity change $\pi_i \pi_f$ between the initial nuclear state of the parent nucleus and the final nuclear state of the daughter nucleus. Allowed and forbidden unique transitions can be calculated without involving the structure of the nuclei by approximating the integral of the lepton wave functions over the entire space by their magnitudes evaluated at the nuclear surface. Given that $L = 1$ if $\Delta J = 0$ for an allowed transition, and $L = \Delta J$ for any $(L-1)^{\text{th}}$ forbidden unique transition, the theoretical shape factor is then

$$C(W) = (2L-1)! \sum_{k=1}^{L} \lambda_k \frac{p^{2(k-1)}\, q^{2(L-k)}}{(2k-1)![2(L-k)+1]!} \quad (3)$$

The λ_k parameters are defined from the Coulomb amplitudes α_k by

$$\lambda_k = \left(\alpha_{-k}^2 + \alpha_k^2\right) \Big/ \left(\alpha_{-1}^2 + \alpha_1^2\right) \quad (4)$$

A usual assumption is to set $\lambda_k = 1$ to avoid calculating these parameters, which can be justified for certain transitions where their energy variation can be weak. This assumption is here referred to as the $\lambda_k = 1$ approximation and was kept as an option in the BetaShape program.

Calculation of beta spectra for forbidden non-unique transitions is far more difficult than for forbidden unique transitions. The approximation described above is no longer valid and the structure of the initial and final nuclear states has to be taken into account. The usual ξ approximation treats a forbidden non-unique transition as a forbidden unique one of identical ΔJ. The validity of this assumption was thoroughly tested in [5] and is used in the BetaShape program. In order to improve the accuracy of the spectrum shapes, the BetaShape program includes a database of 130 experimental shape factors given in [5], with an update for ^{138}La [8].

The calculations also account for the outer radiative corrections $R(Z, W)$, considering the energy loss of beta particles in the electromagnetic field of the nucleus by means of internal bremsstrahlung and virtual photons. These analytical corrections were derived by Sirlin for allowed transitions [9,10]. This correction can be turned off when using BetaShape.

Finally, the spectrum shape is modified by applying the screening correction $S(W, Z)$. The most widespread approach was set out by Rose in [11]. For evaluating the screening effect, a Thomas-Fermi potential V_0 which depends only on the atomic number of the daughter nucleus is subtracted from the total energy W of the beta particle in all the quantities required for the calculation of the spectrum shape, except in the neutrino energy q. This method is well described in [4]. The parameterization of the potential used in the BetaShape program can be found in [5]. A more refined analytical approach was recently investigated in [12] based on the work of Bühring [13]. This correction was adapted to Salvat's potentials [14] which were preferred for their better reliability. This formulation allows the determination of the screened-to-unscreened ratios $F_0 L_0^* / F_0 L_0$ and λ_k^* / λ_k, which were found to be consistent with the ratios given in Table III in [15]. BetaShape allows the choice of the screening correction from either Rose or Bühring, or neither.

2.2. Calculated quantities

First, the transition parameters and their uncertainties are determined from the input ENSDF file: intensity I_β, partial half-life $t = T_{1/2}/I_\beta$, forbiddenness from the spins and parities of the nuclear states, total maximum energy of the beta particle W_0 from the Q-value and the nuclear levels. Beta and neutrino spectra are then calculated according to the options chosen by the user and a measured spectrum is determined from an experimental shape factor if the transition is present in the database.

The total spectrum, as a result of the sum of single spectra weighted by the transition intensities, is determined if the radionuclide decays through more than one transition. If present, the measured spectrum is always preferred. A spectrum determined with the $\lambda_k = 1$ approximation is never considered.

These spectra are integrated to determine the mean energies, the $\log ft$ values and some analysis parameters, defined in [5], that compare calculated and measured spectra, if an experimental shape factor is available. Every integral is determined via a three-point Lagrangian interpolation. The mean energy of a beta spectrum is

$$\bar{E} = m_e \frac{\int_1^{W_0} (W-1) N(W) \mathrm{d}W}{\int_1^{W_0} N(W) \mathrm{d}W} \quad (5)$$

In case of multiple transitions, the mean energy of the total spectrum is also determined. The $\log ft$ value of a β^- transition is calculated from the partial half-life t and

$$f_\beta = \int_1^{W_0} N(W) \mathrm{d}W \quad (6)$$

Uncertainties are determined as in the LogFT program. Due to the non-trivial correlation between the polynomial parameters, the uncertainty from an experimental shape factor is not propagated.

As a β^+ transition is always competing with an electron capture transition, the $\log ft$ value of such a transition has to account for the electron capture contribution

$$f_{\varepsilon/\beta^+} = f_\varepsilon + f_\beta \quad (7)$$

Rigorously, the $\log ft$ value cannot be determined by BetaShape in this case because the electron capture transitions are not treated. However, provided that $I_\beta \neq 0$, it is straightforward to write

$$\log ft = \log\left(\frac{f_\beta}{I_\beta} T_{1/2}\right) + \left(\frac{1 + f_\varepsilon/f_\beta}{1 + I_\varepsilon/I_\beta}\right) \quad (8)$$

The Behrens and Bühring formalism for electron capture is very similar to the one for a beta transition [16]. Introducing the decay constant λ, one has $I_\varepsilon/I_\beta = \lambda_\varepsilon/\lambda_\beta$. For allowed and forbidden unique transitions, the nuclear structure is factored out and appears as a similar constant K for both β^+ and electron capture parts: $\lambda_\beta = K f_\beta$ and $\lambda_\varepsilon = K f_\varepsilon$. The quantity f_ε is the sum of the contribution of each orbital

$$f_\varepsilon = \sum_x n_x C_x f_x \quad (9)$$

where C_x is similar to the shape factor of the β^+ transition, and n_x is the relative occupation number of the orbital x. It is noteworthy that n_x is not taken into account in the LogFT program. Thus, $I_\varepsilon/I_\beta \approx f_\varepsilon/f_\beta$. Consequently, one might expect for allowed and forbidden unique transitions

$$\log ft \approx \log\left(\frac{f_\beta}{I_\beta}T_{1/2}\right) \tag{10}$$

This approximation was studied during the validation process of BetaShape (see Sect. 4).

3. Program structure

The BetaShape program has been written in C++ and consists of six classes, four interfaced programs, 155 functions and a database of 130 experimental shape factors. Information is transferred from one program to another via temporary files, which slightly increases the execution time, but allows easy improvement of the different parts of the code for future versions. The *Tools* class was created for reading, writing and handling strings, numbers and uncertainties throughout the process.

The core of the calculations is performed in four classes:

- *ContWF* calculates the relativistic electron wave functions, the Fermi function and the λ_k parameters;
- *Behrens* calculates the corrections, the theoretical shape factor, the spectra and integrated quantities, and performs spectrum normalisations;
- *ExpSF* checks if the transition is present in the database and if so calculates the normalized spectra and integrated quantities from the experimental shape factor;
- *Residuals* calculates the analysis parameters.

The *bsan* program manages the calculation of a single transition from the input parameters and writes the results in a text file.

An interface has been implemented for dealing with ENSDF files. The *readENSDF* program is the main entrance of BetaShape. The input ENSDF file, which can include more than one radionuclide decay, is sent to the *Ensdf* class where information is read; the transitions to be calculated are determined and sorted by radionuclide; and log files are created for further inspection by the user. Next, the *bsan_mult* program is called for each radionuclide decay, recursively calling *bsan* for each transition; calculates the total spectra and their mean energies; and writes the results in a text file. Then, the *writeENSDF* program is called to write the report files and an updated ENSDF file.

When choices or estimates are necessary, they are explicitly referred to within the log files. For instance, when multiple spins or parities are possible for a nuclear state, the first spin and parity are chosen. Many cases can occur, such as, quantities without uncertainties, unplaced transitions, etc. The default options are Bühring screening, radiative corrections and search for an experimental shape factor are turned on; $\lambda_k = 1$ approximation and calculation of neutrino spectra are turned off. Output precision is six digits and a binning of 300 energies is considered.

4. Validation

Due to the complexity of the code, a benchmark of 23 radionuclides selected to cover a large number of possibilities was used throughout the development: ^{11}C, ^{26}Al, ^{40}K, ^{52}V, ^{60}Co, ^{63}Ni, ^{68}Ga, ^{75}Ge, ^{85}Kr, ^{99}Tc, ^{103}Ru, ^{112}In, ^{137}Cs, ^{138}La, ^{143}Sm, ^{166}Ho, ^{185}W, ^{198}Au, ^{206}Tl, ^{210}Bi, ^{214}Pb, ^{231}Th and ^{241}Pu. This first version of the code was then run over the entire ENSDF database [2]. The code was improved until every bug was fixed and every specific case was treated.

This stabilized version of BetaShape was then compared to LogFT by inspecting the results for all the beta transitions within the database. It should be noticed that LogFT does not check the consistency between the forbiddenness and the spins and parities of the nuclear states given in the input file. Moreover, mean energies and log ft values within the database are sometimes not those from LogFT, depending on the evaluator's choices, and, as LogFT changes β^+ and electron capture intensities, some transitions disappear and others appear compared to the original data. Thus, BetaShape was used to correct the forbiddennesses according to the ξ approximation. LogFT was then run over these preliminary output files from BetaShape, and BetaShape was then finally rerun over the output files of LogFT in order to compare the results of both codes with equivalent input data.

The consistency of the mean energies and log ft values was tested at $k = 1$, 2 and 3, corresponding to confidence levels of 68.3%, 95.4% and 99.7% respectively. A total of 20 066 beta transitions were calculated and compared. When focusing on discrepancies of the mean energies greater than 1%, less than 1% of the values are inconsistent at $k = 1$ and less than 0.5% at $k = 3$, as these were mainly determined from experimental shape factors in BetaShape. Regarding the log ft values which are more than 1% discrepant, 2.5% are inconsistent at $k = 1$ and 1% at $k = 3$.

The approximation given in Eq. (10) to determine the log ft values of β^+ transitions was also tested by inspection of the inconsistent values at $k = 1$ for transitions calculated:

- As allowed: three transitions from measured spectra were found, as well as 17 transitions from 6 432 allowed and 1 257 first forbidden non-unique (0.2%), without any uncertainty on the intensities and with a discrepancy $\leq 2.5\%$.
- As first forbidden unique: no transition appeared from 389 first forbidden unique and 289 second forbidden non-unique.
- As second forbidden unique: only one transition arose, with a discrepancy of 1.3%, from 109 second forbidden unique and 30 third forbidden non-unique (0.7%); this transition is from ^{205}Po decay with an incongruously very small uncertainty which comes from the data.

Transitions with higher forbiddennesses cannot be calculated by the LogFT program. Hence the approximation of Eq. (10) provides consistent results with LogFT for β^+ transitions at the precision level of current nuclear data.

To illustrate the improvements of the BetaShape program, the third forbidden unique β^- transition of ^{40}K is considered as an example. An experimental shape factor is available in the database, measured from 100 to

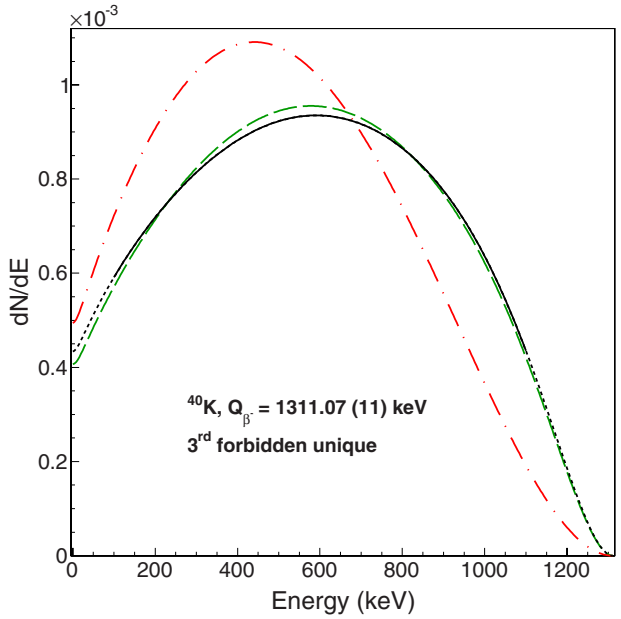

Figure 1. Measured spectrum from the third forbidden unique β^- transition of ^{40}K decay compared with LogFT and BetaShape. Black spectra: from the experimental shape factor [17], solid line within the measured energy range, dotted outside. Red dash dotted spectrum: LogFT (calculated as allowed). Green dashed spectrum: BetaShape (calculated as third forbidden unique).

1100 keV [17]. This transition is calculated by LogFT as an allowed transition, leading to a mean energy $\overline{E} = 508.31$ keV and $\log ft = 18.0417$ (14). BetaShape calculates this transition as third forbidden unique, leading to $\overline{E} = 583.283$ (48) keV and $\log ft = 20.6006$ (14), very close to the results determined from the experimental shape factor $\overline{E} = 583.982$ (48) keV and $\log ft = 20.5788$ (14). The disagreement between the experimental and calculated spectra is 1.2% within the measured energy range. The corresponding beta spectra are given in Fig. 1.

5. Conclusion

The BetaShape program has been developed to improve the accuracy of the nuclear data related to beta emission properties. The theoretical model was implemented with analytical calculations, except for the relativistic electron wave functions which are numerical solutions of the Dirac radial equations. Mean energies, $\log ft$ values, and beta and neutrino spectra for single and multiple transitions, are provided. A database of experimental shape factors is also included and the uncertainties from the input parameters are propagated. Executables for different platforms are available at `http://www.nucleide.org/logiciels.htm`.

This new program was compared to the LogFT program, the standard code used in modern nuclear data evaluations. The vast majority of the results of both codes are consistent, which validates BetaShape. The remaining discrepancies were found to come from the improvements of BetaShape. However, this code does not currently treat electron capture decays, although preliminary results for these transitions, including atomic effects, seem very promising [8]. The inclusion of these calculations within BetaShape will offer a realistic and more accurate replacement to LogFT.

References

[1] R.G. Helmer, E. Browne, M.M. Bé, J. Nucl. Sci. Tech. **39**, 455 (2002)
[2] M.R. Bhat, *Evaluated Nuclear Structure Data File (ENSDF)*, Nucl. Data Sci. Tech. (Springer-Verlag, Berlin, Germany, 1992), Files from the ENSDF database, revised as of December 31, 2015
[3] *LOGFT Program*, `http://www.nndc.bnl.gov/nndcscr/ensdf_pgm/analysis/logft/` (2001), original code from [4]
[4] N.B. Gove, M.J. Martin, Nucl. Data Tables A **10**, 205 (1971)
[5] X. Mougeot, Phys. Rev. C **91**, 055504 (2015), `http://link.aps.org/doi/10.1103/PhysRevC.91.055504`
[6] H. Behrens, W. Bühring, *Electron Radial Wave Functions and Nuclear Beta Decay* (Clarendon, Oxford, 1982)
[7] X. Mougeot, C. Bisch, Phys. Rev. A **90**, 012501 (2014)
[8] F. Quarati, P. Dorenbos, X. Mougeot, Appl. Radiat. Isot. **109**, 172 (2016), ISSN 0969-8043, `http://www.sciencedirect.com/science/article/pii/S0969804316000026`
[9] A. Sirlin, Phys. Rev. **164**, 1767 (1967)
[10] A. Sirlin, Phys. Rev. D **84**, 014021 (2011)
[11] M.E. Rose, Phys. Rev. **49**, 727 (1936)
[12] X. Mougeot, Appl. Radiat. Isot. **109**, 177 (2016), ISSN 0969-8043, `http://www.sciencedirect.com/science/article/pii/S0969804315302591`
[13] W. Bühring, Nucl. Phys. A **430**(1), 1 (1984), ISSN 0375-9474, `http://www.sciencedirect.com/science/article/pii/0375947484901908`
[14] F. Salvat et al., Phys. Rev. A **36**, 467 (1987)
[15] H. Behrens, J. Jänecke, in *Numerical Tables for Beta-Decay and Electron Capture*, edited by H. Schopper, Landolt-Börnstein, New Series, Group I, **4** (Springer Verlag, Berlin, 1969)
[16] W. Bambynek et al., Rev. Mod. Phys. **49**, 77 (1977)
[17] H. Leutz, G. Schulz, H. Wenninger, Z. Phys. **187**(2), 151 (1965), ISSN: 0044-3328, `http://dx.doi.org/10.1007/BF01387190`