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SIMPLE MONTE-CARLO METHODS IMPLEMENTED IN ROOT FOR FITS USING PARAMETERS WITH ERRORS

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In order to extract nuclear excited state lifetimes in trans-fer reaction using the Plunger device, the Doppler Decay Curve Method is in certain cases the only way available, as the shifted peak is not observ-able. However, the problem of extracting this lifetime for levels that have considerable cascade feeding from levels with lifetimes of the same order of magnitude is not trivial. While the Bateman equations provide a physically-transparent way of fitting such curves, there is nonetheless a problem of propagating the errors of the lifetimes of the higher energy levels and of the feeding ratios into the fit and the extraction of the lifetimes. In this article, we have used a Monte Carlo fitting method implemented in ROOT in order to easily and transparently solve this problem and help extract lifetimes with correctly-calculated errors.

Keywords: nuclear lifetimes, plunger, transfer reactions, ROOT, Monte Carlo, fitting

1. Introduction

The determination of lifetimes of nuclear excited states is an important objective of current experimental low-energy nuclear structure research. The lifetimes of such states, besides allowing the determination of spins and parities, also allow the extraction of reduced matrix elements, offering an insight into the complicated inner workings of the nuclear force and nuclear structure.

Currently, there are methods to extract nuclear lifetimes ranging from attoseconds up to thousands of years[1], an amazing 28 orders of magnitude. The Recoil Distance Doppler Shift method can be used to extract lifetimes in the area of fs to ps, and relies on the Doppler shift of γ-rays emitted by a residual nucleus following a nuclear reaction. Following the reaction, the residual will have a velocity of the order of a percent of the speed of light. If the target is thin enough, the residual will escape the target and continue its path. Any γ-rays emitted during flight will have a shifted energy if observed at an angle different from 90° with respect to the direction of the nucleus' velocity.

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In the RDDS method, a special device called plunger is used[2]. The plunger holds a stopper foil (usually gold) at a fixed distance behind the target, being able to maintain the distance with sub-micrometer accuracy and vary it as required. All γ-rays that are emitted after the residual reaches the stopper are not Doppler shifted. The ratio of the shifted and unshifted peaks in an energy spectrum then depends on the target-stopper distance, the velocity of the residual (both of which are easily obtainable) and the lifetime and feeding history of the excited state, which can then be extracted.

In the case of ^{64}Ni, which is a magic nucleus with Z=28, the above situation has the particularity that the gating transition, the $2^{+} -> 0^{+}$ 1345 keV γ-ray, is very short lived. Because the gating is only done on the unshifted peak, this means that the gating eliminates the shifted peaks of the longer-lived levels from the spectra. The γ-transitions emitted in flight from these levels are unlikely to be in coincidence with the unshifted transition from the 1345 keV level, lowering their presence in the gated spectra to the point they are unobservable. However, measuring the normalized intensity of the unshifted peak as a function of the target-stopper distance, the lifetime of the state can be determined by fitting with Bateman's equations[3], as can be seen in Fig.1.

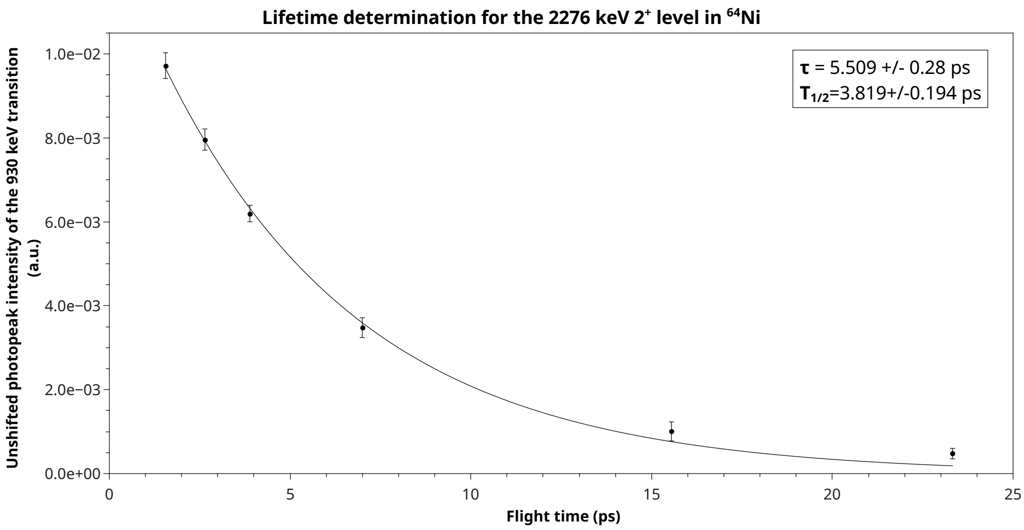

Fig.1. The normalized intensity of the 930 keV $2^{+} \rightarrow 0^{+}$ from ^{64}Ni for six different target-stopper distances from an experiment undertaken in the Nuclear Physics Department of IFIN-HH. The points fit well on a simple exponential decay which is used to extract the lifetime of the level, which is shown in the upper right corner.

Considering the simplest case of a nuclear level with direct feeding only, the normalized intensity of the unshifted peak as a function of the flight time will be given by the well known exponential equation:

$$N_0(t_f) = N_0(0) * e^{-\frac{t_f}{\tau_0}} \tag{1}$$

which is quite straightforward to fit and extract the lifetime. However, in the common case of levels that also have cascade feeding, the situation becomes far more complicated! For example, let us look at a part of the level scheme of ^{64}Ni shown in Fig.2, which shows a cascade of five transitions directly feeding each other. The five levels that are involved in these transitions and whose lifetimes can thus be extracted are marked from 0 to 4. While the extraction of the lifetime of the level labeled 0 is trivial, it gets more complicated down the cascade. Besides the fact that the Bateman equations get far more complicated, the lifetimes and feeding ratios of the levels above also have to be taken into consideration.

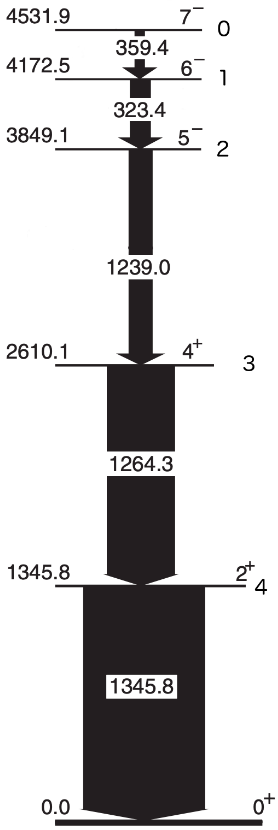

Fig. 2. A part of the level scheme of ^{64}Ni, showing five of the most intense transitions from this nucleus in cascade. While the extraction of the lifetime of the first level (labeled 0) is trivial, for all the other ones, cascade feeding and the lifetimes of the levels above them have to be taken into account. Image taken from [4] and modified.

The Bateman equations giving the population levels for the second and third levels at time t_f are:

$$N_1(t_f) = N_1(0) * e^{-\frac{t_f}{\tau_1}} + N_0(0) * \frac{\tau_1}{\tau_0 - \tau_1} * (e^{-\frac{t_f}{\tau_0}} - e^{-\frac{t_f}{\tau_1}}) \tag{2}$$

$$N_2(t_f) = N_2(0) * e^{-\frac{t_f}{\tau_2}} + N_1(0) * \frac{\tau_2}{\tau_1 - \tau_2} * (e^{-\frac{t_f}{\tau_1}} - e^{-\frac{t_f}{\tau_2}}) +$$
$$+ N_0(0) * \frac{\tau_2}{(\tau_1 - \tau_2)(\tau_0 - \tau_2)(\tau_0 - \tau_1)} * (\tau_0(\tau_1 - \tau_2)e^{-\frac{t_f}{\tau_0}} - \tau_1(\tau_0 - \tau_2)e^{-\frac{t_f}{\tau_1}} + \tau_2(\tau_0 - \tau_1)e^{-\frac{t_f}{\tau_2}}) \tag{3}$$

where $N_1(t_f)$ and $N_2(t_f)$ are the populations of levels 1 and 2 after flight time t_f, $N_0(0)$, $N_1(0)$ and $N_2(0)$ are the initial populations of the levels and τ_0, τ_1 and τ_2 are the lifetimes of the levels.

These are significantly more complicated than the simple exponential in Eq.1, especially through the appearance in the formulas of the lifetimes and feeding ratios from other levels. Even so, this is a simplified case in which each level is fed by only one other transition. In reality, multiple transitions with different lifetimes can feed and depopulate different levels, complicating the formula and the fitting even more.

The number of unshifted γ-rays emitted from a level is not given by formulas 2 and 3, but by:

$$N_{\gamma 1} = N_1(t_f) + N_0(t_f) \tag{4}$$

$$N_{\gamma 2} = N_2(t_f) + N_1(t_f) + N_0(t_f) \tag{5}$$

because, after coming at rest, not only the nuclei which are in the excited state 1 emit an unshifted 323.4 keV γ-ray, but also those that are in excited state 0, which will decay to excited state 1 while at rest.

Using these formulas to fit experimental data and extracting the lifetimes of the levels of interest requires knowledge of the lifetimes of the preceding levels and of the feeding ratios, which can either be extracted from the data or from the same fit. It is certainly preferable to extract the values from other fits and then include them as parameters into the new fit, as this limits the free parameters and improves the quality and errors of the fitting procedure, but this is not always possible.

Less simple, however, is how to correctly and transparently propagate the errors that are associated with the other lifetimes and feeding ratios through the fit. This is crucial in order to be able to publish reliable data with correctly estimated errors. Skipping the propagation of the errors of the other lifetimes and feeding ratios and only using the error from the fitting procedure can lead to a significant underestimation of the error in certain cases.

2. The program and procedure

In order to address this issue, we have devised a simple solution using a Monte Carlo fitting procedure employing the ROOT programming language[7]. Due to the tremendous power of modern-day computers, millions of fits can be done in just a couple of minutes. This allows us to not only fit the data using the other previously extracted parameters, but to also vary these parameters within their errors. All of these values are then used to extract the total error of the fit which contains both the error of the fitting procedure and the propagation of the errors from the previous values used in the fit.

During the experiment, an ^{18}O beam impinged upon a ^{62}Ni target at an energy slightly below the Coulomb barrier in order to suppress fusion [5]. The resulting γ-rays were detected using the RoSphere spectroscopy array [6]. Data was taken for six different target-stopper distances, namely 10, 17, 25, 45, 100 and 150 μm. For each distance, the data was sorted into symmetric γ-γ matrices. A gate was placed on the most intense transition in ^{64}Ni, the $2^+ \rightarrow 0^+$ 1345.8 γ-ray. The unshifted areas of the coincident γ-rays were determined for every observable transition in ^{64}Ni at each distance.

The areas were normalized using the very intense 150 keV transition in ^{77}Kr, which was produced through the competing ^{62}Ni(^{18}O,3n)^{77}Kr fusion evaporation reaction. Due to the long lifetime of this state, it decays almost entirely at rest regardless of the target-stopper distance. The area of this peak is thus proportional to the total number of ions delivered to the target, making it excellent for normalization.

The resulting normalized intensities for each transition were fed to a ROOT program written specifically for this purpose and reproduced in the Appendices. The data format consisted of three columns, these being the flight time, the γ intensities and their errors. The fitting was done from the top down, as the results from the first fit would be used in the second one and so on.

For the top-most transition of 359.4 keV, the intensities were fitted with a simple exponential and no other processing was done. The data points, the fit and the resulting lifetime can be seen in Fig.3 in red.

For the following 323.4-keV transition, formula 4 was used for the fitting procedure. However, parameters τ_0 and $N_0(0)$, which are the lifetime and the population of the preceding level, must be given a value. The lifetime of the level was taken from the previous fit to be 12.514 ps. Instead of trying to extract the initial population of the preceding level, the direct population ratio extracted from a previous thick-target experiment is used instead, with $N_1(0) = f_0 * N_0(0)$. However, this does not account for the fact that τ_0 and f_0 are not precisely determined nor does it allow for the propagation of errors.

Thus, instead of doing a single fit with $\tau_0 = 12.514$ ps and $f_0 = 0.639$, one million fits were made instead. Before each fit, τ_0 and f_0 were initialized using a random Gaussian function centered on their respective values and with

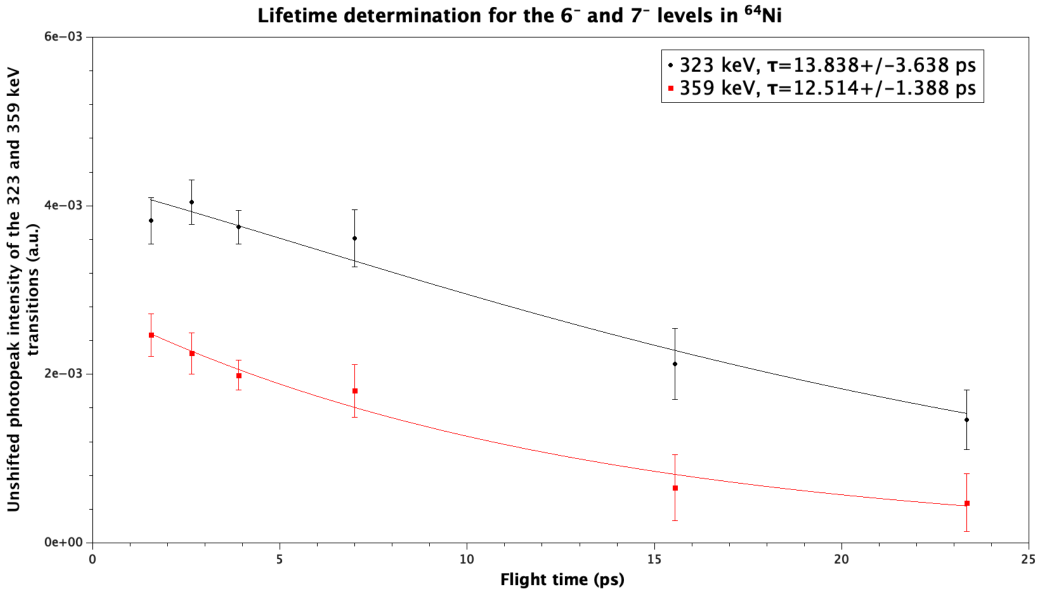

Fig. 3. The data points, fits and lifetimes for the first two transitions from the cascade shown in Fig.2, with an energy of 359 and 323 keV, respectively. The data points from the 359 keV γ-ray were fitted with a simple exponential with no further processing. The data points from the 323 keV transition were fitted with Eq.4 using the ROOT program described in this paper.

σ equal to the previously extracted errors. τ_1 and $N_0(0)$ were treated as free parameters of the fit. For each fit result, τ_1 and its error were used to add 100 points to a histogram, again according to a Gaussian distribution. Only the fits for which the χ^2 was reasonable were kept for further processing.

The result is a histogram in which all the results of the fits are added up, as can be seen in Fig.4. For all the functions used in the example, the resulting distribution in the histogram was a Gaussian. Fitting it with a Gaussian function, the extracted center of the distribution was taken as the final fit value, while σ was considered to be the error of the fit.

As a comparison, for the lifetime of the 323 keV γ-ray, using our method and measured feeding, the extracted value was $\tau_1 = 13.838 \pm 3.638$ ps. With a simple fit, neglecting the errors of the direct feeding ratio and of the lifetime of the previous level, the extracted value is $\tau_1 = 13.94 \pm 3.396$ ps, which is very close. This indicates that the fitting error is dominated by the errors of the data points. However, the difference between the errors is 0.242 ps, which, while no more than 2% of the total value, would have been an important underestimation.

Alternatively, trying to fit the feeding ratio as well instead of extracting it from the data gives erroneous results. With a simple fit but a fitted feeding

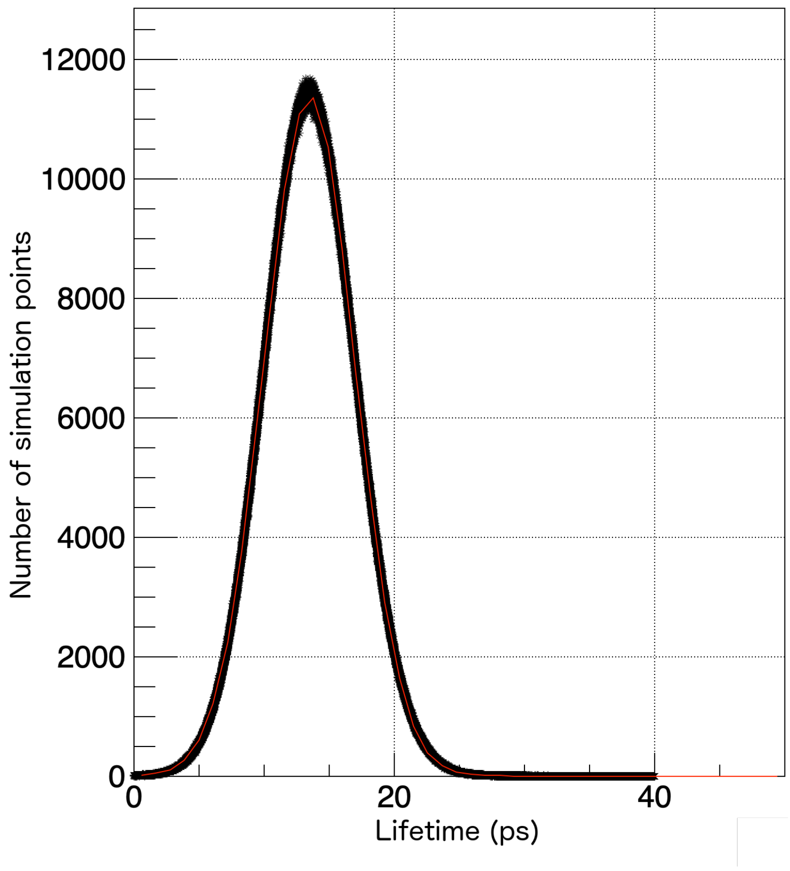

Fig. 4. The resulting histogram following the one million fits of the data from the 323 keV γ-ray. In all of our cases, the points are distributed on a Gaussian. The center of this Gaussian, at 13.838 ps, has been taken as the total fit value and the σ of the Gaussian, $\sigma = 3.638$ ps, as the error of the value.

ratio, the extracted lifetime is $\tau_1 = 22.185 \pm 4.534$ ps, while, with our Monte Carlo fit, the extracted lifetime is $\tau_1 = 22.169 \pm 4.517$ ps, again very close to each other. However, both of these values are completely discarded because the fitted feeding ratio is of the order of 20, in complete disagreement with the data which indicates that $f_0 = 0.558 \pm 0.106$.

Continuing to the next transition in the cascade, the 1239 keV one, formula 5 is used to extract the lifetime. Four parameters are now needed for the fit, being of the ones extracted from previous fits and measurements. These values are $\tau_0 = 12.514 \pm 1.388$ ps, $\tau_1 = 13.838 \pm 3.638$ ps, $f_0 = N_0(0)/N_1(0) = 0.639 \pm 0.187$ and $f_1 = N_1(0)/N_2(0) = 4.79 \pm 1.88$.

For the 1239 keV transition with the parameters given above, this yields a lifetime of $\tau_2 = 21.828 \pm 6.188$ ps, as can be seen in Fig.5. The same fit done with a fitted feeding yields a lifetime of $\tau_2 = 15.754 \pm 34.472$ ps, a significantly worse result due to the increase of the number of parameters that have to be fitted and to the large correlation between the feeding factor and lifetime parameters that have to be fitted. Also, the fitted feeding value f_1 is 1.26 ± 0.77, in clear disagreement with the value extracted from the data of 4.79 ± 1.88. Due to the very large lifetime error and the disagreement in the feeding data, the value obtained with the fitted feedign was discarded from further analysis, even though Fig.5 indicates that this fit was closer to the experimental points that the one with measured feeding, but not by a large degree.

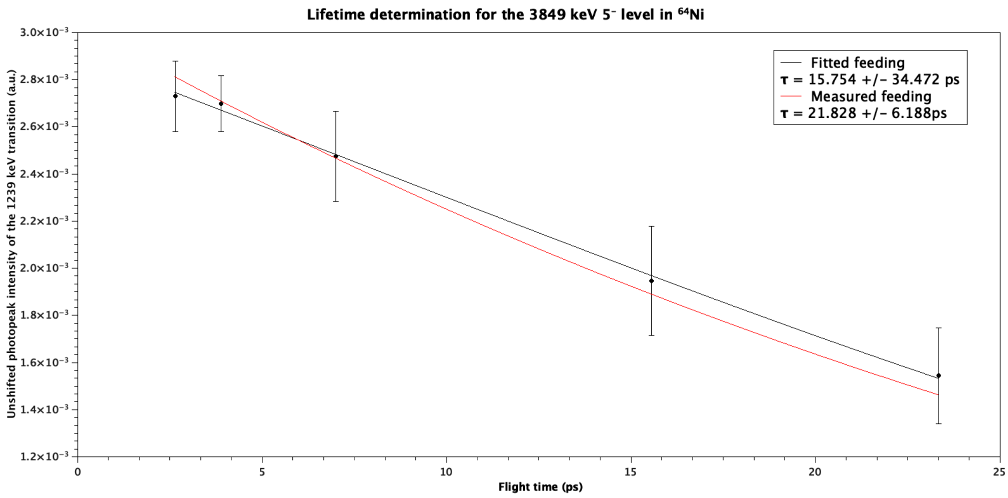

Fig. 5. The intensity of the 1239 keV transition as a func-tion of flight time and two fits used to extract the lifetime. The black line shows a fit in which both the lifetime of the level and the feeding ratio were fitted, yielding a lifetime of $\tau_2 = 15.754 \pm 34.472$ ps. The very large error is due both to the increase of the number of parameters being fitted and to the large correlation between the feeding parameter and the ex-tracted lifetime. Nonetheless, the extracted feeding parameter is 1.26, disagreeing with the extracted value of 4.79. The red line shows the fit obtained with the measured feeding value of $f_1 = 4.79 \pm 1.88$, which yields a lifetime of $\tau_2 = 21.828 \pm 6.188$ ps, which is the adopted value.

The fit was also done with fixed parameters in order to ascertain the importance of the proposed method on the final results. This gave a result of $\tau_2 = 25.10 \pm 4.74$ ps, in agreement with the previous result obtained by varying of the previously extracted values. However, the error from the simple fit is 24% smaller than the one obtained with the method proposed in this paper.

This also proves the rather intuitive conclusion that the contribution of this fitting method to the final error increases with the number of previously-extracted values used in the fit and with the complexity of the function used.

3. χ^2 limiting value

A discussion on the choice of χ^2 limiting value is also warranted. There is no fixed value that can be taken as a limiting value for the fits, as the 'reasonable' χ^2 depend on the number of parameters that are fitted and how well the proposed function can fit the experimental data. A brief study of the χ^2 values that are obtained for each situation (combination of data, function and parameters) is required before each fitting procedure.

For example, for the fitting of the data from the 1239 keV transition presented above, a limiting value of 1 was chosen in order to eliminate fit values with unreasonable χ^2 values that would negatively affect the analysis procedure. The average χ^2 of the accepted fits was 0.08314. However, only 590,272 fits yielded acceptable χ^2 values and were used in the following analysis, while 409,728 fits were rejected due to having χ^2 values of over 1.

Doing the exact opposite of the analysis in the text and taking into account only the fits with χ^2 values of over 1 yields a lifetime for the 1239 keV transition of $\tau_2 = 0.339 \pm 0.335$ ps, nearly two orders of magnitude lower than the value extracted with the fits with a χ^2 value of under 1.

4. Conclusion

In summary, we have developed a simple Monte Carlo fitting procedure in order to correctly propagate parameter errors through fits for the extraction of nuclear lifetimes using the Bateman equations. It is important to note that this procedure is in no way limited to this analysis and can be used for any fitting using parameters with errors.

While, in the present case, the result did not considerably vary due to the inclusion of the errors of the parameters using the Monte Carlo fit, it nonetheless offers a transparent way of accounting for them in the final result. The 170 ps variation in the error between our method and a simple fitting procedure is significant. The use of more complicated functions with more parameters with errors could lead to the opposite situation where the inclusion of the errors correctly identifies that the final result is less accurate or even inconclusive.

The program that has been developed is freely shared at https://github.com/standlucian/montecarlofitting with comments on what each section does. It is important to note that the fitting function can be changed to fit any sort of data and the method is in no way limited to lifetime determinations.

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