A study of additional uncertainties from fit boundaries using a new code for multi-reflection time-of-flight data

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Raw data of the isotopes $^{210-214}$Ra and $^{210-214}$Ac, measured with the RIKEN-KEK multi-reflection time-of-flight mass spectrograph (MRTOF-MS),[1,2] has been analyzed using a new code for mass evaluation. It has been developed to investigate uncertainties of time-of-flight (TOF) fits, which are not covered by the uncertainty provided by the fit routine. Additional effects can occur if the extracted TOF value from the fit depends on the choice of boundary conditions. Such conditions can be the fitting range, and for binned data, the choice of the bin size as well as the choice of bin origin (starting position of the first bin).

The code is a wrapping program around the maximum-likelihood estimator provided by the library ROOT/CERN[3] and enables repeated fits to the TOF data with various bin sizes, bin origins (see bottom of figure), and fitting ranges around the peak center. Due to the change of conditions, every new data fit will converge at a slightly different TOF. However, unless the choice of boundaries is not obviously wrong, as *e.g.*, the fitting range so large that a neighbor peak influences the result, there is no reason to consider any of those choices as incorrect. Such variation of results is not generally covered by the uncertainties obtained from the fitting routine as the optimizer works only with the data and parameter limits given by the user.

For MRTOF-MS spectra recorded over a time span of 20 min up to several hours, another degree of freedom arises when correcting for TOF drifts (temperature and voltage dependent). The data of the reference ions is split into subsets containing a certain number of experimental sweeps, the TOF of the reference ions in each subset is obtained from a fit, and then the data is summed up again with adjusted time origins to eliminate the drifts. However, if not all fluctuation frequencies are resolvable, the variation of the number of sweeps will cause changes in the final mass value, which is not fully predictable. The top of the figure shows the mass results of a selected data set as a function of the number of sweeps for each subset.

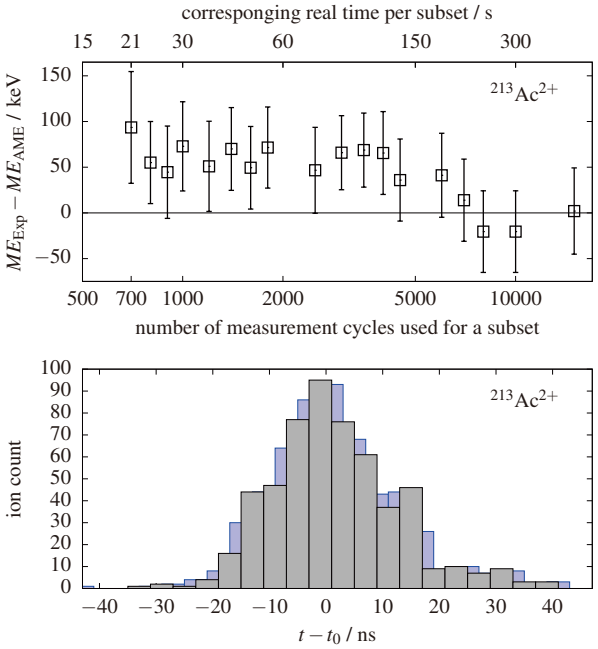

Fig. 1. Top: Scattering of the mass result of a selected $^{213}Ac^{2+}$ data set for various number of sweeps used for the data subsets to perform the TOF drift correction. Bottom: TOF spectrum with 4 ns bin width with two different origins of binning. The time origin of the grey colored spectrum has 2 ns difference from the blue one in the background.

A full analysis with different bin sizes, bin widths, bin origins, and number of sweeps per subset has been performed for all data sets of the measured Ac/Ra isotopes.[4] The result of the full analysis is an additional average scattering, which is covered when multiplying the statistical uncertainty by a factor of about 1.3. This value approaches the Birge ratio of about 1.2 from those isotopes for which a sufficient number of independent data sets could be measured. For low-statistics data, such an evaluation can provide a reasonable estimation of the uncertainty. A thorough future study can give more accurate answer how strong the scattering of mass results can be caused by the choice of the fit boundaries rather than caused by the data itself.

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