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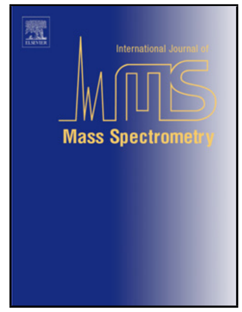


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Author: S. Purushothaman S. Ayet San Andrés J. Bergmann T. Dickel J. Ebert H. Geissel C. Hornung W.R. Plaß C. Rappold C. Scheidenberger Y.K. Tanaka M.I. Yavor

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# Hyper-EMG: A new probability distribution function composed of Exponentially Modified Gaussian distributions to analyze asymmetric peak shapes in high-resolution time-of-flight mass spectrometry

S. Purushothaman[a,*], S. Ayet San Andrés[a,b], J. Bergmann[b], T. Dickel[a,b], J. Ebert[b], H. Geissel[a,b], C. Hornung[b], W. R. Plaß[a,b], C. Rappold[a,b], C. Scheidenberger[a,b], Y. K. Tanaka[a,b], M. I. Yavor[c]

[a]*GSI Helmholtzzentrum für Schwerionenforschung, 64291 Darmstadt, Germany*
[b]*Justus-Liebig Universität Gießen, 35392 Gießen, Germany*
[c]*Institute for Analytical Instrumentation, Russian Academy of Sciences, 190103 St. Petersburg, Russia*

**Abstract**

A new Probability Distribution Function (PDF) called hyper-Exponentially Modified Gaussian (hyper-EMG) is introduced for the analysis of high-resolution spectra from multiple-reflection time-of-flight mass spectrometers. The hyper-EMG consists of a central Gaussian distribution modified by multiple exponential tails with different strengths at one or both sides. The basic statistical properties of the new PDF are given and the analysis of mass spectra containing separated and overlapping peaks is presented. The main requirement is to accurately determine the positions and areas of the individual mass peaks. From the distances of positions the mass values can be determined, from the areas the population of different ground and isomeric states can be obtained. The hyper-EMG has been applied to high-resolution time and mass spectra characterized by mass resolving powers of 140000 and 520000 obtained with $^{133}Cs^{+}$ and $^{39}K^{+}$ ions, respectively. From the measured mass distribution of $^{39}K^{+}$ ions, an overlapping distribution of two peaks with an area ratio of 1:10 and a mass difference of 2.6 ppm (parts-per-million) is generated and analyzed. The results reveal significant advantages of the new PDF for the evaluation of overlapping distributions for accurate mass and area determinations compared with commonly used PDFs which are more than one order of magnitude less accurate. It is obvious that the hyper-EMG can be favorably applied also to other fields.

*Keywords:* Analysis of asymmetric peak shapes, Mass and abundance determination, Hyper-Exponentially Modified Gaussian, Exponentially Modified Gaussian, Mixture distributions, High-resolution mass spectrometry, Multiple-reflection time-of-fight mass spectrometer

## 1. Introduction

The investigation of short-lived exotic nuclei is a major research field in many modern accelerator laboratories worldwide [1]. Exotic nuclei, characterized by extreme proton-to-neutron ratios compared to stable nuclides, reveal novel features of the nuclear force. Therefore, the measured properties of exotic nuclei can contribute to improve substantially the understanding of the strong interaction and the synthesis of the elements in the universe [2]. High-resolution accurate mass measurements of exotic nuclei reflect the nuclear binding energy which determines the structure and stability of the measured species.

New key experimental tools in this field are Multiple-Reflection Time-Of-Flight Mass Spectrometers (MR-TOF-MS) tailored to measure the mass and abundance of exotic nuclides [3–7]. The ground-state mass of a nucleus is a basic property. However, in some investigations the masses of excited states are also of high interest in nuclear spectroscopy and reaction studies. The lifetime of the excited (isomeric) states [8] can have a large range, e.g., from nanoseconds to many years. Depending on the excitation energy and the resolution of the spectrometer the two mass populations can overlap and must be disentangled for at least two reasons: firstly to assign unambiguously the value of the ground-state mass and secondly to deduce in addition the population of the isomeric state and the excitation energy. From these requirements, it is obvious that the positions and the areas of the observed overlapping distributions must be accurately determined.

In MR-TOF mass spectrometry the measured time distributions are converted into mass distributions and the corresponding areas can yield abundances of isotopes, reaction probabilities for their production and finally also the population of the observed ground and excited states. A critical part of the anal-

*Corresponding author
*Email address:* S.Purushothaman@gsi.de (S. Purushothaman)