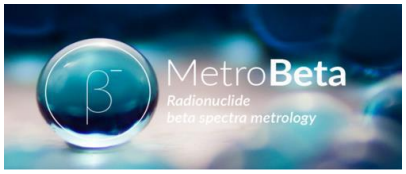

EMPIR
EURAMET
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Deliverable 1

Grant Agreement number	15SIB10	
Project short name	MetroBeta	
Deliverable title	Papers on the improved theoretical computation methods submitted to a peer-reviewed journals	
Lead partner	CEA	
Due and actual dates	May 2019	August 2019

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1 Introduction

The first objective of this deliverable is to provide the state of the art computation method of the single-nucleon energy levels and wave functions in the spherical doubly magic nuclei. This has been done using the phenomenological nuclear mean-field approach known for its more than satisfactory description of the experimental data employing the so-called Woods-Saxon potential. We have written and tested the corresponding computer codes solving the Schrödinger mean field equation with different variants of the Woods-Saxon Hamiltonian. The improvements mentioned in the title concern mainly the issue of the control of the predictive power of the corresponding Hamiltonian. We performed the adjustments of the Hamiltonian parameters using various variants of the spin-orbit potential to assure possibly the best empirical description of the observables of interest. Special effort has been undertaken to optimise the parameterisations via removing parametric correlations since, as it is well known from the so-called inverse-problem theory in applied mathematics, the modelling containing parametric correlations gives uncontrollably diverging predictions in the areas away from the parameter adjustment zones.

Our results were published in three articles in refereed journals, which are mentioned in what follows together with brief comments.

Reference 1

Narrowing the confidence intervals in nuclear structure predictions through elimination of parametric correlations; I. Dedes and J. Dudek, Acta Physica Polonica B Proceedings Supplement, Vol. 10, 51 (2017)

As it can be shown rigorously within the inverse problem theory, a subdomain of applied mathematics, existence of the parametric correlations among the model parameters excludes the possibility of stable predictions of the modelling. We have examined the improvements of the predictive power via: a) establishing the presence and the character of the parametric correlations within the model of interest, and b) eliminating the parametric correlations using the adapted Monte-Carlo algorithms.

Reference 2:

Predictive power of theoretical modelling of the nuclear mean field: examples of improving predictive capacities; I. Dedes and J. Dudek, Physica Scripta 93 044003 (2018)

We examine the improvements of the performance of the Hamiltonian by replacing the purely phenomenological spin-orbit potential by the microscopic one depending on the nucleonic densities and employing the self-consistency conditions. We demonstrated how to drastically reduce the number of independent parameters (1 instead of 6) using Monte Carlo approach to eliminate the parametric correlations without worsening the r.m.s. deviations for the test quantities.

Reference 3

Propagation of the nuclear mean-field uncertainties with increasing distance from the parameter adjustment zone: Applications to super-heavy nuclei; I. Dedes and J. Dudek, Phys. Rev. C 99, 054310 (2019)

It is very well known that even with the best-parameterised models the prediction uncertainties increase with increasing distance between the prediction zone and the parameter adjustment zone. To obtain the most stringent test conditions we need to find the testing zones lying possibly farthest away from the adjustment areas. To this end we have applied our test to the heaviest nuclei available in the context – the super-heavy nuclei. Illustrations of the description quality are given.

The second objective of this deliverable is to specifically calculate beta transitions regardless of their nature, whether it be allowed, forbidden unique, or forbidden non-unique. Reaching this objective requires to include the nuclear structure component within the calculation of beta decays. The

Behrens and Bühring formalism has then been thoroughly investigated. All equations needed for the beta decay calculations have been derived very carefully, for both beta minus and beta plus transitions. In addition, the same work has been done for electron capture decays, which always compete with beta plus decays. Focus has been made on single particle transition matrix elements, which are the building blocks needed for including, in the future, more complicated description of the nuclear structure. A specific calculation code has been developed with different optimization algorithms. Partial half-lives and log ft values, which are integrated quantities of the beta spectrum, are calculated. Nucleon wave functions have been determined from either a non-relativistic or a relativistic harmonic oscillator. Results highlight the success and the limits of this model and pave the way of future work for high-precision calculations of beta decays with very accurate nuclear structure modelling.

In the two references below, we have performed calculations to investigate the sensitivity of our theoretical modelling to the inclusion of the nuclear component. The studies have been focused on beta plus and electron capture transitions.

Reference 4

Direct determination of the ^{138}La *β-decay Q value using Penning trap mass spectrometry*; R. Sandler, G. Bollen, J. Dissanayake, M. Eibach, K. Gulyuz, A. Hamaker, C. Izzo, X. Mougeot, D. Puentes, F.G.A. Quarati, M. Redshaw, R. Ringle, S. Schwarz, I. Yandow, Phys. Rev. C 100, 014308 (2019)

Reference 5

Towards high-precision calculation of electron capture decays; X. Mougeot, Applied Radiation and Isotopes (accepted)

2 Paper abstract and identifier

We refer to the articles in the order introduced in Section 1 above.

Reference 1

ABSTRACT:

As it is well-known, the existence of correlations among the parameters of mathematical models such as typical physics theories implies that any attempt of optimization of the parameters becomes impossible or highly unstable. When this happens, one says that the parameter determination (usually referred to as inverse problem) becomes an ill-posed mathematical problem. In this article, we suggest a regularization method of ill-posed or nearly ill-posed inverse problems in the context of the nuclear mean-field applications with the help of the Monte Carlo methods. We present the approach and illustrate its numerical results on the example of the parameter adjustments of the phenomenological Woods–Saxon Hamiltonian in the ^{208}Pb nucleus treated as a test case.

http://dx.doi.org/10.5506/APhysPolBSupp.10.51 or
http://www.actaphys.uj.edu.pl/fulltext?series=Sup&vol=10&page=51

Reference 2

ABSTRACT:

We examine the effects of the parametric correlations on the predictive capacities of the theoretical modelling keeping in mind the nuclear structure applications. The main purpose of this work is to illustrate the method of establishing the presence and determining the form of parametric correlations within a model as well as an algorithm of elimination by substitution (see text) of parametric correlations. We examine the effects of the elimination of the parametric correlations on the stabilization of the model predictions further and further away from the fitting zone. It follows that the choice of the physics case and the selection of the associated model are of secondary importance in this case. Under these circumstances we give priority to the relative simplicity of the underlying mathematical algorithm, provided the model is realistic. Following such criteria, we focus specifically on an important but relatively simple case of doubly magic spherical nuclei. To profit from the algorithmic simplicity we chose working with the phenomenological spherically symmetric Woods–Saxon mean-field. We employ two variants of the underlying Hamiltonian, the traditional one involving both the central and the spin orbit potential in the Woods–Saxon form and the more advanced version with the self-consistent density-dependent spin–orbit interaction. We compare the effects of eliminating of various types of correlations and discuss the improvement of the quality of predictions ('predictive power') under realistic parameter adjustment conditions.

http://dx.doi.org/10.1088/1402-4896/aab085

Reference 3

ABSTRACT:

We combine the framework of the inverse problem theory and the Monte Carlo approach to formulate exact mathematical models that enable estimates of the uncertainty distributions for modeling predictions. We illustrate and discuss in particular what we refer to as the "NO GO property." When the uncertainties of data constituting the input to the parameter adjustment procedures exceed certain critical value(s), even an exact modeling looses its stochastic reliability; its further use may provide "acceptably looking" r.m.s. deviations in the fitting zone with very likely meaningless, because they are unstable, predictions outside of it. We examine confidence intervals for intraneous (inside of the adjustment zone) and extraneous (outside of the adjustment zone) predictions and we demonstrate that "satisfactory" r.m.s. deviations in the intraneous modeling regime offer generally null certitude about the quality of extraneous predictions. Even though not entirely unknown, this property requires strong emphasizing since ignoring it has lead to misleading conclusions and confusing messages in the literature. We generalize our considerations to the realistic nuclear mean-field simulations of the properties of the nucleonic mean-field energies in spherical nuclei. We predict quantitatively the deterioration with increasing mass of the nucleonic-energy confidence intervals in superheavy nuclei. We show a strong dependence of those confidence intervals on the quantum characteristic of nucleonic states and provide detailed illustrations. In particular we demonstrate that, in the realistic predictions for the superheavy nuclei with the phenomenological Woods-Saxon Hamiltonian for up to $Z \approx 114$ or so, one obtains relatively stable predictions of the single-particle spectra with N 180, while approaching the NO GO zone of this model for further increasing neutron numbers. Thus the main area of today's interest within the instrumental reach for the superheavy nuclei studies remains, according to these estimates for the Woods-Saxon modeling, within the stability zone.

http://dx.doi.org/10.1103/PhysRevC.99.054310

Reference 4

ABSTRACT:

Background: The understanding and description of forbidden decays provides interesting challenges for nuclear theory. These calculations could help to test underlying nuclear models and interpret experimental data.

Purpose: Compare a direct measurement of the ^{138}La β-decay Q value with the β-decay spectrum end-point energy measured by Quarati et al. using $LaBr_3$ detectors [Appl. Radiat. Isot. 108, 30 (2016)]. Use new precise measurements of the ^{138}La β-decay and electron capture (EC) Q values to improve theoretical calculations of the β-decay spectrum and EC probabilities.

Method: High-precision Penning trap mass spectrometry was used to measure cyclotron frequency ratios of ^{138}La, ^{138}Ce and ^{138}Ba ions from which β-decay and EC Q values for ^{138}La were obtained.

Results: The ^{138}La β-decay and EC Q values were measured to be Q = 1052.42(41) keV and Q_{EC} = 1748.41(34) keV, improving the precision compared to the values obtained in the most recent atomic mass evaluation [Wang, et al., Chin. Phys. C 41, 030003 (2017)] by an order of magnitude. These results are used for improved calculations of the ^{138}La β-decay shape factor and EC probabilities. New determinations for the ^{138}Ce 2EC Q value and the atomic masses of ^{138}La, ^{138}Ce, and ^{138}Ba are also reported.

Conclusion: The ^{138}La β-decay Q value measured by Quarati et al. is in excellent agreement with our new result, which is an order of magnitude more precise. Uncertainties in the shape factor calculations for ^{138}La β-decay using our new Q value are reduced by an order of magnitude. Uncertainties in the EC probability ratios are also reduced and show improved agreement with experimental data.

https://doi.org/10.1103/PhysRevC.100.014308

Reference 5

ABSTRACT:

Based on previous study, the calculation of electron capture decays has been improved by considering a more accurate atomic model with precise atomic energies, and different radiative corrections have been tested. The computer code has been revised in order to greatly speed-up the calculation and has then been coupled with the BetaShape code. The influence of the nuclear component has also been explored using a simple nuclear model. All the calculations are compared with precise measurements available in the literature.

Accepted for publication in Applied Radiation and Isotopes.