Science Bulletin xxx (2018) xxx–xxx

Contents lists available at ScienceDirect

Science Bulletin

journal homepage: www.elsevier.com/locate/scib

Article

High precision nuclear mass predictions towards a hundred kilo-electron-volt accuracy

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ARTICLE INFO

Article history:
Received 22 February 2018
Received in revised form 23 April 2018
Accepted 2 May 2018
Available online xxxx

Keywords:
Nuclear masses
Nuclear effective interactions
Fourier analysis
Radial basis function approach

ABSTRACT

Mass is a fundamental property and an important fingerprint of atomic nucleus. It provides an extremely useful test ground for nuclear models and is crucial to understand energy generation in stars as well as the heavy elements synthesized in stellar explosions. Nuclear physicists have been attempting at developing a precise, reliable, and predictive nuclear model that is suitable for the whole nuclear chart, while this still remains a great challenge even in recent days. Here we employ the Fourier spectral analysis to examine the deviations of nuclear mass predictions to the experimental data and to present a novel way for accurate nuclear mass predictions. In this analysis, we map the mass deviations from the space of nucleon number to its conjugate space of frequency, and are able to pin down the main contributions to the model deficiencies. By using the radial basis function approach we can further isolate and quantify the sources. Taking a pedagogical mass model as an example, we examine explicitly the correlation between nuclear effective interactions and the distributions of mass deviations in the frequency domain. The method presented in this work, therefore, opens up a new way for improving the nuclear mass predictions towards a hundred kilo-electron-volt accuracy, which is argued to be the chaos-related limit for the nuclear mass predictions.

1. Introduction

Nucleus is a very small but dense object in an atom. It contains almost all mass of an atom, and hence becomes the major origin of masses in our world. Known as the famous Einstein mass-energy relation $E = mc^2$, the tiny "mass defect" in atomic nuclei gives the energies that fuel the stars, including our sun, and further provides the energies for the lives on the earth [1]. Moreover, nuclear mass is a key nuclear physics input for nuclear astrophysics in understanding the origin of elements in our universe [2], the composition of the most compact objects known-neutron stars [3], the neutrino cooling of the neutron star crusts [4], etc. Due to the lack of nuclear properties for most nuclei related to the rapid neutron capture process (r-process), the origin of heavy elements is still an unsolved physics question [5,6], which is one of the 11 greatest unanswered questions of physics [7]. High-precision determination of nuclear mass has always been extremely important for nuclear physicists [8–11], since it plays an essential role in determining the limits of nuclear landscape [12], understanding the nuclear interaction and the behavior of neutron-rich matter [13,14], and studying the nuclear shell structure [15].

With the construction and upgrade of radioactive ion beam facilities, great progress has been made in recent years in the measurements of nuclear masses, which have reached very high precision [15–18] and have been available for very exotic nuclei [13,19–22]. The nucleus is a finite quantum many-body system that is composed of two types of interacting fermions in which the underlying force is poorly understood. Thus the prediction of nuclear mass is a great and longstanding challenge for theoretical models. The accurate mass prediction is largely hampered by the absence of an exact theory of nuclear interaction and the difficulties inherent to quantum many-body calculations. Therefore, various models have been or are being developed to predict nuclear masses. Although the *ab initio* calculations can be used to predict the nuclear masses, they are only applicable to the light nuclei or those nuclei near magic numbers [23–27]. For the whole nuclear chart, a

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https://doi.org/10.1016/j.scib.2018.05.009
2095-9273/

Please cite this article in press as: Niu Z et al. High precision nuclear mass predictions towards a hundred kilo-electron-volt accuracy. Sci Bull (2018), https://doi.org/10.1016/j.scib.2018.05.009

classical nuclear mass model—liquid drop model—was developed [28,29] soon after the confirmation of the constituents of nucleus, i.e., the discovery of neutron [30]. Since then, comprehensive efforts have been devoted to this investigation. There are so far mainly three kinds of global nuclear mass models: the macroscopic (e.g., Bethe-Weizsäcker (BW) model [28,29,31]), macroscopic-microscopic (e.g., finite-range droplet model (FRDM) [32] and Weizsäcker-Skyrme (WS) model [33]), and microscopic mass models (e.g., Skyrme Hartree-Fock-Bogoliubov (HFB) [34] and relativistic mean-field (RMF) models [35,36]). The macroscopic mass models well describe the bulk properties of nuclear mass, while they lack detailed information of nuclear shell structure and hence give relatively large root-mean-square (rms) deviations. By including the microscopic shell corrections, the macroscopic-microscopic mass models have achieved the best accuracy in nuclear mass descriptions, although this kind of hybrid models is generally inconsistent in their macroscopic and microscopic parts. The microscopic mass models are much involved, while they are usually believed to have a better ability of extrapolation.

About 80 years' continuous efforts by several generations of theoreticians have resulted in a remarkable success in the development of nuclear models. The rms values, defined by the deviations between model predictions and experimental data [37], are reduced from about 3 million electron volts (MeV) for the BW model [31] to about 300 kilo electron volts (keV) for the WS4 model [33]. Comparison of rms values in different models is shown in Fig. 1. The best accuracy of 300-keV level achieved by the WS4 macroscopic-microscopic model [33] is already a great challenge for the pure microscopic mass models, especially for those based on the covariant density functionals, which are usually believed to have a better ability of extrapolation. However, such an accuracy is still not good enough for the studies of exotic nuclear structure and astrophysical nucleosynthesis, which demand an accuracy better than 100 keV [8]. From the estimate of statistical fluctuations of nuclear ground-state energies [38,39], the possible accuracy limit of theoretical calculations is expected to be tens of keV. Therefore, there are still a high demand and a large room for improving the existing nuclear mass models even for the best available one. Correspondingly, in this work, we would like to raise the following questions: what are the main limitations of present models? Microscopically, which parts of nuclear effective interactions are still heavily missing or need better treatment in the available theories? The answers to these questions are crucial for the breakthroughs in the coming studies in nuclear physics and astrophysics.

Based on thousands of measured nuclear masses [37], it has been aware that there are systematic large deviations from experimental data in various global mass models, e.g., around magic nuclei. Depending on specific model, these deviations often show quite different patterns in both magnitudes and distribution over the nuclear chart as a function of proton and neutron numbers. In other words, it is difficult to find universal regulations that hold for different models for improving their accuracy. This motivates us to explore a novel view of the deviations between the calculated results and experimental data.

The Fourier spectral analysis provides a different view from the frequency domain, which has been widely used in many fields of engineering, such as electronics, telecommunication, and optics [40]. In particular, in the field of image processing, it is found that the frequency spectra of various pictures can show similar structures when they share common features. This makes the Fourier spectral analysis an effective way to find universal regulations of image processing, and thus plays an important role in image denoising, compression, and recognition. In fact, nuclear mass deviations between model predictions and experimental data can be treated as an image processing problem. We will first analyze the deviations by the Fourier spectral analysis in the conjugate space of frequency. As a step further, we will employ the radial basis function (RBF) approach to study the deviations coming from different frequency domains. The RBF approach is a powerful interpolation method, in which complicated nonlinear functions are described with linear combination of radial basis functions. It can well describe the smooth surface and has been successfully used in time series prediction, control of nonlinear systems, three-dimensional reconstruction in computer graphics [41], even in nuclear mass predictions [42–44]. Guided by the Fourier spectral analysis and the RBF approach, in this work, we will show a general and systematic strategy for improving the accuracy of nuclear mass predictions from several MeV to less than 100 keV.

2. Discrete Fourier transform

To investigate the deviations between the calculated results and experimental data in the conjugate frequency space, we would perform the two-dimensional discrete Fourier transform of the mass differences [45]. The amplitude of discrete Fourier transform is defined as

$$F_{kl} = \frac{1}{Z_{\mathrm{m}}N_{\mathrm{m}}}\sum_{Z=8}^{Z_{\mathrm{m}}}\sum_{N=8}^{N_{\mathrm{m}}}\left(M_{\mathrm{exp}}^{Z,N} - M_{\mathrm{th}}^{Z,N}\right)\mathrm{e}^{-\mathrm{i}2\pi\left[\frac{(k-1)(Z-1)}{Z_{\mathrm{m}}}+\frac{(l-1)(N-1)}{N_{\mathrm{m}}}\right]}, \tag{1}$$

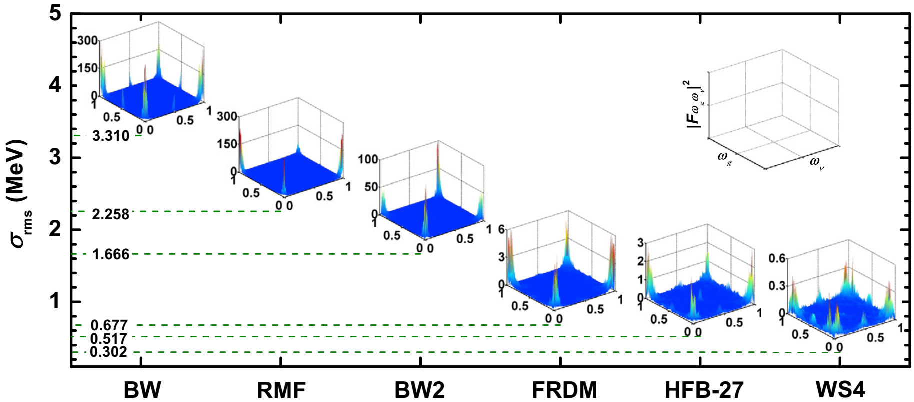

Fig. 1. (Color online) Squared amplitudes $|F_{\omega_\pi\omega_\nu}|^2$ of the discrete Fourier transforms of the mass differences between the experimental data and the predictions of various models, plotted against proton frequency ω_π and neutron frequency ω_ν. The rms deviations of these mass models are marked on the vertical axis. Here we only take into account the nuclei with proton number $Z \geqslant 8$ and neutron number $N \geqslant 8$ listed in the Atomic Mass Evaluation (AME2016).

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