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Study of the Duflo-Zuker Nuclear Mass Model under Multiple Physical Constraints

Authors: Ye Weihu, Qian Yibin, Qian Yibin

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Abstract

Nuclear masses play a very important role in nuclear physics and nuclear astrophysics research. Although current theoretical models can describe the masses of known nuclides reasonably well, many controversies persist regarding the extrapolation of different models, particularly concerning predictions in the neutron-rich region. This paper reviews our main achievements in recent years on the extrapolation of nuclear mass models, namely, employing rigorous multi-objective optimization algorithms to incorporate nuclear mass differences, α-decay energies, and local mass relations as constraints, thereby alleviating the overfitting problem in mass models and enhancing their extrapolation capability to a certain extent.

Full Text

Preamble

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Study of Multiple Physical Constraints on the Duflo-Zuker Nuclear Mass Model

Ye Weihu[1], Qian Yibin[1]
([1] School of Physics, Nanjing University of Science and Technology, Nanjing 210094, China)

Abstract

Nuclear mass plays a crucial role in both nuclear physics and nuclear astrophysics. Although current theoretical models can describe the masses of known nuclides reasonably well, significant discrepancies remain in their extrapolations,

particularly for neutron-rich regions. This paper reviews our recent work on improving the extrapolation capabilities of nuclear mass models through rigorous multi-objective optimization algorithms. By incorporating mass differences, α-decay energies, and local mass relations as constraints, we mitigate overfitting issues in mass models and enhance their predictive power for extrapolation.

Keywords: nuclear mass; α-decay energy; multi-objective optimization

Introduction

Nuclear mass (or binding energy) serves as both an effective probe for studying nuclear structure information and a key physical quantity in astrophysics for investigating the origin of heavy elements. On one hand, nuclear masses provide critical insights into nucleon correlations, shell effects, and deformation [**?**]. On the other hand, precise nuclear masses constitute essential input for nucleosynthesis network calculations, which is crucial for addressing one of the 21st century' s eleven major unsolved physics problems: "How are the elements from iron to uranium produced in the universe?" Consequently, mass measurement has remained a hot topic in nuclear science research.

Experimentally, masses of approximately 2,500 nuclides can be obtained through direct or indirect measurements, while theoretical predictions suggest that 7,000–10,000 nuclides could exist in nature [**?**, **?**]. However, these unknown nuclides are concentrated in the proton drip-line region, neutron-rich region, and superheavy nuclear region, where target nuclei have short lifetimes and small production cross-sections, making precise mass measurements technically challenging. For the foreseeable future, masses of unstable nuclides will continue to rely on theoretical models.

Nuclear mass theoretical models can generally be divided into two categories: global and local. Global models with reasonable accuracy include macroscopic-microscopic and pure microscopic models. The macroscopic term in macroscopic-microscopic models describes the smooth component of binding energy, while the microscopic term typically refers to shell and pairing energy corrections. The classic concept of pure microscopic models involves specifying a nucleon interaction potential field and solving the Schrödinger equation in the non-relativistic framework or the Dirac equation in the relativistic framework. Commonly used global models include the Duflo-Zuker (DZ) model [**?**], the finite-range droplet model [**?**], and mean-field theory [**?**], with standard deviations of approximately 300–600 keV [**?**]. Local models, by contrast, indirectly obtain masses of unknown nuclides using mass relations between neighboring nuclei, achieving theoretical precision within about 150 keV. These include the famous Garvey-Kelson (GK) relations [**?**, **?**], residual neutron-proton interaction formulas [**?**, **?**], and isospin multiplet mass equations [**?**, **?**], among others. Domestic research groups have made many important discoveries and extensions in local mass relations, including studies on generalizing GK relations to determine optimal extrapolation paths [**?**, **?**] and research on mirror

nucleus extrapolation formulas [**?**, **?**]. Further details on local mass relations can be found in recent review articles [**?**].

Although global models possess significantly broader and deeper physical concepts than local models, local models achieve far higher binding energy precision within certain mass number regions. In recent years, with the emergence of interdisciplinary research between nuclear physics and machine learning, the accuracy of nuclear mass models has improved dramatically [**?**], reaching within 100 keV and thus satisfying the precision requirements for nucleosynthesis calculations. However, researchers have raised a critical question: Is there a correlation between a model' s precision on known nuclides and its predictive power in unknown regions?

Unfortunately, systematic studies by Sobiczewski et al. based on dozens of popular mass models revealed weak correlations between precision on known nuclides and predictive capability in unknown regions [**?**]. This suggests that solely pursuing binding energy precision may not improve predictive power for unknown nuclei. Additionally, mass models suffer from internal contradictions inherent to parameterized models, namely overfitting. For instance, although DZ-type mass models achieve high accuracy in binding energy calculations, their precision for mass-related quantities such as α-decay energies is relatively low [**?**]. Moreover, extrapolations from different mass models differ significantly, with discrepancies reaching several tens of MeV near the neutron drip line [**?**]. These phenomena indicate non-negligible overfitting problems in mass models. While overfitted models can perfectly reproduce training data, their errors increase with extrapolation distance.

The primary approach to mitigating overfitting is providing more fitting samples, which prevents algorithms from "over-learning" in specific intervals and helps achieve global rather than local optima for free parameters. Therefore, we introduce multi-objective optimization algorithms into nuclear mass modeling, using α-decay energies and GK relations as important constraints. This paper aims to enhance the extrapolation capabilities of mass models by introducing multiple physical constraints, thereby reducing the enormous uncertainties associated with long-distance extrapolation.

2. Model Introduction and Algorithm

The Duflo-Zuker (DZ) series represents one of the most widely used mass models due to its high theoretical accuracy and extrapolation performance, with computational costs far lower than other models of comparable precision. The DZ series includes DZ10, DZ28, DZ33, etc. [**?**, **?**]. This paper uses the DZ10 model as an example to present results under multi-objective optimization.

2.1 DZ10 Model

The DZ10 model expresses the ground-state binding energy of a nucleus as:

$$BE_{DZ10} = a_{1V}C + a_2(M+S) - a_3 + a_{6V}TS + a_{7s}3 - a_8 + a_{4V}P - a_{5V}T + a_{9s}4 + a_{10}d_4$$

where a_i are free parameters determined through fitting; a_1, a_4, a_5, and a_6 represent Coulomb energy, pairing energy, symmetry energy, and symmetry energy correction in the liquid-drop model, respectively; the remaining terms represent microscopic valence nucleon corrections.

2.2 Multi-Objective Optimization Algorithm

In professional and daily life, people frequently face optimization problems, such as maximizing corporate profits or minimizing living costs. However, since objectives are often interrelated, maximizing one objective inevitably reduces benefits for other related objectives, necessitating trade-offs between conflicting goals. Optimization problems considering two or more objectives simultaneously are called multi-objective optimization problems, widely applied in economics, engineering, and other disciplines [**?**]. Multi-objective optimization algorithms define the Pareto front, also known as the set of non-dominated solutions. This set contains a series of solutions determined by different trade-off relationships among objectives. No solution in the non-dominated set can simultaneously optimize all objectives. The core concept involves finding as many compromise solutions as possible under conflicting objective functions to provide users with ample choices.

Generally, a multi-objective optimization problem can be expressed as:

$$F(x) = (f_1(x), \ldots, f_m(x)) x \subset \Omega lb \leq x_i \leq ub$$

where $f_i(x)$ are objective functions; $x = (x_1, x_2, \ldots, x_m)$ are decision variables; each decision variable is constrained within upper and lower bounds in the solution space. Since multi-objective optimization involves comparing multiple objective functions, individual superiority cannot be determined by comparing a single function value as in single-objective optimization. The Pareto dominance relationship constitutes the core principle of multi-objective optimization algorithms, defining superiority between individuals in the solution space. Assuming two individuals s and t exist in the solution space, individual s dominates (is superior to) individual t if and only if $\forall i = 1, 2, \ldots, m, f_i(s) \leq f_i(t)$, and $\exists j \in [1, 2, \ldots, m]$ such that $f_j(s) < f_j(t)$.

3. Results and Analysis

3.1 Constraints from α-Decay Energies

Currently, the Non-dominated Sorting Genetic Algorithm-II (NSGA-II) remains the most widely used and cited second-generation evolutionary algorithm [**?**, **?**]. Therefore, this study employs NSGA-II for multi-objective optimization of

binding energies and α-decay energies. The α-decay energy is given by the mass difference between parent and daughter nuclei:

$$Q_\alpha = BE(Z-2, N-2) + BE_\alpha - BE(Z, N)$$

The objective function is constructed from the standard deviation between theoretical and experimental values:

$$\sigma_K = \sqrt{\sum_{i=1}^{\hat{N}} (K_{\text{expt.}} - K_{\text{theo.}})^2}$$

where σ_k represents the standard deviation formula between theoretical and experimental values; $\hat{N}$ is the number of experimental samples (2,340 binding energies and 275 even-even nucleus α-decay energies); k denotes binding energy or other physical quantities. Experimental data for binding energies and α-decay energies are taken from the Atomic Mass Evaluation AME2020 [**?**].

[Figure 1: see original paper] shows the non-dominated solution results for the DZ10 model obtained through the NSGA-II algorithm, with horizontal and vertical axes representing standard deviations of binding energy and α-decay energy, respectively. The upper-leftmost solution represents the optimal binding energy precision but worst α-decay energy precision, while the lower-rightmost solution represents the opposite. The relationship between binding energy and α-decay energy precision is clearly conflicting: improving binding energy precision comes at the cost of degrading α-decay energy precision. This reveals that conventional single-objective algorithms fitting binding energy parameters prioritize local optimization of mass accuracy rather than global optimization considering multiple physical quantities, potentially exacerbating overfitting and degrading extrapolation performance beyond the training set. Furthermore, incorporating α-decay energy data yields solutions with superior α-decay energy calculation capabilities. Since α-decay energy is a crucial determinant of α-decay lifetimes —a 0.01 MeV uncertainty in α-decay energy can affect half-lives by an order of magnitude—these model-derived α-decay-favored solutions can support predictions of α-decay energies in heavy and superheavy nuclei.

In recent years, due to large discrepancies between different theoretical models in regions beyond experimental data, theorists have needed to quantify model uncertainties through systematic and statistical uncertainty analyses. Based on these dozens of non-dominated solutions, we can determine the model' s statistical uncertainty. Table 1 presents the parameter uncertainties for the DZ10 model, where the second column shows statistical uncertainties and the third column provides parameters for the mass-optimal solution.

Based on the statistical characteristics of the non-dominated solution set, [Figure 2: see original paper] systematically presents physical information including

new nuclear boundaries, two-neutron separation energies, and extrapolation differences among non-dominated solutions. First, drip lines can be determined where nucleon separation energies become negative. Since even-even nuclei are generally more stable than odd-A nuclei, drip lines determined by two-nucleon separation energies encompass those determined by single-nucleon separation energies. In the figure, $P(S_{2n} < 0)$ represents the probability that a nuclide is unbound based on two-neutron separation energy, while $P(S_{2p} < 0)$ represents the corresponding probability based on two-proton separation energy. Second, we systematically calculate two-neutron separation energies for non-dominated solutions and take weighted averages, with magnitudes indicated by the color bar. Third, we compute binding energy differences using parameter sets from the mass-optimal solution and the second-best mass solution (the two uppermost adjacent solutions in [Figure 1: see original paper]), shown in the lower-right subplot. This subplot clearly shows that extrapolation differences do not exceed 0.5 MeV in regions with experimental data and proton-rich areas, but increase significantly in superheavy and neutron-rich regions. Since these two solutions are heavily biased toward mass precision, they may exacerbate overfitting during large-scale extrapolation, ultimately degrading model differences. Therefore, we select two solutions from the intermediate region of [Figure 1: see original paper] to compute extrapolation differences. Comparing the subplot in [Figure 2: see original paper] with [Figure 3: see original paper] reveals that extrapolation differences from the intermediate region are noticeably smaller than those from the mass-optimal group, indicating that using non-dominated solutions balancing binding energy and α-decay energy yields smaller uncertainties during extrapolation.

3.2 Constraints from Garvey-Kelson Relations

Building upon the previous discussion, we can further explore constraints on mass models by introducing local mass formulas. This study employs the Garvey-Kelson relation as an additional constraint on the nuclear mass model. Previously, J. Barea et al. proposed attaching local-type constraints to global model fitting to enhance coherence between neighboring nuclei and improve predictive power during extrapolation [**?**], though their methods were relatively crude and redundant. Subsequently, global models typically treated GK relations as posterior samples rather than constraints. Leveraging the advantages of multi-objective optimization algorithms, we implement the Garvey-Kelson relation as a strict constraint for more detailed analysis of mass models.

The GK relation is expressed as:

$$\Delta M_{GK} = M(N{+}2, Z{-}2){-}M(N, Z){+}M(N, Z{-}1){-}M(N{+}1, Z{-}2){+}M(N{+}1, Z){-}M(N{+}2, Z{-}1)$$

where ΔM_{GK} is a constant uncertainty (typically within \$±\$150 keV) after cancellation through addition and subtraction of six neighboring nuclides. Based

on this equation, we extracted several hundred experimental $\Delta M_{\text{expt.}}$ values from AME2020 and computed standard deviations with theoretical $\Delta M_{\text{theo.}}$ values from the DZ10 model. In practice, numerous GK relation variants exist (dozens) based on assumptions of residual nucleon interaction cancellation. This study simply adopts the above equation as a feasible case to demonstrate the viability of using GK relations for multi-objective mass model constraints; other GK variants could be substituted, though this requires future verification.

[Figure 4: see original paper] presents the non-dominated solution set obtained through multi-objective optimization using binding energy, α-decay energy, and GK relations, with the mass-optimal solution enclosed in a cyan box. While we have argued that balanced solutions among multiple physical quantities may be more reliable for extrapolation, this claim requires further confirmation through detailed analysis. Given the large number of non-dominated solutions, identifying those with greater physical significance and more reliable extrapolation values becomes crucial. Neutron-rich nuclides, with their large isospin asymmetry, pose significant challenges for both theoretical predictions and experimental measurements, and discrepancies between different theoretical models often concentrate in neutron-rich regions.

First, we extract recent experimental mass data for neutron-rich nuclei not yet included in AME2020 [**?**]. Using the DZ10 mass-optimal solution as a theoretical baseline, we compute standard deviations for these nuclei and retain non-dominated solutions that yield better precision than this baseline, classifying them as a "potential solution set." Although the total number of non-dominated solutions reaches several hundred, only a few dozen potential solutions are selected. Table 2 presents systematic analysis results for the potential solution set from both local and global perspectives: rows 2–4 address local neutron-rich nuclear data, while the final three rows address overall fitting sample data. Row 2 shows standard deviations computed with the mass-optimal solution; row 3 shows the best standard deviation from the potential solution set; row 4 provides statistical analysis of binding energy standard deviations for all potential solutions (mean and variance); rows 5–7 show statistical analyses for binding energies, α-decay energies, and GK relations in the fitting sample. The best potential solution improves the precision for neutron-rich nuclear masses by approximately 70% compared to the mass-optimal solution. Furthermore, row 4 shows small variations with mean values concentrated in intermediate regions (balanced zones) for α-decay energy and GK relations, validating our argument that globally balanced solutions across multiple physical quantities are more likely to provide stable and reliable extrapolation values.

Previously, using two globally optimal solutions balancing binding energy and α-decay energy, we found that binding energy differences during extrapolation were reduced, indicating some mitigation of overfitting. Naturally, we must examine binding energy differences among non-dominated solutions obtained under constraints from binding energy, α-decay energy, and GK relations (i.e., more physical data). [Figure 3: see original paper] subplot (b) shows binding

energy differences computed from two randomly selected solutions in the potential solution set (intermediate region). Compared to subplot (a), subplot (b) exhibits smaller differences during extrapolation, demonstrating the feasibility of incorporating GK relations in reducing extrapolation uncertainties.

The synthesis of superheavy nuclei (SHN) represents a frontier research topic in nuclear physics, with α-decay being the primary decay mode for SHN. We performed theoretical calculations of α-decay energies for SHN ($Z \geq 104$) based on the potential solution set. [Figure 5: see original paper] shows the distribution of standard deviations for α-decay energies of all SHN computed by the potential solution set. The distribution roughly follows a Gaussian shape, with the mass-optimal solution positioned in the middle-to-rear section, while most potential solutions concentrate to its left and a minority to its right. This indicates that potential solutions are more likely to yield more precise α-decay energies for superheavy nuclei than the mass-optimal solution.

Nuclear shell evolution has been a major international research focus, with studies showing that weakly bound nuclides far from the β-stability line may exhibit shell structure evolution. The DZ mass model incorporates complex valence nucleon calculations for shell structures, with pre-inputted shell information at Z(N) = 8, 20, 28, 50, 82, N = 126, 184, while new magic numbers observed experimentally are not yet included. This study makes a preliminary attempt by adding a neutron shell at N = 152 to DZ10 and computing α-decay energies for $126 \leq N \leq 184$, though results show relatively large deviations from experimental values, requiring further future investigation.

Conclusion

This study aims to alleviate overfitting in nuclear mass models and reduce enormous uncertainties during long-distance extrapolation by introducing strict physical constraints. Within the multi-objective optimization framework, incorporating α-decay energies and the local mass formula Garvey-Kelson relation significantly improves α-decay energy precision and enhances model extrapolation capabilities. Additionally, new nuclear boundaries and model statistical uncertainties are derived from the statistical characteristics of the multi-objective method. From the vast non-dominated solution set, we identify solutions with greater extrapolation capability (termed "potential solutions") and perform rigorous statistical analyses, demonstrating that globally balanced solutions across multiple physical quantities exhibit higher predictive power than single mass-optimal solutions. The introduction of these physical constraints mitigates overfitting to some extent, thereby improving model reliability during extrapolation and providing theoretical support for reliable predictions of neutron-rich nuclei.

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