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Predicting Nuclear Masses Using Continuous Bayesian Probability Estimators

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Abstract

In recent years, machine learning methods have been widely applied to the prediction of nuclear masses. Based on the Continuous Bayesian Probability (CBP) estimator, combined with Bayesian Model Averaging (BMA), the description of nuclear masses by theoretical models has been improved. In the CBP method, the difference between theoretical and experimental nuclear mass values is treated as a continuous variable; kernel density estimation is employed to generate its prior and conditional probability density functions, and Bayes' theorem is used to determine the posterior probability density function. In global optimization and extrapolation analyses, the CBP method significantly improves the accuracy of theoretical model predictions. Furthermore, the BMA method assigns weights to each model based on their predictive performance for benchmark nuclei, balancing the advantages of each model in different regions. The reliability of the BMA method's corrections was evaluated by predicting the two-neutron drip line positions of Ca isotopes. The combination of CBP and BMA methods provides an effective approach for predicting nuclear masses in unknown regions and can be applied to the study of other nuclear properties.

Full Text

Preamble

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Predicting Nuclear Masses Using a Continuous Bayesian Probability Estimator

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Abstract [Background]: In recent years, machine learning methods have been widely applied to the predictions of nuclear masses. [Purpose]: This study employs the continuous Bayesian probability (CBP) estimator and Bayesian model averaging (BMA) to optimize the descriptions of sophisticated nuclear mass models. [Methods]: The CBP estimator treats the residual between theoretical and experimental values of nuclear masses as a continuous variable, deriving its posterior probability density function (PDF) from Bayesian theory. The BMA method assigns weights to models based on their predictive performance for benchmark nuclei, thereby balancing each model's unique strengths. [Results]: In global optimization, the CBP method improves the Hartree-Fock-Bogoliubov (HFB) model by approximately 90%, and the relativistic mean-field (RMF) and semi-empirical formulas by 70% and 50%, respectively. In extrapolation analysis, the CBP method improves prediction accuracy for HFB models, RMF models, and semi-empirical formulas by approximately 80%, 55%, and 50%, respectively, demonstrating strong generalization ability. To assess BMA reliability, the two-neutron separation energy for Ca isotopes was extrapolated to predict its two-neutron drip line. [Conclusions]: The proposed methods provide an effective way to accurately predict nuclear mass, with potential applications to research on other nuclear properties.

Key Words: Machine learning, Nuclear masses, Continuous Bayesian probability estimator, Bayesian model averaging

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Nuclear mass represents one of the most fundamental physical quantities in nuclear physics. Precise nuclear mass data not only advances theoretical research on nuclear structure [1-4] but also provides critical support for understanding nuclear decay [5-9], nucleosynthesis processes [10,11], and related research in nuclear astrophysics [12,13]. Currently, experimental nuclear mass measurements primarily employ two methods. The first involves nuclear mass spectrometry techniques that determine mass by measuring flight time or cyclotron frequency [14-17]. The second extracts nuclear masses by analyzing Q-values from nuclear reactions or decays [18,19]. While significant progress has been achieved in recent years, the expansion of known nuclear masses has slowed due to difficulties in producing short-lived target nuclei. Most nuclear masses in neutron-rich regions far from stability remain unmeasured [20-22], requiring theoretical model predictions for unknown regions [23].

Nuclear mass theoretical models can be broadly categorized into two classes. The first comprises microscopic nuclear structure models with parameter sets, such as non-relativistic Hartree-Fock-Bogoliubov (HFB) models [24-28] (SkP [29], SLy4 [30], etc.) and relativistic mean-field (RMF) models [31-37] (NL3*

[38], NLSH [39], etc.). The second includes macroscopic semi-empirical formulas and macroscopic-microscopic models that further incorporate microscopic effects, such as the Weizsäcker-Skyrme (WS*) formula [40], Duflo-Zuker (DZ) formula [41,42], and the finite-range droplet model (FRDM) [43,44]. However, the complexity of theoretical models increases significantly as demands for calculation precision grow.

In recent years, machine learning has been extensively applied to study physical quantities in nuclear physics [44-53]. Notable progress has been achieved in predicting nuclear masses and neutron drip line positions [54-55]. Machine learning models can be divided into two categories: generative models and discriminative models. Generative models learn the joint probability distribution of data to generate new data, such as Gaussian processes (GP) [56-58] and Naive Bayesian Probability (NBP) classifiers [59-62]. Discriminative models directly rely on conditional probability distributions to classify data into different categories, such as decision trees (DT) [63], support vector machines (SVM) [64], and neural networks (NN) [65-69]. Algorithm selection depends on dataset characteristics. Generative models are more suitable when training data is limited because they model the complete data distribution and may capture more information [70,71]. As a generative model, the NBP method has been proposed to improve theoretical predictions of nuclear masses and charge radii [59-62].

Building upon the Naive Bayesian Probability classifier, this work applies the Continuous Bayesian Probability (CBP) estimator [72] to improve theoretical descriptions of nuclear masses. In the CBP framework, the deviation between experimental data and theoretical results—i.e., the mass residual—is treated as a continuous variable, thereby considering contributions from all experimental data. Bayesian formula is applied to obtain the posterior probability density function (PDF) of residuals, from which nuclear mass estimates are derived. To further enhance prediction stability, this study employs Bayesian Model Averaging (BMA) to comprehensively consider predictions from different models [73-75]. BMA is an optimization method that evaluates predictive performance of various theoretical models and performs weighted averaging, which has been used to provide quantified predictions in nuclear physics research.

This work applies the CBP method to optimize three categories of theoretical models: HFB models, RMF models, and semi-empirical formulas. Systematic analysis of CBP performance in global optimization and extrapolation is conducted. For global optimization, the complete dataset comprises 868 even-even nuclei with experimental mass data from the 2020 Atomic Mass Evaluation (AME2020). For extrapolation analysis, the learning set includes 768 even-even nuclei present in AME2003 [77], while the validation set contains 100 newly added even-even nuclei from AME2020. After CBP refinement, BMA assigns weights to each theoretical model based on their predictive performance for six benchmark nuclei: ^{14}O , ^{28}Ne , ^{82}Ru , ^{112}Zr , ^{178}Pt , and ^{280}Ds . Results demonstrate that the CBP method combined with BMA effectively improves theoretical descriptions of nuclear masses and can predict masses in unknown regions

of the nuclear chart.

The paper is organized as follows: Section 1 details the theoretical framework of CBP and BMA methods; Section 2 presents prediction results and discussion; Section 3 provides conclusions.

1 Theoretical Framework

This section introduces the theoretical framework of the Continuous Bayesian Probability (CBP) estimator and Bayesian Model Averaging (BMA). In the CBP method, residuals of theoretical nuclear mass values are treated as continuous variables. Bayesian formula calculates and predicts the posterior probability density function of residuals for target nuclei, from which residual estimates are obtained. In BMA, a method for assigning weights to different models based on Bayesian theorem is proposed, which can be used to construct formulas for calculating averaged masses. Additionally, this work proposes corresponding accuracy evaluation criteria and uncertainty assessment standards.

1.1 Continuous Bayesian Probability Estimator

Bayes' theorem provides an effective method for calculating posterior probabilities of target values based on sample sets. Assuming mutual independence among events, the multivariate Bayes theorem for calculating posterior probability density functions can be expressed as:

$$p(X_1, X_2, \dots, X_m | Y) = \frac{p(Y | X_1, X_2, \dots, X_m) p(X_1, X_2, \dots, X_m)}{\int p(Y | X_1, X_2, \dots, X_m) p(X_1, X_2, \dots, X_m) dX_1 \dots dX_m}$$

where $p(X_1, X_2, \dots, X_m)$ is the prior probability density function representing the probability density of events X_i occurring, and $p(Y | X_1, X_2, \dots, X_m)$ is the likelihood probability density function representing the probability of event Y occurring given X_i .

Treating nuclear mass residuals as continuous variables improves nuclear mass description using Eq. (1). Event Y denotes the nuclear mass residual δ , a continuous random variable. Events X_i represent the proton number Z and neutron number N of target nuclei. Assuming independence between variables Z and N , the posterior probability density function $p(\delta | Z_t, N_t)$ for a target nucleus with proton number Z_t and neutron number N_t is given by Eq. (2):

$$p(\delta | Z_t, N_t) = \frac{p(Z_t | \delta) p(N_t | \delta) p(\delta)}{\int p(Z_t | \delta) p(N_t | \delta) p(\delta) d\delta}$$

The likelihood probability density functions $p(Z_t | \delta)$ and $p(N_t | \delta)$ in Eq. (2) can be derived from univariate Bayes formulas:

$$p(Z_t|\delta) = \frac{p(\delta|Z_t)p(Z_t)}{\int p(\delta|Z_t)p(Z_t)d\delta}$$

$$p(N_t|\delta) = \frac{p(\delta|N_t)p(N_t)}{\int p(\delta|N_t)p(N_t)d\delta}$$

In Eqs. (3) and (4), the prior probabilities $p(Z_t)$ and $p(N_t)$ represent the frequencies of proton number Z_t and neutron number N_t in the training set, respectively.

The likelihood probability density functions $p(\delta|Z_t)$ and $p(\delta|N_t)$ can be obtained through kernel density estimation (KDE):

$$p(\delta|Z_t) = \frac{1}{n_Z} \sum_{i=1}^{n_Z} K\left(\frac{\delta - \delta_i}{h_Z}\right)$$

$$p(\delta|N_t) = \frac{1}{n_N} \sum_{i=1}^{n_N} K\left(\frac{\delta - \delta_i}{h_N}\right)$$

where the kernel function is:

$$K(t) = \frac{1}{\sqrt{2\pi}} e^{-t^2/2}$$

In Eqs. (5)-(7), h_Z and h_N are bandwidth parameters, and n_Z (n_N) denotes the number of nuclei in the training set with proton number Z_t (neutron number N_t). Similarly, the prior probability density function $p(\delta)$ in Eqs. (2)-(4) can also be calculated using KDE:

$$p(\delta) = \frac{1}{n} \sum_{i=1}^n K\left(\frac{\delta - \delta_i}{h_\delta}\right)$$

where n is the total number of nuclei in the training set. In Eqs. (5)-(7), δ_i represents the mass residual of a single nucleus in the training set. The bandwidth parameters h_δ , h_Z , and h_N depend on factors such as the distribution range of mass residuals, dataset size, and noise levels.

To incorporate local relationships between neighboring nuclei, a weighting function $\omega(Z_t, N_t; Z_i, N_i)$ is introduced when calculating likelihood and prior probability density functions. This function contains two parameters, ρ and ε . Parameter ρ influences the extrapolation distance of predictions. Based on the distribution of nuclei in the selected dataset across the nuclear chart, ρ is set to 4. Parameter ε affects the stability of the posterior probability density function; this study selects $\varepsilon = 10^{-10}$. The weighting function adjusts the weights of data

points during likelihood estimation but does not appear in the overall Bayesian framework, thus minimally impacting the feature independence assumption. By introducing the weighting function, the prior probability density function $p(\delta)$ and likelihood probability density functions $p(\delta|Z_t)$ and $p(\delta|N_t)$ become:

$$p(\delta) = \frac{1}{\sum_{i=1}^n \omega_i} \sum_{i=1}^n \omega_i K\left(\frac{\delta - \delta_i}{h_\delta}\right)$$

$$p(\delta|Z_t) = \frac{1}{\sum_{i=1}^{n_Z} \omega_i} \sum_{i=1}^{n_Z} \omega_i K\left(\frac{\delta - \delta_i}{h_Z}\right)$$

$$p(\delta|N_t) = \frac{1}{\sum_{i=1}^{n_N} \omega_i} \sum_{i=1}^{n_N} \omega_i K\left(\frac{\delta - \delta_i}{h_N}\right)$$

Combining Eqs. (2)-(11) determines the posterior probability density function, and calculating its expectation value yields the final residual prediction for the target nucleus:

$$\delta_{\text{pred}} = \int \delta \cdot p(\delta|Z_t, N_t) d\delta$$

Finally, adding the predicted residual to the theoretical mass value $E_{\text{th}}(Z, N)$ gives the corrected mass prediction:

$$E_{\text{corr}}(Z, N) = E_{\text{th}}(Z, N) + \delta_{\text{pred}}(Z, N)$$

1.2 Bayesian Model Averaging

To combine the respective advantages of different theoretical models and comprehensively consider each model's predictive performance across different regions, Bayesian Model Averaging (BMA) is introduced based on the CBP method. BMA is an optimization algorithm that selects the best statistical model from a set of candidate models. This study employs six theoretical models to obtain mass residuals, including non-relativistic HFB models, relativistic RMF models, and semi-empirical formulas. Since prediction results differ among models, BMA determines each model's weight based on its predictive performance for target nuclei to reduce these differences.

Given a set of candidate models $\{M_1, M_2, \dots, M_K\}$, Bayes' theorem determines the weight assigned to each model:

$$P(M_k|D) = \frac{P(D|M_k)P(M_k)}{\sum_{i=1}^K P(D|M_i)P(M_i)}$$

In this study, dataset D contains six benchmark nuclei: ^{14}O , ^{28}Ne , ^{82}Ru , ^{112}Zr , ^{178}Pt , and ^{280}Ds , which are used to evaluate theoretical model accuracy across the nuclear chart. The prior probability $P(M_k)$ is set to $1/K$, while the likelihood $P(D|M_k)$ is determined by each model's predictive performance for benchmark nuclei. The corrected residual $\delta_{\text{corr},j}$ represents the residual for benchmark nucleus j after correction by theoretical model M_k . The final average mass result for nucleus (Z_t, N_t) through BMA is:

$$E_{\text{corr}}(Z_t, N_t) = \sum_{k=1}^K E_{\text{corr},k}(Z_t, N_t)P(M_k|D)$$

1.3 Evaluation Criteria and Uncertainty

The root-mean-square (RMS) deviation σ_{rms} measures the deviation between model-corrected results and experimental data:

$$\sigma_{\text{rms}} = \sqrt{\frac{1}{n} \sum_{i=1}^n (E_{\text{exp},i} - E_{\text{corr},i})^2}$$

In the CBP method, prediction uncertainty originates from the posterior probability density function. The uncertainty for nucleus (Z, N) is defined as:

$$\sigma(Z, N) = \sqrt{\int (\delta - \delta_{\text{pred}})^2 p(\delta|Z, N) d\delta}$$

The standard for calculating BMA method uncertainty is shown in Eq. (19):

$$\sigma_{\text{BMA}}(Z, N) = \sqrt{\sum_{i=1}^K \sigma_i^2(Z, N)P(M_i|D)}$$

2 Results and Discussion

This section presents optimization results for theoretical nuclear masses using CBP and BMA methods. First, three theoretical models provide original theoretical results: HFB models (SLy4 and SkP parameters) [78], RMF models (NL3* and NLSH parameters) [79], and semi-empirical formulas (DZ10 and WS* models). The CBP method then optimizes these original results, evaluating global optimization and extrapolation predictive capabilities. Finally, based on each model's performance for benchmark nuclei, BMA balances predictive differences among models across regions.

2.1 Global Optimization Capability of CBP Method

The complete set used in this section consists of 868 even-even nuclei with experimental masses from AME2020, covering proton numbers $Z \geq 8$. First, each nucleus' s original theoretical mass E_{th} and original mass residual $\delta_{\text{pre}} = E_{\text{exp}} - E_{\text{th}}$ are calculated using six models. The CBP method then optimizes nuclear mass predictions. Each target nucleus' s training set contains the remaining 867 nuclei from AME2020. Equations (3)-(11) calculate the prior probability density functions $p(\delta)$, $p(\delta|Z_t)$, and $p(\delta|N_t)$, followed by Eq. (2) to obtain the posterior probability density function $p(\delta|Z_t, N_t)$. The optimized mass for each target nucleus is finally derived using Eqs. (12) and (13).

Bandwidth parameters h_δ , h_Z , and h_N in Eqs. (9)-(11) depend on the distribution of original mass residuals δ_{pre} . Larger bandwidth parameters yield smoother, more reliable calculations but may dilute fine variations caused by physical effects. Smaller bandwidth parameters capture subtle residual changes more precisely but are susceptible to noise. In the complete dataset, most δ_{pre} values range from 0 to 20 MeV, while differences in δ_{pre} among isotopes and isotones mostly range from 0 to 5 MeV. Selecting bandwidth parameters within these ranges optimizes prediction performance.

Based on distribution characteristics of δ_{pre} from six theoretical models, final parameters are selected as $h_\delta = 5.00$ MeV, $h_Z = 1.00$ MeV, and $h_N = 2.00$ MeV to maximize physical effect capture while maintaining strong generalization.

demonstrates CBP's global optimization capability. σ_{pre} represents the standard deviation of original theoretical model predictions for even-even nuclei in the complete set, while σ_{post} gives the standard deviation after CBP correction. The improvement factor $\Delta = (\sigma_{\text{pre}} - \sigma_{\text{post}})/\sigma_{\text{pre}}$ quantitatively measures precision enhancement.

For HFB models with SkP and SLy4 parameters, optimized standard deviations σ_{post} are approximately 0.63 MeV and 0.80 MeV, respectively, representing about 88% improvement. For RMF models with NL3* and NLSH parameters, σ_{post} decreases to approximately 0.30 MeV and 0.58 MeV, respectively, achieving nearly 80% reduction. For semi-empirical formulas, CBP reduces σ_{post} to approximately 0.52 MeV, with improvements exceeding 60%. shows that different nuclear mass model categories exhibit different posterior standard deviations σ_{post} , and models within the same category tend to converge to similar σ_{post} values regardless of their original σ_{pre} .

Previous work applied the Naive Bayesian Probability (NBP) classifier to nuclear mass prediction by converting the problem into a classification task. K-means clustering determined residual cluster centers, with Bayes' theorem selecting the class center with maximum posterior probability as the predicted residual. In contrast, the CBP method uses kernel density estimation to determine prior and likelihood probability density functions, then applies Bayes' theorem to obtain the posterior probability density function. The expectation value

calculated across the entire residual distribution serves as the target nucleus residual estimate. By treating residuals as continuous variables and considering all residual contributions rather than discretizing them, CBP demonstrates superior optimization performance.

To visually demonstrate CBP optimization effects across regions, [Figure 1: see original paper] compares mass residuals before and after CBP correction. Left panels show original theoretical residuals, while right panels display corrected residuals for each model. CBP achieves significant corrections across all theoretical models, particularly in heavy nuclear regions and near drip lines where initial residuals were large. This phenomenon is explained by CBP's theoretical framework: building upon global theoretical descriptions, CBP employs statistical methods to consider regional correlation effects among nuclei with the same proton number Z or neutron number N , enabling effective correction of original theoretical results. In light nuclear regions, corrected mass precision decreases slightly due to more discrete original residual distributions, fewer nucleons, and weaker regional correlations between neighboring nuclei and target nuclei. As more nuclear masses are precisely measured experimentally, CBP's optimization capability is expected to improve significantly.

2.2 Extrapolation Capability of CBP Method

Compared to global description, model extrapolation stability carries greater uncertainty. This section investigates CBP's extrapolation capability. The learning set comprises 768 even-even nuclei from AME2003, while the validation set includes 100 newly measured even-even nuclei from AME2020. Prior and likelihood probabilities are calculated using learning set data, then CBP predicts masses for the 100 validation nuclei. Bandwidth parameters h_δ , h_Z , and h_N in extrapolation match those from global optimization in Section 2.1.

shows standard deviations σ_{pre} and σ_{post} for training and validation sets, along with improvement factors Δ . For semi-empirical formulas, the WS* model's training set standard deviation is 0.52 MeV, reducing to 0.31 MeV after CBP optimization, while validation set standard deviation decreases from 0.98 MeV to 0.58 MeV, both achieving 41% improvement. Comparing improvement factors between training and validation sets demonstrates CBP's strong stability for unknown data.

Beyond semi-empirical formulas, CBP exhibits good extrapolation capability for microscopic models like HFB and RMF. Before CBP optimization, HFB and RMF models show only slight standard deviation increases in the validation set compared to the training set, indicating inherent extrapolation ability. After CBP optimization, both models' validation set standard deviations reduce to approximately 1.50 MeV, with improvement factors strongly consistent with training set results, confirming CBP's robustness in extrapolation.

CBP's optimization in the validation set is slightly lower than in the training set because most validation nuclei lie at the nuclear chart edges, where fewer nuclei

share identical proton and neutron numbers with training set nuclei, reducing prediction precision. As more nuclear masses are measured precisely across the chart, CBP accuracy will further improve.

Results demonstrate CBP's strong extrapolation capability for accurately predicting unknown nuclear masses, attributed to two factors. First, theoretical mass models based on nuclear interactions effectively capture fundamental physical principles of atomic nuclei, describing overall mass variation trends. Second, CBP can probe finer nuclear structures and unknown physical effects. This detailed capture capability enables CBP to optimize theoretical predictions, and show that CBP inherits theoretical model advantages while supplementing local correlation characteristics between nuclei, providing reliable predictions in regions lacking experimental data and demonstrating potential for application to other physical quantities like charge radii.

2.3 Further Optimization with BMA Method

CBP-improved mass models exhibit excellent predictive performance near the stability line, while each theoretical model performs best in specific drip-line regions. Therefore, BMA is needed to comprehensively consider various model advantages. BMA evaluates each model's performance on benchmark nuclei to assign weights, balancing predictive differences among theoretical models. To assess BMA reliability, this section predicts the two-neutron drip line for Ca isotopes.

Based on 868 even-even nuclei from the complete set, different theoretical models combined with CBP predict masses for six benchmark nuclei: ^{14}O , ^{28}Ne , ^{82}Ru , ^{112}Zr , ^{178}Pt , and ^{280}Ds , covering light to heavy regions and proton-rich to neutron-rich extremes across the nuclear chart. Corrected mass residuals δ_{corr} for these benchmark nuclei are calculated, and Gaussian distributions are constructed using Eq. (15) to evaluate each model's predictive capability. shows predicted residuals for six benchmark nuclei and model weights from BMA.

As an evaluation criterion, model weights $P(M_k|D)$ are derived from Bayes' formula. shows that NLSH, DZ10, and WS* models combined with CBP perform excellently on six benchmark nuclei and receive higher weights, while SLy4, SkP, and NL3* models show poorer performance with lower weights. Eq. (16) then optimizes predictions for 100 validation nuclei. After BMA optimization, the validation set's standard deviation decreases to 0.52 MeV, superior to any individual model's CBP-corrected result in , demonstrating higher prediction precision.

Continuing the previous discussion, this section uses BMA to predict the two-neutron drip line for Ca isotopes. [Figure 2: see original paper] shows two-neutron separation energy predictions for Ca isotopes. The solid line represents BMA's average prediction, while shaded bands indicate associated uncertainties. In known regions ($N \leq 40$), BMA predictions highly agree with experimental data, successfully capturing the neutron magic number $N = 28$. For the heav-

most discovered Ca isotope ^{60}Ca , the predicted existence probability is 1.0. In unknown regions ($N > 40$), BMA extrapolation determines the probability of nuclear existence, defined as $P_{\text{ex}}(Z, N) = P(S_{2n}(Z, N) > 0)$, representing the proportion of positive separation energies within the error band. Results are shown in the inset. For ^{74}Ca , $P_{\text{ex}} = 0.04$, indicating uncertain existence. Additionally, BMA's posterior predictions place the two-neutron drip line for Ca isotopes at ^{74}Ca with an existence probability of 0.04.

3 Conclusion

This work combines the Continuous Bayesian Estimator (CBP) and Bayesian Model Averaging (BMA) to improve six theoretical nuclear mass models. The main innovations are twofold: First, CBP introduces continuous probability density functions to deeply explore local mass relationships among nuclei with identical proton and neutron numbers. Second, BMA comprehensively considers different theoretical models' predictive performance across the nuclear chart, further improving nuclear mass prediction precision. In global optimization, CBP improves HFB models by approximately 90% and RMF and semi-empirical formulas by 70% and 50%, respectively. In extrapolation analysis, CBP improves prediction accuracy for HFB, RMF, and semi-empirical formulas by approximately 80%, 55%, and 50%, demonstrating strong robustness. Since each theoretical model exhibits different predictive performance in specific regions, BMA assigns weights based on benchmark nucleus predictions. To evaluate BMA reliability, extrapolation results for Ca isotope two-neutron separation energies are presented, predicting their two-neutron drip line. Overall, CBP and BMA significantly improve nuclear mass descriptions. Theoretical nuclear models describe main mass variation trends, while CBP combined with BMA provides reliable corrections. Results show that CBP and BMA can support mass predictions for exotic nuclei near drip lines and apply to other nuclear research fields such as nuclear charge radii, nuclear reactions, and nuclear astrophysics.

Author Contributions: Tan Kaizhong performed calculations and drafted the manuscript; Gao Wanqing organized literature and planned manuscript structure; Liu Jian guided and reviewed the work.

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