Improvement of nuclear semi-empirical mass formula by including shell effect

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Date: 2025-04-16T09:21:15+00:00

Abstract

Shell effect plays an important role in nuclear mass predictions especially for the nuclei around the magic numbers. In this study, a new mass formula with semi-empirical shell correction terms is constructed to improve the mass description of the Bethe-Weizs"{a}cker (BW) formula. For nuclei with Z, $N \geqslant 8$, the root mean square (rms) deviation of the new formula with respect to the latest nuclear mass evaluation dataset AME2020 is 0.887 MeV, inducing a 72.23% reduction compared to the rms deviation of 3.194 MeV for the formula BW. The deviations between the theoretical predictions and the experimental data are within 1.5 MeV for 91.90% of the nuclei. In addition, the new formula significantly improves the predictions of the binding energies for magic nuclei, the rms deviation of the new formula for the binding energy of magic nuclei is only 1.065 MeV, which is a 80.80% reduction compared to that of the formula BW.

Full Text

Preamble

Improvement of the Nuclear Semi-Empirical Mass Formula by Including Shell Effects

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(Dated: April 16, 2025)

Shell effects play an important role in nuclear mass predictions, especially for nuclei around magic numbers. In this study, we construct a new mass formula with semi-empirical shell correction terms to improve the mass description of the Bethe-Weizsäcker (BW) formula. For nuclei with Z, N > 8, the root-mean-square (rms) deviation of the new formula relative to the latest nuclear mass evaluation dataset AME2020 is 0.887 MeV, representing a 72.23% reduction compared to the rms deviation of 3.194 MeV for the BW formula. The deviations between theoretical predictions and experimental data are within 1.5 MeV for 91.90% of nuclei. In addition, the new formula significantly improves predictions of binding energies for magic nuclei; the rms deviation for magic nuclei is only 1.065 MeV, which is an 80.80% reduction compared to that of the BW formula.

PACS numbers: 21.10.Dr, 31.15.bu

Introduction

Nuclear mass is one of the most fundamental physical quantities in nuclear physics [**?**, **?**], widely used to extract nuclear effective interactions [**?**] and various nuclear structure information such as pairing correlation [**?**], shell effects [**?**, **?**], and deformation [**?**, **?**]. From nuclear mass, one can easily calculate various nucleon separation energies, reaction and decay energies, which determine the positions of the drip lines [**?**] and serve as key inputs for rapid neutron-capture process (r-process) simulations.

The uncertainty in nuclear mass has a large influence on β-decay half-lives [**?**] and neutron capture rates [**?**], significantly affecting abundance distributions in r-process simulations [**?**]. In conclusion, nuclear mass plays an important role in both nuclear physics and nuclear astrophysics [**?**, **?**].

Various theoretical models predict more than 7000 nuclei on the nuclear chart [**?**], but only about 3000 nuclear masses have been experimentally measured [**?**], and many nuclear masses involved in r-process simulations remain unmeasured. This increases the necessity of developing mass models with reliable extrapolation capabilities. Currently, various mass models have been developed with rms deviations ranging from 0.3 to 3 MeV. There are mainly three kinds of nuclear mass models: macroscopic, microscopic, and macroscopic-microscopic models.

The earliest nuclear mass model was the traditional liquid-drop model, i.e., the Bethe-Weizsäcker (BW) semi-empirical formula, which is a macroscopic model that treats the nucleus as a charged liquid droplet [**?**, **?**]. Since it does not account for microscopic shell corrections, large deviations exist between nuclear mass predictions and experimental data around magic nuclei. The BW formula was subsequently developed by including various correction terms [**?**, **?**], with the improved version achieving an rms deviation of about 1.6 MeV. Based on the macroscopic model, the Strutinsky method [?] is used to extract shell correction energies, leading to the development of macroscopic-microscopic models. The finite-range droplet model (FRDM) [?, ?] has an rms deviation of about 0.6 MeV relative to experimental mass data and is often used as input for r-process simulations. In addition, a series of Weizsäcker-Skyrme (WS) models have been developed by accounting for isospin effects [?], mirror nuclei constraints [?], and surface diffuseness effects (WS4) [?], with the WS4 mass model achieving an rms deviation of about 0.3 MeV.

However, macroscopic-microscopic models must ensure self-consistency between macroscopic and microscopic terms. Microscopic models study atomic nuclei at the nucleon level and can provide various nuclear ground-state properties including nuclear mass within a uniform framework [?], and are therefore often believed to have more reliable extrapolation capabilities.

In a non-relativistic framework, a series of Hartree-Fock-Bogoliubov (HFB) microscopic mass models have been developed with rms deviations of 0.5–0.8 MeV using Skyrme [?, ?] or Gogny forces [?]. Microscopic mass models in the relativistic framework include relativistic mean-field (RMF) models [?, ?], relativistic continuum Hartree-Bogoliubov (RCHB) [?], and deformed relativistic Hartree-Bogoliubov theory in continuum (DRHBc) [?, ?, ?]. For these relativistic microscopic mass models, although the accuracy with respect to experimental data now achieves nearly 1 MeV [?, ?, ?], these models are still very time-consuming for large-scale systematic calculations.

In recent years, with the rapid development of artificial intelligence, machine learning (ML) methods have also been widely used to study nuclear properties [?], such as β-decay half-lives [?, ?], α-decay half-lives [?], fission yields [?, ?], charge radii [?, ?], and nuclear reaction cross sections [?]. Currently, ML methods such as Bayesian neural network (BNN) [?], kernel ridge regression (KRR) [?, ?], Light Gradient Boosting Machine (LightGBM) [?], and Gaussian process [?] have been used to study nuclear mass, with mass models based on these ML methods achieving rms deviations of about 0.1 MeV relative to experimental data. Although machine learning models have high prediction accuracy in known regions, the physical basis of ML methods is unclear, which may affect their extrapolation abilities [?]. For example, radial basis functions (RBF) [?, ?] and KRR methods were found to have reliable extrapolation distances not far from the known region [?].

This study focuses on constructing shell correction terms to improve the prediction ability of the semi-empirical mass formula for magic nuclei. Each term in the semi-empirical mass formula has a clear physical meaning, making it easy to identify the specific contribution of each term to the binding energy. In addition, its high efficiency and low computational cost enable calculation of all nuclear masses in a very short time, which is highly useful for systematically studying uncertainties and sensitivities in the r-process. The new mass formula proposed in this work has an rms deviation of 0.887 MeV relative to experimental data in AME2020 [?] for nuclei with Z, N $>$ 8, representing a 72.23%

reduction compared to the semi-empirical BW formula and 45.42% lower than the rms deviation of the empirical formula proposed in Ref. [**?**], with mass predictions significantly improved particularly for magic nuclei.

The paper is organized as follows. Section II introduces the BW semi-empirical mass formula and the construction of shell correction terms. Results and discussion are presented in Section III. Finally, summary and perspectives are given in Section IV.

Theoretical Framework

The traditional semi-empirical mass formula BW accounts for volume energy, surface energy, Coulomb energy, and symmetry energy. The binding energy B for a nucleus with proton number Z and neutron number N (mass number $A = Z + N$) can be calculated from these four terms:

$$B = a_{vA} + a_{sA}^{2/3} + a_{cZ}^{2A^{-1/3}} + a_{\mathrm{sym}}(N-Z)^{2A^{-1}}, \tag{1}$$

where a_i denotes free parameters determined by fitting experimental nuclear masses.

In Ref. [**?**], the exchange Coulomb term $a_{\mathrm{xc}}Z^{4/3}A^{-1/3}$, the Wigner term $a_w|N-Z|A^{-1}$, the pairing term $\delta a_{pA}^{-1/2}$, the surface symmetry term $a_{\mathrm{st}}(N-Z)^{2A^{-4/3}}$, the curvature term $a_{rA}^{1/3}$, and shell correction terms $a_{mP}+b_{mP}^2$ based on the BW formula are added. In this paper, this model is denoted as the mass formula BWK. In the above expressions, δ and P are given by:

$$\delta = (-1)^Z + (-1)^N,$$

$$P = \frac{\nu_p \nu_n}{\nu_p + \nu_n},$$

where ν_p and ν_n are the numbers of valence nucleons, i.e., the differences between the nucleon numbers Z and N and the nearest magic number (the proton and neutron magic numbers are taken to be 2, 8, 20, 28, 50, 82, 126 and 2, 8, 20, 28, 50, 82, 126, 184 as in Ref. [**?**]). The new formula obtained by removing the shell correction terms $a_{mP} + b_{mP}^2$ from formula BWK is denoted as formula BWK*.

In Fig. 1, we investigate the effect of the shell correction terms $a_{mP} + b_{mP}^2$ in formula BWK on binding energy predictions. In general, this term provides a large improvement in binding energy predictions, reducing the rms deviation by about 0.8 MeV. In particular, it improves predictions for some deformed nuclei, such as those in the regions $32 \le Z \le 41$ and $34 \le N \le 45$, $34 \le Z \le 47$, and $57 \le N \le 73$. In addition, formula BWK also improves prediction ability for binding energies of some magic nuclei with $N = 28, 50$.

However, the predictions of formula BWK are worse for nuclei with $Z \geq 50, 82$, overestimating experimental binding energies by more than 4 MeV, while predictions for some doubly magic nuclei are underestimated by more than 4 MeV. Moreover, the shell correction energies between semi-magic and doubly magic nuclei should be different, while the shell correction terms $a_{mP}+b_{mP}^2$ are always 0 for both semi-magic and doubly magic nuclei. Therefore, it is necessary to construct a new shell correction term that reflects the difference in shell correction energies between semi-magic and doubly magic nuclei.

To construct appropriate shell correction terms for magic nuclei, we study the differences between experimental binding energies of magic nuclei and BWK predictions as a function of the number of valence nucleons, shown in Fig. 2. The binding energy residuals of the semi-empirical formula BWK are found to have an approximate linear relationship with the number of valence nucleons when the mass number $A > 56$.

Therefore, the linear term of valence nucleons $c_m(\nu_n+\nu_p)$ is used to describe the residuals of semi-magic nuclear binding energies. The new formula is denoted as F1, with the form:

$$B = a_{vA}+a_{sA}^{2/3}+a_{cZ}^{2A^{-1/3}}+a_{\mathrm{sym}}(N-Z)^{2A^{-1}}+\delta a_{pA}^{-1/2}+a_{\mathrm{xc}}Z^{4/3}A^{-1/3}+a_w|N-Z|A^{-1}+a_{\mathrm{st}}(N-Z)^{2A^{-4/3}}+a_{rA}^{1/3}+a_{mP}+$$

The exponential term $e_{m1}e^{e_{m2}(\nu_n^2+\nu_p^2)}$ is introduced to describe such residuals for doubly magic nuclei, similar to Refs. [**?**, **?**], denoted as F2. *Isospin dependence is further introduced in formula F2* as in Ref. [**?**], and the new formula is denoted as F2. The specific expressions for semi-empirical formulas F2* and F2 are:

$$B = a_{vA}+a_{sA}^{2/3}+a_{cZ}^{2A^{-1/3}}+a_{\mathrm{sym}}^{I}I_s^{2Af}+\delta_{np}a_{pA}^{-1/3}+a_{\mathrm{xc}}Z^{4/3}A^{-1/3}+a_{rA}^{1/3}+a_{mP}+b_{mP}^2+c_m(\nu_n+\nu_p)+e_{m1}e^{e_{m2}(\nu_n^2+\nu_p^2)},$$

where a_{sym}^I, I, and f_s are defined as:

$$a_{\mathrm{sym}}^I = c_{\mathrm{sym}}\left(1 - k\frac{N-Z}{A}\right),$$

$$I = \frac{N-Z}{A},$$

$$f_s = 1 + \kappa_s\left(\left(I - \frac{0.4}{A^{1/3}}\right)^2 - \frac{I^4}{2+|I|A}\right)A^{1/3}.$$

From Fig. 1(b), it is seen that the residuals of doubly magic nuclei are negative in the light-mass region, positive in the heavy-mass region, and near zero in the medium-mass region. This means that the residuals of binding energies are different for magic nuclei in different regions. To describe the differences between magic nuclei in different regions, a δ_{shell} factor is introduced in the coefficient of the exponential term, and the new formula obtained is named BWN, with the expression:

$$B = a_{vA}+a_{sA}^{2/3}+a_{cZ}^{2A^{-1/3}}+a_{\text{sym}}^{I}I_s^{2Af}+\delta_{np}a_{pA}^{-1/3}+a_{\text{xc}}Z^{4/3}A^{-1/3}+a_{rA}^{1/3}+a_{mP}+b_{mP}^{2}+c_m(\nu_n+\nu_p)+e_{m1}\delta_{\text{shell}}e^{e_{m2}(\nu_n^2+\nu_p^2)}$$

where δ_{shell} is defined as:

$$\delta_{\text{shell}} = \begin{cases} -1, & Z, N \in [8, 24]; \\ 1, & Z \in [8, 24] \& N \in (24, 66]; \\ 1, & Z \in (24, 39] \& N \in [8, 66]; \\ 0, & \text{elsewhere.} \end{cases}$$

The parameters of each semi-empirical formula (BW, BWK*, BWK, F1, F2*, F2, and BWN) are determined by fitting to experimental data in AME2020 [**?**], as shown in Table I. The accuracy of the semi-empirical formula is evaluated by the rms deviation, defined by:

$$\sigma_{\text{rms}}(B) = \sqrt{\frac{\sum(B_{\text{exp}} - B_{\text{th}})^2}{n}},$$

where B_{exp} and B_{th} are experimental and theoretical binding energies, respectively, and n is the number of experimental data for nuclei with $Z, N > 8$.

Results and Discussion

The rms deviations of binding energies for each semi-empirical formula are shown in Table I. From Table I, it is seen that the rms deviation of the newly proposed formula BWN is 0.887 MeV, which is 72.23% and 45.42% lower than the mass formulas BW and BWK, respectively. Since the rms deviations of formulas F2* and F2 are similar, isospin dependence in the symmetry energy and pairing energy terms in formula F2 does not improve accuracy in the known region, although their differences may become large in unknown regions.

Furthermore, compared to formula F2, the introduction of δ_{shell} in formula BWN can reduce the rms deviation by approximately 0.2 MeV without including additional parameters, which indicates the importance of employing different shell corrections in different mass regions.

The rms deviation can only roughly reflect the accuracy of a semi-empirical mass formula. To show more details, the differences between experimental binding energies and predictions calculated by mass formulas F1, F2*, and F2 are shown in Fig. 3.

Compared with Fig. 1(b), it can be found from Fig. 3(a) that the introduction of the linear terms $c_m(\nu_n + \nu_p)$ improves the prediction ability of the formula for nuclei with proton numbers around 50 and 82, reducing the rms deviation by about 0.4 MeV. From Fig. 3(a), it can be seen that the exponential term with a constant coefficient provides a slight improvement for some superheavy nuclei, such as nuclei with $Z > 82$ and $N > 126$, but does not significantly improve prediction accuracy for doubly magic nuclei. Furthermore, comparing Fig. 3(b) and (c), we find that the effect of isospin dependence of the symmetry energy and pairing energy term on mass description is small in the known mass region, with the rms deviation decreasing by about 0.03 MeV.

The mass description of the newly proposed mass formula BWN is compared with the mass formula BW in Fig. 4. It can be seen that the binding energy predictions of formula BW have large deviations from experimental binding energies for magic nuclei and most deformed nuclei. Around doubly magic nuclei, the predictions of mass formula BW are always underestimated by more than 4 MeV compared to experimental binding energies, while they are overestimated by more than 4 MeV in deformation regions, such as $31 \leq Z \leq 39$ and $35 \leq N \leq 47$, $38 \leq Z \leq 47$ and $55 \leq N \leq 69$, and $Z \geq 82$ and $N \geq 126$.

In addition, the binding energy residuals calculated by formula BW show odd-even staggering structures due to the lack of odd-even pairing correction, with smaller and larger differences appearing alternately.

Compared to mass formula BW, it can be seen from Fig. 4(b) that formula BWN significantly improves the description of nuclear binding energies for nuclei near magic numbers and deformed nuclei. Based on mass formula F2, mass formula BWN further accounts for differences between doubly magic nuclei in different regions by introducing δ_{shell}, significantly improving mass description in the region around doubly magic nuclei and improving prediction accuracy of nuclear binding energies in the $8 < Z < 20$, $8 < N < 20$ region. The rms deviations of mass formula BWN predictions relative to experimental binding energies are 0.887, 0.838, and 1.065 MeV for the three datasets: $Z, N > 8$; $A > 60$; and magic nuclei, respectively, which represents reductions of 72.23%, 73.35%, and 80.08% compared to mass formula BW.

In Fig. 5, the differences between experimental binding energies and predictions of the three mass formulas BW, BWK, and BWN are shown as functions of proton number and neutron number. The differences between experimental binding energies and predictions of mass formula BW are very large in the light nuclei region and in regions with proton numbers $Z = 50, 82$ or neutron numbers $N = 50, 82, 126$, even reaching more than 15 MeV. In addition to the region around traditional magic numbers, large differences between experimental binding energies and BW predictions are also found for some nuclei, such as those around $Z = 34, 90$ or $N = 40, 145$. By including other correction terms, mass formula BWK reduces binding energy residuals for most nuclei, but its predictions are not more accurate than BW for some nuclei, e.g., those with $100 \leq N \leq 120$.

Based on mass formula BWK, BWN is obtained by including new shell correction terms, further improving nuclear mass descriptions for magic nuclei. The rms deviations of formulas BW and BWK with respect to magic nuclei are 5.346 MeV and 2.729 MeV, respectively, while the corresponding rms deviation of mass formula BWN is only 1.065 MeV, representing reductions of 80.80% and 60.97% compared to formulas BW and BWK, respectively. In addition, the differences between experimental binding energies and BWN predictions are almost always within 1.5 MeV. The percentage of nuclei for which predictions of BW, BWK, and BWN deviate from experimental data by less than 1.5 MeV is 41.88%, 70.21%, and 91.90%, respectively.

Summary and Perspectives

In summary, a new semi-empirical mass formula is proposed by including new shell correction terms. The shell correction terms in the new mass formula contain three components: the quadratic polynomial of P, the linear term of valence nucleons, and the exponential term of valence nucleons. The quadratic polynomial terms of P improve binding energy predictions for most deformed nuclei and some magic nuclei. The linear term for the number of valence nucleons is used to improve the prediction ability of the mass formula for semi-magic nuclei, especially nuclei with proton numbers near 50 and 82, reducing the rms deviation by approximately 0.4 MeV. The introduction of an exponential term with a constant coefficient did not obviously improve the prediction ability of the mass formula for doubly magic nuclei, but binding energy residuals were significantly reduced for doubly magic nuclei by accounting for differences between different doubly magic nuclei, with the exponential term reducing the rms deviation by about 0.2 MeV.

Compared with mass formulas BW and BWK, the rms deviation of the new mass formula relative to experimental data for nuclei with $Z, N > 8$ is reduced by 72.23% and 45.42%, respectively, falling to 0.887 MeV. The rms deviation of the newly proposed formula with respect to magic nuclei is only 1.065 MeV, representing reductions of 80.80% and 60.97% compared to formulas BW and BWK, respectively. In addition, nuclei whose experimental binding energies deviate from predictions of mass formulas BW, BWK, and the new mass formula by less than 1.5 MeV account for 41.88%, 70.21%, and 91.90% of the total number of nuclei, respectively.

In conclusion, the new mass formula significantly improves the description of nuclear binding energies, especially for magic nuclei. In the future, we will further consider the effect of deformation on binding energy. In addition, since the semi-empirical formula enables large-scale calculations of nuclear masses in a short time, it is well suited for studies of the sensitivity of r-process abundances to nuclear masses, which could deepen our understanding of the origin of heavy elements.

Acknowledgments

This work was partly supported by the National Natural Science Foundation of China under Grants No. 11935001, No. 11875070, and No. 12375109, the Anhui project (Z010118169), the Key Research Foundation of Education Ministry of Anhui Province under Grant No. 2023AH050095, the University Synergy Innovation Program of Anhui Province under Grant No. GXXT-2023-007, and the University Natural Science Outstanding Youth Research Projects of Anhui Province under Grant No. 2022AH030039.

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