Further improvements on a global nuclear mass model

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Abstract

The semi-empirical macroscopic-microscopic mass formula is further improved by considering some residual corrections. The rms deviation from 2149 known nuclear masses is significantly reduced to 336 keV, even lower than that achieved with the best of the Duflo-Zuker models. The α-decay energies of super-heavy nuclei, the Garvey-Kelson relations and the isobaric multiplet mass equation (IMME) can be reproduced remarkably well with the model, and the predictive power of the mass model is good. With a systematic study of 17 global nuclear mass models, we find that the quadratic form of the IMME is closely related to the accuracy of nuclear mass calculations when the Garvey-Kelson relations are reproduced reasonably well. Fulfilling both the IMME and the Garvey-Kelson relations seems to be two necessary conditions to improve the quality of the model prediction. Furthermore, the α-decay energies of super-heavy nuclei should be used as an additional constraint on the global nuclear mass models.

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I. INTRODUCTION

The precise calculation for nuclear masses is of great importance for not only nuclear physics but also nuclear astrophysics. In nuclear physics, the synthesis of super-heavy nuclei [1–3] and nuclear symmetry energy [4, 5] attracted much attention in recent years. Accurate predictions for the shell corrections and $\alpha$-decay energies of super-heavy nuclei are urgently required for the synthesis of new super-heavy nuclei. Simultaneously, nuclear masses include important information on nuclear symmetry energy [6, 7] which closely relates to the structure of nuclei and the dynamical process of nuclear reactions. In addition, the r-process abundances in nuclear astrophysics depend strongly on the nuclear masses of extremely neutron-rich nuclei and the shell-structure data of neutron magic nuclei. Some nuclear mass models have been developed with rms deviations of about several hundreds to a thousand keV with respect to all known nuclear masses. The most successful global mass models include: 1) various macroscopic-microscopic mass models such as the finite range droplet model (FRDM) [8], the extended Bethe-Weizsäcker (BW2) formula [9] and the Weizsäcker-Skyrme (WS) mass models proposed very recently by Wang et al. [10, 11]; 2) various microscopic mass models based on the mean-field concept such as the non-relativistic Hartree-Fock-Bogoliubov (HFB) approach with the Skyrme energy-density functional [12] or the Gogney forces and the relativistic mean-field (RMF) model [13]; and 3) the Duflo-Zuker (DZ) mass models [14, 15] which are successful for describing known masses, with an accuracy at the level of 360 keV. For known masses, the predictions from these global mass models are close to each other. However, for neutron drip line nuclei and super-heavy nuclei, the differences of the calculated masses from these models are quite large. It is therefore necessary to perform a systematic study of these models to check the reliability for extrapolations.

Besides the global mass models, some local relations and equations such as the isobaric multiplet mass equation (IMME) [16, 17], the Garvey-Kelson (GK) relations [18, 19] and the residual proton-neutron interactions [20, 21] are used to analyze the isospin-symmetry breaking effects and the consistency of nuclear mass predictions. It is thought that the binding energies of extremely proton-rich nuclei can be predicted at the level of $100 \sim 200$ keV based on the IMME [16]. As the IMME is a basic prediction leading from the isospin concept, testing the validity of this equation is of fundamental importance. On the other
hand, it is shown that the GK relations which are obtained from an independent-particle picture and the charge-symmetry of nuclear force, are satisfied to a very high level of accuracy by known masses, with an rms deviation of about 100 keV [19]. It is of crucial importance to incorporate these local relations and equations in the global nuclear mass models for exploring the missing physics and the constraints in the models.

In our previous works [10, 11], we proposed a semi-empirical nuclear mass formula based on the macroscopic-microscopic method together with the Skyrme energy-density functional, with an rms deviation of 441 keV for 2149 known masses. The isospin and mass dependence of the model parameters such as the symmetry energy coefficient and the constraint between mirror nuclei from the isospin symmetry in nuclear physics play an important role for improving the accuracy of the mass calculation. In this work, the formula will be further improved by considering some residual corrections of nuclei. With some empirical considerations for these residual corrections, we find both the precision and the consistency of the mass formula can be significantly improved. The paper is organized as follows: In Sec. II, the mass formula and some corrections are briefly introduced. In Sec. III, calculated nuclear masses from the proposed model are presented and compared to the results from other mass models. In Sec. IV, a number of global nuclear mass models are systematically tested by using the Garvey-Kelson relations and the IMME. Finally, a summary is given in Sec. V.

II. THE NUCLEAR MASS MODEL AND SOME CORRECTIONS

In this mass formula, the total energy of a nucleus is written as a sum of the liquid-drop energy, the Strutinsky shell correction $\Delta E$ and the residual correction $\Delta_{\text{res}}$.

$$E(A, Z, \beta) = E_{\text{LD}}(A, Z) \prod_{k \geq 2} (1 + b_k \beta_k^2) + \Delta E(A, Z, \beta) + \Delta_{\text{res}}.$$  \hspace{1cm} (1)

The liquid-drop energy of a spherical nucleus $E_{\text{LD}}(A, Z)$ is described by a modified Bethe-Weizsäcker mass formula,

$$E_{\text{LD}}(A, Z) = a_v A + a_s A^{2/3} + E_C + a_{\text{sym}} I^2 A + a_{\text{pair}} A^{-1/3} \delta_{np} + \Delta_{\text{IV}}$$  \hspace{1cm} (2)

with the isospin asymmetry $I = (N - Z)/A$, the Coulomb energy,

$$E_C = a_c \frac{Z^2}{A^{1/3}} \left(1 - 0.76 Z^{-2/3}\right)$$  \hspace{1cm} (3)
FIG. 1: (Color online) (a) Positions of some known doubly-magic nuclei (squares). The stars denote the predicted tetrahedral doubly-magic nuclei in Refs. [23, 24]. (b) Shell corrections of nuclei with WS [10]. The solid line shows the position of $N = 1.37Z + 13.5$.

and the symmetry energy coefficient,

$$a_{\text{sym}} = c_{\text{sym}} \left[ 1 - \frac{\kappa}{A^{1/3}} + \frac{\xi}{2} - \frac{|I|}{2 + |I|A} \right].$$  \hfill (4)

The $a_{\text{pair}}$ term empirically describes the pairing effect (see Ref. [10] for details). The terms with $b_k$ describe the contribution of nuclear deformation (including $\beta_2$, $\beta_4$ and $\beta_6$) to the macroscopic energy. Mass dependence of the curvatures $b_k$ in Eq. (1) is written as [10],

$$b_k = \left( \frac{k}{2} \right) g_1 A^{1/3} + \left( \frac{k}{2} \right)^2 g_2 A^{-1/3},$$  \hfill (5)

according to the Skyrme energy-density functional, which greatly reduces the computation time for the calculation of deformed nuclei.

In addition, we propose an empirical correction term $\Delta W$ in $E_{\text{LD}}$ to consider the Wigner-like effect of heavy nuclei [22] which is due to the approximate symmetry between valance-proton and valance-neutron. In [10, 11], we found that some heavy doubly-magic nuclei surprisingly lie along a straight line $N = 1.37Z + 13.5$ (see Fig.1), which is called shell stability line of heavy nuclei. Furthermore, some predicted tetrahedral doubly-magic nuclei [23, 24] [stars in Fig.1(a)] also lie near the line. The shell corrections of nuclei obtained with WS [10] are shown in Fig.1(b), and they are approximately symmetric along the shell stability line, i.e. the shell correction of doubly-magic nucleus $^{164}\text{Pb}$ is close to that of $^{176}\text{Sn}$. In other words, the change of the shell energy by adding several neutrons to the...
doubly-magic nucleus $^{208}\text{Pb}$ is close to that by adding several protons to $^{208}\text{Pb}$ because of the charge-independence of nuclear force and the fact that the Coulomb interaction is weak relative to the strong interaction. To consider the symmetry and interaction between valance-proton and valance-neutron, we phenomenologically write the Wigner-like term as,

$$
\Delta_W = c_w \left( e^{\|I\|} - e^{-\|\eta\|} \right).
$$

(6)

Where, $\eta = \frac{\Delta Z \Delta N}{Z_m}$ denotes the effective distance of a nucleus to the shell stability line. The values of $\Delta Z$, $\Delta N$ and $Z_m$ are uniquely determined by a rectangle [see the green rectangle in Fig.1(a)] based on the position of a nucleus under consideration and the shell stability line. Similar to the known Wigner effect causing a cusp for light nuclei near the $N = Z$ line, the Wigner-like term $\Delta_W$ causes a cusp for heavy nuclei limited to the close vicinity of the shell stability line, which reduces the rms deviation with respect to masses by about 5%.

The microscopic shell correction

$$
\Delta E = c_1 E_{sh} + |I| E'_{sh}
$$

(7)

is obtained with the traditional Strutinsky procedure [25] by setting the order $p = 6$ of the Gauss-Hermite polynomials and the smoothing parameter $\gamma = 1.2\hbar \omega_0$ with $\hbar \omega_0 = 41A^{-1/3}$ MeV. $E_{sh}$ and $E'_{sh}$ denote the shell energy of a nucleus and of its mirror nucleus, respectively. The $|I|$ term in $\Delta E$ is to take into account the mirror nuclei constraint [11] from the isospin symmetry, with which the accuracy of the mass model can be significantly improved (by 10%). The single-particle levels are obtained under an axially deformed Woods-Saxon potential [26]. Simultaneously, the isospin-dependent spin-orbit strength is adopted based on the Skyrme energy-density functional,

$$
\lambda = \lambda_0 \left( 1 + \frac{N_i}{A} \right)
$$

(8)

with $N_i = Z$ for protons and $N_i = N$ for neutrons, which strongly affects the shell structure of neutron-rich nuclei and super-heavy nuclei.

Some other residual corrections caused by the microscopic shell effect are empirically written as a sum of three terms,

$$
\Delta_{\text{res}} = \Delta_M + \Delta_P + \Delta_T.
$$

(9)

The first term $\Delta_M$ is to further consider mirror nuclei effect. In our previous work [11], we found that the shell correction difference $|\Delta E - \Delta E'|$ between a nucleus and its mirror
nucleus is small due to the isospin symmetry in nuclear physics. Here, we empirically write

$$\Delta_M = c_2(S + S_1)(1 - I^2A),$$  \hspace{1cm} (10)

with

$$S = \frac{(\Delta E - \Delta E')^2}{T(T+1)}. \hspace{1cm} (11)$$

Here, $T = \left|\frac{N-Z}{2}\right|$ denotes the isospin of a nucleus, and we set $S = 0$ for nuclei with $N = Z$. $S_1$ is the corresponding value of a neighboring isobaric nucleus $(A, Z_1)$ with $Z_1 = Z + 1$ for $N < Z$ cases and $Z - 1$ for $N \geq Z$ cases. The $\Delta_M$ term effectively describes the residual mirror nuclei and isospin effect in nuclei and significantly improves the accuracy of mass calculation by about 50 keV.

The second term $\Delta_P$ further considers the residual pairing corrections of nuclei which may be phenomenologically given by the second differences of the masses. That is, in addition to the $a_{\text{pair}}$ term in $E_{LD}$ for describing the pairing correction, we further consider the term

$$\Delta_P = \frac{1}{2} \frac{\partial^2 E_{\text{sh}}}{\partial A^2} \bigg|_T$$

with a step size of $\Delta A = 2$ in the calculations. This term improves the smoothness of the mass surface assumed in the Garvey-Kelson relations [18], and simultaneously reduces the rms deviation by about 4% and 6% with respect to the masses and the neutron separation energies, respectively. In addition, for describing the influence of triaxial (or tetrahedral) deformation [23, 24] effectively, we proposed a parameterized formula in our previous work [11]. Here the formula is slightly extended to include the contribution of the protons, $\Delta_T = -0.7 \left[ \cos \left(2\pi \frac{N}{10}\right) + \cos \left(2\pi \frac{N}{20}\right) + \cos \left(2\pi \frac{Z}{52}\right) \right] A^{-1/3}$ MeV.

**III. CALCULATED MASSES FROM THE MODEL**

Based on the 2149 ($N$ and $Z \geq 8$) measured nuclear masses AME2003 [27], we obtain the optimal model parameters which is labelled as WS3 and listed in Table I. We show in Table II the rms deviations $\sigma(M)$ between the 2149 experimental masses and predictions of some models (in keV). $\sigma(S_n)$ denotes the rms deviation to the 1988 measured neutron separation energies $S_n$. $\sigma(Q_\alpha)$ in Table II denotes the rms deviation with respect to the $\alpha$-decay energies of 46 super-heavy nuclei ($Z \geq 106$) [11]. $\sigma(GK)$ presents the rms deviation with respect to the GK mass estimates and $\sigma(b)$ denotes the rms deviation from the formula
### TABLE I: Model parameters of the mass formula WS3.

| Quantity | Value  | Quantity | Value  |
|----------|--------|----------|--------|
| $a_v$ (MeV) | $-15.5485$ | $g_1$ | $0.01037$ |
| $a_s$ (MeV) | $17.4663$ | $g_2$ | $-0.5071$ |
| $a_c$ (MeV) | $0.7128$ | $V_0$ (MeV) | $-45.2092$ |
| $c_{\text{sym}}$ (MeV) | $29.1174$ | $r_0$ (fm) | $1.3848$ |
| $\kappa$ | $1.3437$ | $a$ (fm) | $0.7617$ |
| $\xi$ | $1.1865$ | $\lambda_0$ | $26.6744$ |
| $a_{\text{pair}}$ (MeV) | $-6.2299$ | $c_1$ | $0.6454$ |
| $c_w$ (MeV) | $1.0490$ | $c_2$ (MeV$^{-1}$) | $1.6179$ |

### TABLE II: rms $\sigma$ deviations between data AME2003 [27] and predictions of some models (in keV).

| | ETF2[28] | BW2[9] | FRDM[8] | HFB-17[12] | DZ10[14] | WS[10] | WS*[11] | DZ31[14] | DZ28[15] | WS3 |
|---|---|---|---|---|---|---|---|---|---|
| $\sigma(M)$ | $3789$ | $1594$ | $656$ | $581$ | $561$ | $516$ | $441$ | $362$ | $360$ | $336$ |
| $\sigma(S_n)$ | $1300$ | $586$ | $399$ | $506$ | $342$ | $346$ | $332$ | $299$ | $306$ | $286$ |
| $\sigma(Q_\alpha)$ | $557$ | $1233$ | $566$ | $-$ | $916$ | $284$ | $263$ | $1052$ | $936$ | $248$ |
| $\sigma(GK)$ | $24$ | $129$ | $337$ | $496$ | $100$ | $151$ | $165$ | $115$ | $133$ | $131$ |
| $\sigma(b)$ | $2734$ | $759$ | $-$ | $-$ | $870$ | $283$ | $450$ | $630$ | $-$ | $449$ |

The line $\sigma(M)$ refers to all the 2149 measured masses, the line $\sigma(S_n)$ to the 1988 measured neutron separation energies $S_n$, the line $\sigma(Q_\alpha)$ to the $\alpha$-decay energies of 46 super-heavy nuclei. $\sigma(GK)$ presents the rms deviation with respect to the GK mass estimates. $\sigma(b)$ denotes the rms deviation from the formula [16] $b_{\text{fit}} = 0.710A^{2/3} - 0.946$ for the $b$ coefficients of 179 neutron drip line nuclei.

ETF2 denotes the extended Thomas-Fermi approach including all terms up to second order in the spatial derivatives [28] together with the Skyrme force SkP [29], in which the deformations and shell corrections of nuclei are not involved. BW2 means the extended Bethe-Weizsäcker formula [9] in which the shell corrections of nuclei are described as a function of valence-nucleon number assuming the magic numbers being 2, 8, 20, 28, 50, 82, 126, 184. FRDM and HFB-17 denote the finite-range droplet model [8] and the latest Hartree-Fock-Bogoliubov (HFB) model with the improved Skyrme energy-
FIG. 2: (Color online) (a) Deviations of calculated nuclear masses from the experimental data as a function of neutron number. The squares and the solid circles denote the results of FRDM and WS3, respectively. (b) The same as (a), but with the results of DZ28 model for comparison.

density functional [12], respectively. DZ10, DZ28 and DZ31 denote the Duflo-Zuker mass models with 10, 28 and 31 parameters, respectively [14, 15].

The rms deviation from the 2149 masses with WS3 is remarkably reduced to 336 keV, much smaller than the results from the finite range droplet model (FRDM) and the latest HFB-17 calculations, even lower than that achieved with the best of the Duflo-Zuker models. In Fig. 2, we show the deviations from the experimental masses as a function of neutron number. The squares and the solid circles in Fig.2(a) denote the results from the FRDM and WS3, respectively. The accuracy of mass calculation especially for light nuclei is significantly improved in the WS3 model. The open circles in Fig.2(b) denote the results from the DZ28 model. Compared to the DZ28 model, the rms deviations from masses and neutron separation energies are reduced by 7%. To further test the extrapolation of our mass model, we also calculate the average deviation from four very recently measured masses for $^{63}$Ge, $^{65}$As, $^{67}$Se, and $^{71}$Kr [30]. Our result is 118 keV, much smaller than the results from DZ28 (321 keV) and FRDM (680 keV).

It is known that the $\alpha$-decay energies of super-heavy nuclei [1] have been measured with a high precision, which provides us with useful data for testing our mass model. The rms
FIG. 3: (Color online) $\alpha$-decay energies of some super-heavy nuclei calculated with WS3 (solid curve) and DZ28 (open circles). The squares denote the experimental data taken from [11] (and references therein).

deviation $\sigma(Q_\alpha)$ with respect to the $\alpha$-decay energies of 46 super-heavy nuclei from the WS3 model is remarkably reduced to 248 keV. The difference between the calculated $\alpha$-decay energies of the super-heavy nuclei and the measured data is within $\Delta Q_\alpha = \pm 0.4$ MeV for odd-Z nuclei. The corresponding results from Sobiczewski [31] and FRDM are $\pm 0.8$ and $\pm 1.0$ MeV, respectively. Here, we would like to emphasize that the experimental data of $\alpha$-decay energies are not involved in the fit for the model parameters. We also note that the rms deviations $\sigma(Q_\alpha)$ with the extended Bethe-Weizsäcker (BW2) formula and the DZ mass models are large, which might be due to the difficulty in determining the right shell closures after $^{208}$Pb in these models where the shell corrections of nuclei are described as a function of valence-nucleon number. Fig. 3 shows the calculated $\alpha$-decay energies of some super-heavy nuclei with the WS3 (solid curve) and DZ28 models (open circles), respectively. The results from the WS3 model look much better than those from the DZ28 model, although both models give similar rms deviation for known masses.

In Fig. 4 we show the deviations of the calculated total energies of nuclei at their ground state with WS3 from the results of (a) FRDM, (b) DZ28, (c) WS* and (d) HFB-17, respectively. The shades denote the region with deviations smaller than 2 MeV. One sees that the
FIG. 4: (Color online) Deviations of the calculated nuclear total energies at ground state in this work from the results of (a) FRDM, (b) DZ28, (c) WS* and (d) HFB-17, respectively. The calculated masses with FRDM, DZ28, WS* and HFB-17 are taken from [8], [15], [11] and [12], respectively. The shades denote the region with deviations smaller than 2 MeV.

results from WS3, FRDM, DZ28 and WS* are relatively close to each other, and the results from HFB-17 model deviate obviously from WS3 calculations for extremely neutron-rich nuclei. We also note that the binding energies of super-heavy nuclei around $N \sim 170$ and $Z \sim 100 - 110$ with DZ28 are significantly larger by about 4 MeV than those with WS3, which leads to the deviations in the calculation of the $\alpha$-decay energies (see Fig. 3) between the two models. Because the predictions from different models towards the neutron-drip line tend to diverge [32], it is necessary to analyze the systematic errors from the various mass models for nuclei near the neutron drip line. In Fig. 5 we show the rms deviations with respect to the masses as a function of average neutron-separation energy $\langle S_n \rangle$ of nuclei based on the masses from different mass models. The shades present the average standard deviation errors of the measured masses [27]. One sees that the rms deviations from the FRDM, HFB-17, DZ28 and WS3 increase systematically for nuclei approaching the neutron drip line (i.e., the neutron separation energy $S_n \sim 0$), which indicates that the systematic errors for the neutron drip line nuclei from these mass models expect to be much larger.
FIG. 5: (Color online) rms deviation with respect to the masses as a function of average neutron-separation energy of nuclei. The shades present the average standard deviation errors of the measured masses [27].

The rms deviation $\sigma(M)$ from the FRDM and HFB-17 are about 1.4 and 1.0 MeV for nuclei with $S_n \approx 1$ MeV, respectively. The corresponding results from WS3 and DZ28 are about 0.8 and 0.9 MeV, respectively. The experimental errors are about 0.4 MeV for the masses of nuclei near the neutron drip line, and the tendency of the errors for both experimental data and the model calculations is similar with decreasing of $S_n$ of nuclei. For nuclei approaching the proton drip line (with large value for $S_n$), the rms deviations from DZ28 and WS3 are about 0.45 MeV, and the result from the FRDM reaches about 1 MeV. Fig. 5 indicates that the model WS3 is relatively reliable for describing the masses of nuclei far from the $\beta$-stability line.

Furthermore, to check the predictive power of various models, we follow Ref. [32] and study the quantity $Y = \frac{\sigma(2003) - \sigma(1995)}{\sigma(2003)}$, as a measure of the predictive power of the mass formulas fitted to the 1995 data. Here, $\sigma(1995)$ and $\sigma(2003)$ denote the rms deviation to the masses of the AME1995 [33] and AME2003 [27], respectively. Fig. 6 shows the values
FIG. 6: (Color online) A comparison of the predictive power of the various models. The vertical axis denotes the quantity $Y = \frac{\sigma(2003) - \sigma(1995)}{\sigma(2003)}$, as a measure of the predictive power of the mass formulas fitted to the 1995 data. Here, $\sigma(1995)$ and $\sigma(2003)$ denote the rms deviation to the masses of the AME1995 [33] and AME2003 [27], respectively. See Table II for more information.

FIG. 7: (Color online) A comparison of rms deviation with respect to the masses from AME2003 with the various models. The bars with shades are for the 2149 measured masses and the gray bars denote the rms deviations to the evaluated masses (marked by #) in AME2003. For the HFB-17 model, only the masses of nuclei with $Z \leq 110$ are involved in the calculation.
of $Y$ with various mass model listed in Table II. Large positive value for $Y$ indicates the deterioration for prediction of “new” masses in 2003 compilation. One can see from Fig. 6 that the predictive power of FRDM, HFB-17 and WS3 seems to be relatively better than those of DZ10 [14] and ETF2. In Fig. 7, we show a comparison of the rms deviation with respect to the masses from AME2003 with the various models. The bars with shades denote the rms deviation to the 2149 measured masses and the gray bars denote that to about 900 evaluated masses (marked by #) in AME2003. One sees that the predicted masses from WS3 are relatively close to the evaluated masses in AME2003, with an rms deviation of 0.8 MeV (the evaluated masses in AME2003 are not involved in the fit for the model parameters). The corresponding rms deviations from the three models BW2, DZ10 and DZ28 in which one needs to determine the magic numbers in the calculations are obviously large than the others, like the large rms deviations with respect to the $\alpha$-decay energies of super-heavy nuclei from these three models [see the values of $\sigma(Q_\alpha)$ in Table II]. Figs. 2, 3, 5 and 6 demonstrate that the proposed model in this work has a relatively high accuracy and good predictive power for a description of the masses of the drip line nuclei and the super-heavy nuclei.

IV. CONSTRAINTS ON MASS MODELS FROM LOCAL RELATIONS

In this section, we perform a systematic test of the global nuclear mass models by using the Garvey-Kelson relations and the isobaric multiplet mass equation. We mainly compare the results from the mass models mentioned previously. We first check the Garvey-Kelson (GK) relations based on the obtained mass tables from these mass models. It is known that the GK relation can not be used to cross the $N = Z$ line. Therefore, we suitably select five of the neighbors in GK relation for each nucleus to avoid crossing the $N = Z$ line. We use the following GK relations:

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

$$- M(N + 1, Z - 2) - M(N + 2, Z - 1) : \text{for } N \geq Z \text{ cases } \quad (13)$$

and

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

$$- M(N - 1, Z + 2) - M(N - 2, Z + 1) : \text{for } N < Z \text{ cases } \quad (14)$$
Here, $M(N, Z)$ denotes the mass excess of a nucleus with neutron number $N$ and charge number $Z$. $\sigma$(GK) in Table II presents the rms deviation of the calculated masses by the indicated mass models from the GK mass estimates according to Eqs.(13) and (14).

It is known that the ETF approach or the Hartree-Fock-Bogoliubov (HFB) approach [34] based on the traditional Skyrme force without further improvements describe the nuclear masses rather poorly, although the GK relations are reproduced very well. With a series of improvements on the force, the latest HFB-17 model [12] can reproduce the nuclear masses with an accuracy of 581 keV. However the deviation of the calculated masses from the GK mass estimates becomes relatively large as mentioned in [18]. This indicates that more constraints are still required for further testing the reliability of the mass models, in addition to the GK relations. In other words, fulfilling the GK relations is a necessary but not sufficient condition to improve the quality of the model prediction.

At the same time, we study the isobaric multiplet mass equation (IMME) which is widely used to study the isospin-symmetry breaking effect in nuclei. In the IMME, the binding energy ($BE$) of a nucleus is expressed as

$$BE(T, T_z) = a + bT_z + cT_z^2,$$

with $T_z = (N - Z)/2$. It is known that the IMME is valid if the Coulomb interaction and charge-nonsymmetric parts of the nucleon-nucleon interaction are weak relative to the strong interaction, and it is generally assumed that the quadratic term in the equation is adequate [4, 16, 17]. The $b$ coefficients for light nuclei can be extracted from the measured binding energies of pairs of mirror nuclei [16],

$$b = \frac{BE(T = T_z) - BE(T = -T_z)}{2T}$$

with the isospin $T = |N - Z|/2$. Based on the liquid-drop model, one can roughly estimate the value of the coefficient $b \sim a_c A^{2/3}$. Here, $a_c$ denotes the Coulomb energy coefficient in the liquid-drop model. In [16], Ormand proposed a formula

$$b_{fit} = 0.710A^{2/3} - 0.946$$

for the $b$ coefficients by fitting the experimental data of $A < 60$. In Fig. 8 (a), we show the extracted $b$ coefficients of nuclei in the IMME from mirror nuclei with $A \leq 75$ according to Eq.(16). Here, the experimental binding energies of mirror nuclei are taken from AME2003
FIG. 8: (Color online) (a) $b$ coefficients of nuclei in the IMME as a function of mass number. The solid squares and the solid curve denote the extracted results from mirror nuclei with $A \leq 75$ according to Eq.(16) and those from the empirical formula $b_{\text{fit}} = 0.710A^{2/3} - 0.946$, respectively. The solid (open) circles denote the extracted results by fitting the measured binding energies with parabolas for a series of isobaric even-$A$ (odd-$A$) nuclei. See text for details. (b) The same as (a), but with the results from some mass models for comparison. The crosses, the open circles and the filled circles denote the results for 179 neutron drip line nuclei from ETF2, DZ10 and WS3 calculations, respectively.

[27] and the four very recently measured masses for $^{63}$Ge, $^{65}$As, $^{67}$Se, and $^{71}$Kr in Ref. [30]. It seems to be that the $b$ coefficients are roughly constant for a given $A$. The solid curve denotes the results of the $b_{\text{fit}}$ from Eq.(17). For intermediate and heavy nuclei, the $b$ coefficients could be extracted by fitting the measured binding energies of a series of isobaric nuclei with parabolas. Here, we remove the shell corrections [11] and the Wigner energies (about $47|I|$ MeV) [35] of nuclei from the measured binding energies of nuclei before performing a parabolic fitting in order to eliminate the oscillations in the results. The solid (open) circles denote the extracted results for a series of isobaric even-$A$ (odd-$A$) nuclei, with 95% confidence interval given by the error bars. One can see that the trend of the $b$ coefficients with $A$ can be reasonably well described by the empirical formula $b_{\text{fit}}$, which indicates that the IMME is valid for both light and heavy nuclei in general. The residual oscillations in the $b$ coefficients might come from the deformations of nuclei.
According to the macroscopic-microscopic mass model, the binding energy of a nucleus can be expressed as

\[ BE(A, T_z) = \tilde{a} + \tilde{b} T_z + \tilde{c} T_z^2 + B_{sh} + B_{wig} + B_{def} + \ldots \]  (18)

Here, the mass-dependent coefficients \( \tilde{a} \), \( \tilde{b} \) and \( \tilde{c} \) can be directly obtained from the liquid-drop formula, and \( \tilde{b} \sim a_c A^{2/3} \). \( B_{sh} \), \( B_{wig} \) and \( B_{def} \) denote the shell correction, the Wigner energy and the deformation energy of a nucleus, respectively. From Eqs.(15) \( \sim \) (18) and Fig. 8(a), we learn that: 1) the shell correction difference between a nucleus and its mirror nucleus is small due to the isospin symmetry in nuclear physics as mentioned in our previous work [11]; 2) the Wigner energy of a nucleus equals generally to that of its mirror nucleus since it is usually expressed as a function of \(|I|\); and 3) the deformation energy of a nucleus might be close to the value of its mirror nucleus. The mirror nuclei effects from the isospin symmetry could give a strong constraint on nuclear mass models.

The crosses, the open circles and the filled circles in Fig. 8(b) denote the calculated results with Eq.(16) for 179 neutron drip line nuclei (\( Z \geq 8 \) and \( N \leq 200 \)) from ETF2, DZ10 and WS3 calculations, respectively. The results from WS3 are relatively close to the values of \( b_{\text{fit}} \) (with an rms deviation of 449 keV), which indicates that the IMME with quadratic form is generally satisfied in this model. For extremely neutron-rich nuclei, the results (crosses) from the traditional Skyrme EDF obviously deviate from the values of \( b_{\text{fit}} \). From Fig. 9(a), we note that the change of \( b_{\text{fit}} - b \) with the isospin \( T \) for the 179 neutron drip line nuclei is quite different with different models. For the Skyrme EDF calculations the difference \( b_{\text{fit}} - b \) increases soon with the isospin \( T \) (we draw the same conclusion with Skyrme HFB codes HFBRAD [36] and HFBTHO [37]). Without special consideration for the isospin-symmetry restoration in the traditional Skyrme EDF, the calculated surface diffuseness of protons becomes abnormally large in extremely proton-rich nuclei to reduce the huge Coulomb repulsion, which causes the large deviations from \( b_{\text{fit}} \). These investigations show that the exploration of the IMME in the neutron-rich nuclei might provide us with very useful information for testing the mass models.

Closely relating to the IMME, the Coulomb energies (direct term) of nuclei are investigated simultaneously. Fig. 9(b) shows the Coulomb energy coefficient defined as \( a_c = E_C A^{1/3} Z^{-2} \) with different models as a function of \((N - Z)/2\) for Pb isotopes. Here, \( E_C \) denotes the calculated Coulomb energy of a nucleus with a certain mass model. The
FIG. 9: (Color online) (a) Deviations of the calculated $b$ coefficients with DZ10, ETF2 and WS3 models from $b_{\text{fit}} = 0.710A^{2/3} - 0.946$ [16], as a function of isospin. (b) Coulomb energy coefficient $a_c = E_C A^{1/3} Z^{-2}$ obtained with different models as a function of $(N - Z)/2$.

open circles and the solid line denote the values of $a_c$ with DZ10 and WS3, respectively. The squares and the crosses denote the results from the HFBTHO [37] and the ETF2 [28] approach with the Skyrme force SkP [29], respectively. Similar to Fig. 9(a), the trends are quite different with different models. The coefficient $a_c$ in this work is a constant. In DZ mass models, the isospin effect in the Coulomb energy calculation is involved by the isospin-dependent charge radius $R_c \propto A^{1/3}(1 - 0.25I^2)$, which causes the reduction of the effective coefficient $a_c$ for neutron-rich nuclei (see the open circles). On the contrary, the values of $a_c$ obviously increase with increasing neutron number in the Skyrme energy-density functional calculations. It is because for extremely proton-rich nuclei the surface diffuseness of protons increases sharply to reduce the huge Coulomb repulsion and causes the reduction of $a_c$ consequently. Comparing Fig. 9(a) to (b), one finds that the change of $b_{\text{fit}} - b$ with the isospin $T$ is roughly consistent with that of the Coulomb energy coefficient $a_c$. The Coulomb energy coefficient might be used as a sensitive quantity to study the mass models and the isobaric multiplet mass equation.

In addition, for exploring the correlation among the IMME, the GK relation and the accuracy of the nuclear mass models, we systematically study the rms deviations of calculated $b$ coefficients with Eq.(16) and the nuclear masses by 17 nuclear mass models, including
different versions of liquid drop models [8, 9, 38, 39], the Duflo-Zuker mass models (DZ10 and DZ31 [14]), the ETF2 approach with different Skyrme forces, the WS, WS* and WS3 models. We use $\sigma(b)$ for describing the rms deviation of the calculated $b$ coefficients by a certain mass model from $b_{\text{fit}}$ for the 179 neutron drip line nuclei. The rms deviations $\sigma(b)$ obtained from ETF2, DZ10, DZ31 [14] and WS3 are 2734, 870, 630 and 449 keV, respectively. The values of $\sigma(M)$ and $\sigma(GK)$ from some mass models are presented in Table II previously. In Fig. 10, we show the values of $\sigma(GK)/\sigma(b)$ as a function of $\sigma(GK)/\sigma(M)$. Each of solid circles represents the calculated result from a nuclear mass model and all of circles are located in between two dashed lines. A general tendency of $\sigma(GK)/\sigma(b)$ increasing with $\sigma(GK)/\sigma(M)$ is clearly shown, which exhibits a strong correlation between the quadratic form of the IMME and the accuracy of the mass model when the GK relations are reproduced reasonably well. In other words, reducing the deviation from the IMME could be a way to improve the accuracy of mass predictions if the $\sigma(GK) \sim 100$ keV. Fulfilling both the IMME and the GK relations seems to be two necessary conditions to improve the reliability of mass calculations for known nuclei and the extremely neutron-rich nuclei.
IV. SUMMARY

We proposed an extension of our earlier global nuclear mass model which significantly improves its ability to describe nuclear masses across the periodic table and puts it at least on a par with the very best empirical mass models on the market. With some additional correction terms, including mirror nuclei effect due to the isospin symmetry, Wigner-like effect from the symmetry between valance-neutron and valance-proton, corrections for pairing effects and those from triaxial deformation of nuclei, the rms deviations from 2149 measured masses and 1988 neutron separation energies are significantly reduced to 336 and 286 keV, respectively. As a test of the extrapolation of the mass model, the α-decay energies of 46 super-heavy nuclei have been systematically studied. The rms deviation with the proposed model reaches 248 keV, much smaller than the result 936 keV from the DZ28 model. Furthermore, through studying the rms deviations to the masses of nuclei approaching the drip lines and the predictive power of the mass formulas fitted to the AME1995 data, we find that the results from the proposed model are satisfactory. In addition, with a systematic study of 17 global nuclear mass models, we find that the quadratic form of the IMME is closely related to the accuracy of nuclear mass calculations when the Garvey-Kelson relations are reproduced reasonably well. Fulfilling both the IMME and the Garvey-Kelson relations seems to be two necessary conditions to improve the quality of the model prediction. Furthermore, the α-decay energies of super-heavy nuclei should be used as an additional constraint on the global nuclear mass models.

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