Further improvements on a global nuclear mass model

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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 seem to be two necessary conditions for improving the quality of the model prediction. Furthermore, the α-decay energies of super-heavy nuclei should be used as an additional constraint on global nuclear mass models.

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I. INTRODUCTION

The precise calculation for nuclear masses is of great importance, not only for nuclear physics but also for nuclear astrophysics. In nuclear physics, the synthesis of super-heavy nuclei [1–3] and nuclear symmetry energy [4,5] has attracted much attention in recent years. Accurate predictions for the shell corrections and α-decay energies of super-heavy nuclei are urgently required for the synthesis of new super-heavy nuclei. At the same time, nuclear masses include important information on nuclear symmetry energy [6,7], which closely relates to the structure of nuclei and the dynamic 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 hundred keV to a few MeV with respect to all known nuclear masses. The most successful global mass models include the following: (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 recently by Wang *et al.* [10,11]; (2) various microscopic mass models based on the mean-field concept such as the nonrelativistic Hartree-Fock-Bogoliubov (HFB) approach with the Skyrme energy-density functional (EDF) [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 their 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 100–200 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, plays an important role in 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 that 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

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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 ΔE, and the residual correction $\Delta_{\rm res}$ as follows:

$$E(A,Z,\beta) = E_{\rm LD}(A,Z)\prod_{k\geqslant 2}\left(1+b_k\beta_k^2\right) + \Delta E(A,Z,\beta) + \Delta_{\rm res}. \tag{1}$$

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

$$E_{\rm LD}(A,Z) = a_v A + a_s A^{2/3} + E_C + a_{\rm sym} I^2 A + a_{\rm pair} A^{-1/3}\delta_{np} + \Delta_W, \tag{2}$$

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

$$E_C = a_c \frac{Z^2}{A^{1/3}}(1 - 0.76Z^{-2/3}), \tag{3}$$

and the symmetry energy coefficient

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

The $a_{\rm pair}$ term empirically describes the pairing effect (see Ref. [10] for details). The terms with b_k describe the contribution of nuclear deformation (including β_2, β_4, and β_6) to the macroscopic energy. The mass dependence of the curvatures b_k in Eq. (1) is written as [10]

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

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 Δ_W in $E_{\rm LD}$ to consider the Wigner-like effect of heavy nuclei [22], which is due to the approximate symmetry between valence proton and valence neutron. Surprisingly, in Refs. [10,11] we found that some heavy doubly magic nuclei lie along a straight line $N = 1.37Z + 13.5$ (see Fig. 1), which is called the 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 the doubly magic nucleus ^{164}Pb is close to that of ^{176}Sn. In other words, the change of the shell energy by adding several neutrons to the doubly magic nucleus ^{208}Pb is close to that of adding several protons to ^{208}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 valence proton and valence neutron, we phenomenologically write the

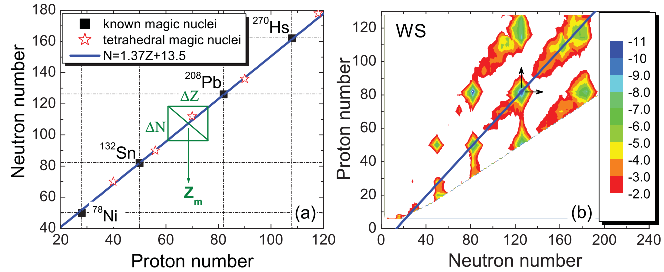

FIG. 1. (Color online) (a) Positions of some known doubly magic nuclei (squares). The stars denote the predicted tetrahedral doubly magic nuclei in Refs. [23,24]. (b) Shell corrections of nuclei with WS [10]. The solid line shows the position of $N = 1.37Z + 13.5$.

Wigner-like term as

$$\Delta_W = c_{\rm w}(e^{|I|} - e^{-|\eta|}), \tag{6}$$

where $\eta = \frac{\Delta Z\,\Delta N}{Z_{\rm m}}$ denotes the effective distance of a nucleus to the shell stability line. The values of ΔZ, ΔN, and $Z_{\rm m}$ 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, which causes a cusp for light nuclei near the $N = Z$ line, the Wigner-like term Δ_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

$$\Delta E = c_1 E_{\rm sh} + |I| E'_{\rm sh} \tag{7}$$

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. $E_{\rm sh}$ and $E'_{\rm sh}$ denote the shell energy of a nucleus and of its mirror nucleus, respectively. The $|I|$ term in ΔE 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,

$$\lambda = \lambda_0\left(1 + \frac{N_i}{A}\right), \tag{8}$$

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,

$$\Delta_{\rm res} = \Delta_M + \Delta_P + \Delta_T. \tag{9}$$

The first term, Δ_M, is to further consider the 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

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
$c_{\rm sym}$(MeV)	29.1174	r_0 (fm)	1.3848
κ	1.3437	a (fm)	0.7617
ξ	1.1865	λ_0	26.6744
$a_{\rm pair}$ (MeV)	−6.2299	c_1	0.6454
$c_{\rm w}$ (MeV)	1.0490	c_2 (MeV^{-1})	1.6179

physics. Here, we empirically write

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

with

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

Here, $T = |\frac{N-Z}{2}|$ 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 $N \geqslant Z$ cases. The Δ_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 Δ_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 $a_{\rm pair}$ term in $E_{\rm LD}$ for describing the pairing correction, we further consider the term

$$\Delta_P = \frac{1}{2}\frac{\partial^2 E_{\rm sh}}{\partial A^2}\bigg|_T, \tag{12}$$

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 parametrized formula in our previous work [11]. Here the formula is slightly extended to include the contribution of the protons, $\Delta_T = -0.7[\cos(2\pi \frac{N}{16}) + \cos(2\pi \frac{N}{20}) + \cos(2\pi \frac{Z}{52})]A^{-1/3}$ MeV.

III. CALCULATED MASSES FROM THE MODEL

Based on the 2149 (N and $Z \geqslant 8$) measured nuclear masses from the atomic mass evaluation of 2003 (AME2003) [27], we obtain the optimal model parameters, which are labeled 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 α-decay energies of 46 super-heavy nuclei ($Z \geqslant 106$) [11]. σ(GK) presents the rms deviation with respect to the GK mass estimates, and $\sigma(b)$ denotes the rms deviation from the formula [16] $b_{\rm fit} = 0.710A^{2/3} - 0.946$ for the b coefficients of 179 neutron drip-line nuclei, which will be discussed in the next section. Here, 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 is the extended Bethe-Weizsäcker formula [9], in which the shell corrections of nuclei are described as a function of the valence-nucleon number assuming the magic numbers are 2, 8, 20, 28, 50, 82, 126, and 184. FRDM and HFB-17 denote the finite-range droplet model [8] and the latest HFB model with the improved Skyrme energy-density functional [12], respectively. DZ10, DZ28, and DZ31 denote different versions of the Duflo-Zuker mass models, with 10, 28, and 31 parameters, respectively.

Remarkably, the rms deviation from the 2149 masses with WS3 is reduced to 336 keV, which is much smaller than the results from the FRDM and the latest HFB-17 calculations, and 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 the WS3 model, 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, which is much smaller than the results from DZ28 (321 keV) and FRDM (680 keV).

TABLE II. The rms σ deviations between data AME2003 [27] and predictions of some models (in keV). The line $\sigma(M)$ refers to all 2149 measured masses, the line $\sigma(S_n)$ to the 1988 measured neutron separation energies S_n, and the line $\sigma(Q_\alpha)$ to the α-decay energies of 46 super-heavy nuclei. σ(GK) presents the rms deviation with respect to the GK mass estimates. $\sigma(b)$ denotes the rms deviation from the formula [16] $b_{\rm fit} = 0.710A^{2/3} - 0.946$ for the b coefficients of 179 neutron drip-line nuclei.

	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
σ(GK)	24	129	337	496	100	151	165	115	133	131
$\sigma(b)$	2734	759	–	–	870	283	450	630	–	449

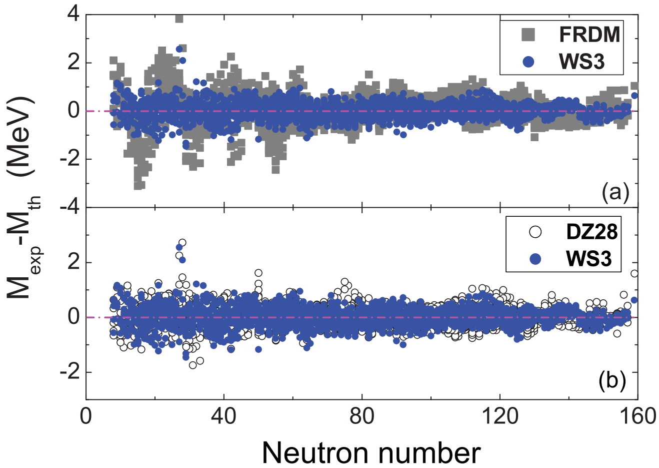

FIG. 2. (Color online) (a) Deviations of calculated nuclear masses from the experimental data as a function of neutron number. The squares and the solid circles denote the results of FRDM and WS3, respectively. (b) The same as (a), but with the results of the DZ28 model for comparison.

It is known that the α-decay energies of super-heavy nuclei [1] have been measured with accuracy at several ten keV to a few hundred keV, which provides us with useful data for testing our mass model. It is remarkable that the rms deviation $\sigma(Q_\alpha)$, with respect to the α-decay energies of 46 super-heavy nuclei from the WS3 model, is reduced to 248 keV. The difference between the calculated α-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 ± 0.8 and ± 1.0 MeV, respectively. Here, we would like to emphasize that the experimental data of α-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. Figure 3 shows the calculated α-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 deviations 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 stippling denotes the region with deviations smaller than 2 MeV. One sees that the results from WS3, FRDM, DZ28, and WS* are relatively close to each other, and the results from the HFB-17 model obviously deviate 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 α-decay energies (see Fig. 3) between the two models. Because the predictions from different models toward the neutron drip line tend to

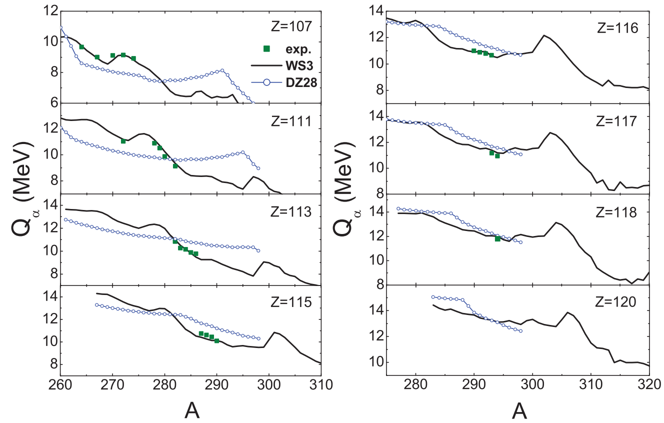

FIG. 3. (Color online) α-decay energies of some super-heavy nuclei calculated with WS3 (solid curve) and DZ28 (open circles). The squares denote the experimental data taken from [11] (and references therein).

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 lower striped area represents the average standard deviation errors of the measured masses [27]. One sees that the rms deviations from 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 can be expected to be much larger than those for stable nuclei. The rms deviation $\sigma(M)$ from 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

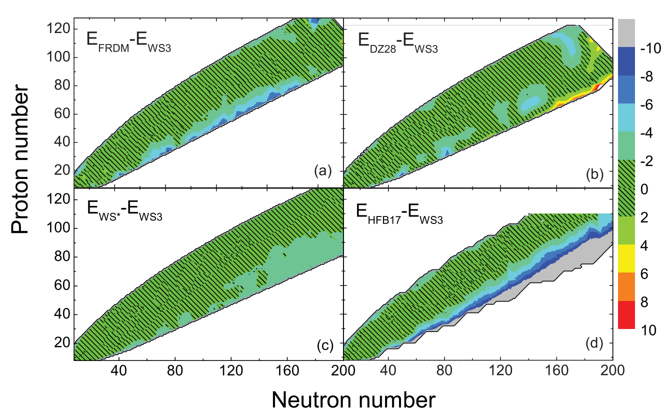

FIG. 4. (Color online) Deviations of the calculated nuclear total energies at the ground state in this work from the results of (a) FRDM, (b) DZ28, (c) WS*, and (d) HFB-17, respectively. The calculated masses with FRDM, DZ28, WS*, and HFB-17 are taken from [8,11,12,15], respectively. The stippling denote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

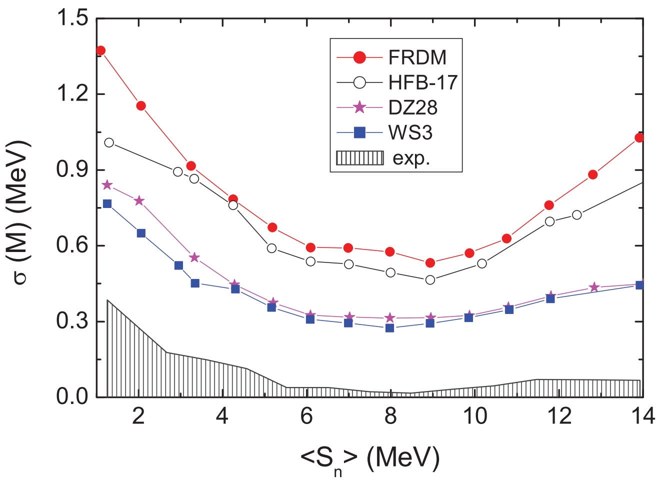

FIG. 5. (Color online) The rms deviation with respect to the masses as a function of average neutron-separation energy of nuclei. The lower striped area represents the average standard deviation errors of the measured masses [27].

similar for decreasing 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 FRDM reaches about 1 MeV. Figure 5 indicates that the model WS3 is relatively reliable for describing the masses of nuclei far from the β-stability line.

Furthermore, to check the predictive power of various models, we follow Lunney and colleagues [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 AME1995 [33] and AME2003 [27], respectively. Figure 6 shows the values of Y with various mass models listed in Table II. A large positive value for Y indicates the deterioration for prediction of "new" masses in the 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

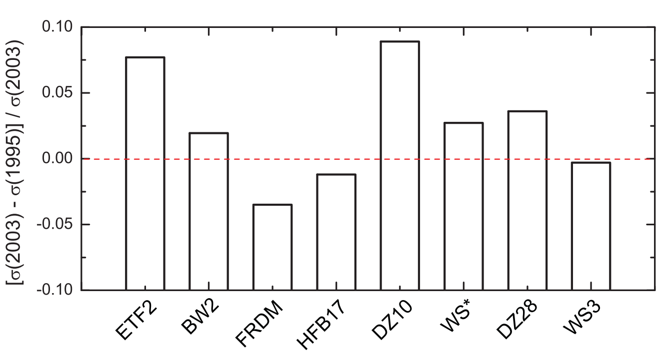

FIG. 6. (Color online) A comparison of the predictive power of the various models. The vertical axis denotes the quantity $Y = \frac{\sigma(2003)-\sigma(1995)}{\sigma(2003)}$, as a measure of the predictive power of the mass formulas fitted to the 1995 data. Here, $\sigma(1995)$ and $\sigma(2003)$ denote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

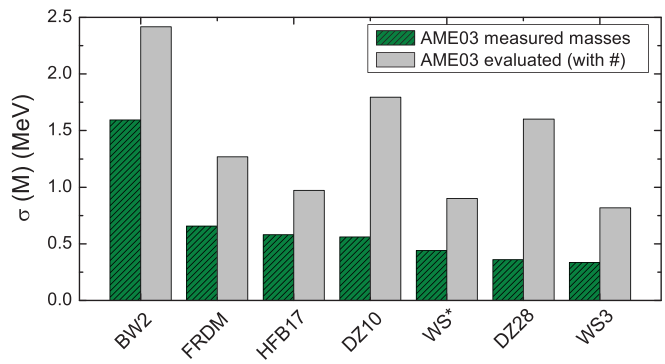

FIG. 7. (Color online) Comparison of rms deviation with respect to the masses from AME2003 with the various models. The dark (green) striped bars are for the 2149 measured masses and the gray bars denote the rms deviations to the evaluated masses (marked by #) in AME2003. For the HFB-17 model, only the masses of nuclei with $Z \leqslant 110$ are involved in the calculation.

rms deviation with respect to the masses from AME2003 with the various models. The striped bars 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 larger than the others, such as the large rms deviations with respect to the α-decay energies of super-heavy nuclei from these three models [see the values of $\sigma(Q_\alpha)$ in Table II]. Figures 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 drip-line nuclei and 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 compare the results from the mass models mentioned previously. We first check the Garvey-Kelson relations based on the obtained mass tables from these mass models. It is known that the GK relation cannot be used to cross the $N = Z$ line. Therefore, we select five suitable neighbors in the GK relation for each nucleus to avoid crossing the $N = Z$ line. We use the following GK relations:

$$\begin{aligned} M_{\rm GK}(N,Z) = {} & M(N+1,Z) + M(N,Z-1) \\ & + M(N+2,Z-2) - M(N+1,Z-2) \\ & - M(N+2,Z-1), \quad \text{for} \quad N \geqslant Z \quad \text{cases}, \end{aligned} \tag{13}$$

and

$$M_{\rm GK}(N,Z) = M(N-1,Z) + M(N,Z+1) + M(N-2,Z+2) - M(N-1,Z+2) - M(N-2,Z+1), \quad \text{for} \quad N < Z \quad \text{cases.} \tag{14}$$

Here, $M(N,Z)$ denotes the mass excess of a nucleus with neutron number N and charge number Z. σ(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 HFB approach [34] based on the traditional Skyrme force without further improvements describes 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 insufficient condition for improving the quality of the model prediction.

At the same time, we study the isobaric multiplet mass equation, 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

$$\mathrm{BE}(T,T_z) = a + bT_z + cT_z^2, \tag{15}$$

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],

$$b = \frac{\mathrm{BE}(T=T_z) - \mathrm{BE}(T=-T_z)}{2T}, \tag{16}$$

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. Ormand [16] proposed the formula

$$b_{\rm fit} = 0.710A^{2/3} - 0.946 \tag{17}$$

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 $A \leqslant 75$ according to Eq. (16). Here, the experimental binding energies of mirror nuclei are taken from AME2003 [27] and the four very recently measured masses for ^{63}Ge, ^{65}As, ^{67}Se, and ^{71}Kr in Ref. [30]. It seems that the b coefficients are roughly constant for a given A. The solid curve denotes the results of the $b_{\rm fit}$ 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

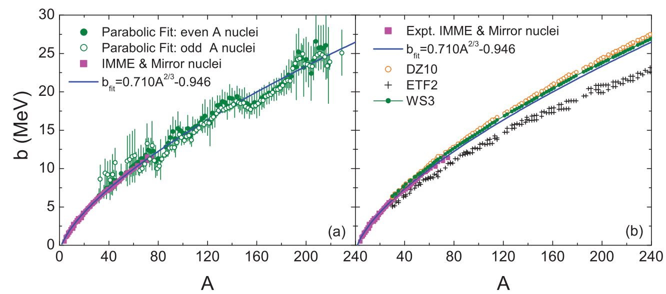

FIG. 8. (Color online) (a) b coefficients of nuclei in the IMME as a function of mass number. The solid squares and the solid curve denote the extracted results from mirror nuclei with $A \leqslant 75$ according to Eq. (16) and those from the empirical formula [16] $b_{\rm fit} = 0.710A^{2/3} - 0.946$, 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.

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 $b_{\rm fit}$, 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

$$\mathrm{BE}(A,T_z) = \tilde{a} + \tilde{b}\,T_z + \tilde{c}\,T_z^2 + B_{\rm sh} + B_{\rm wig} + B_{\rm def} + \cdots. \tag{18}$$

Here, the mass-dependent coefficients $\tilde{a}$, $\tilde{b}$, and $\tilde{c}$ can be directly obtained from the liquid-drop formula and $\tilde{b} \sim a_c A^{2/3}$. $B_{\rm sh}$, $B_{\rm wig}$, and $B_{\rm def}$ denote the shell correction, the Wigner energy, and the deformation energy of a nucleus, respectively. From Eqs. (15)–(18) and Fig. 8(a), we learn the following: (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 generally equals 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 be 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 ($Z \geqslant 8$ and $N \leqslant 200$) from ETF2, DZ10, and WS3 calculations, respectively. The results from WS3 are relatively close to the values of $b_{\rm fit}$ (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

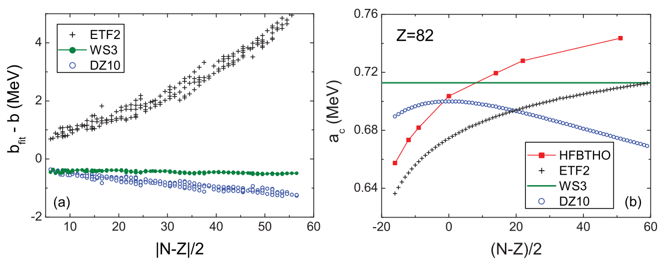

FIG. 9. (Color online) (a) Deviations of the calculated b coefficients with DZ10, ETF2, and WS3 models from $b_{\rm fit} = 0.710A^{2/3} - 0.946$ [16], as a function of isospin. (b) The Coulomb energy coefficient $a_c = E_C A^{1/3} Z^{-2}$ obtained with different models as a function of $(N - Z)/2$.

traditional Skyrme EDF obviously deviate from the values of $b_{\rm fit}$. From Fig. 9(a), we note that the change of $b_{\rm fit} - b$ with the isospin T for the 179 neutron drip-line nuclei is quite different with different models. For the Skyrme EDF calculations the difference $b_{\rm fit} - b$ increases soon with the isospin T (and 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 $b_{\rm fit}$. 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.

In close relation to the IMME, the Coulomb energies (direct terms) of nuclei are investigated simultaneously. Figure 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 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] approaches 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 involves 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). In contrast, the values of a_c obviously increase with increasing neutron number in the Skyrme energy-density functional calculations. This is because for extremely proton rich nuclei, the surface diffuseness of protons increases sharply to reduce the huge Coulomb repulsion and as a result causes the reduction of a_c. Comparing Fig. 9(a) to 9(b), one finds that the change of $b_{\rm fit} - b$ 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 from 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, and 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 $b_{\rm fit}$ 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 $\sigma(\rm GK)$ from some mass models are presented in Table II. In Fig. 10, we show the values of $\sigma(\rm GK)/\sigma(b)$ as a function of $\sigma(\rm GK)/\sigma(M)$. Each of the solid circles represents the calculated result from a nuclear mass model and all of the circles are located in between two dashed lines. A general tendency of $\sigma(\rm GK)/\sigma(b)$ increasing with $\sigma(\rm GK)/\sigma(M)$ 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 $\sigma(\rm GK) \sim 100$ keV. Fulfilling both the IMME and the GK relations seems to be two necessary conditions for improving the reliability of mass calculations for known nuclei and the extremely neutron rich nuclei.

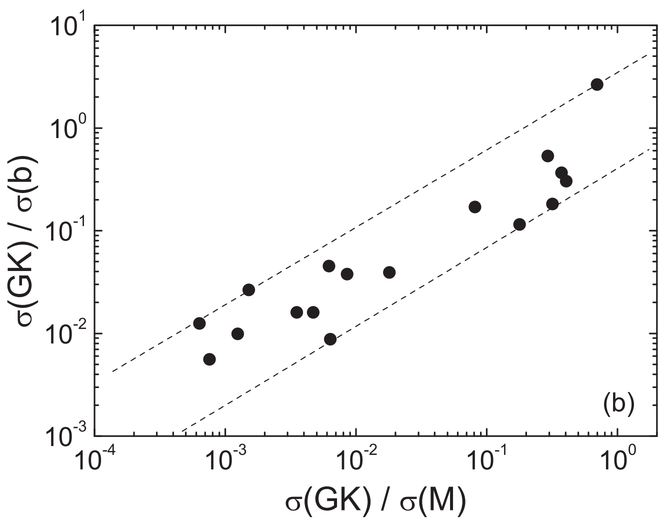

FIG. 10. Values of $\sigma(\rm GK)/\sigma(b)$ as a function of $\sigma(\rm GK)/\sigma(M)$ from 17 different models (solid circles). Dashed lines are to guide the eyes.

V. 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 available. With some additional correction terms, including the mirror nuclei effect due to isospin symmetry, the Wigner-like effect from the symmetry between valence neutron and valence proton, and the 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, which is much smaller than the result of 936 keV from the DZ28 model. Furthermore, by 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 for improving the quality of the model prediction. Furthermore, the α-decay energies of super-heavy nuclei should be used as an additional constraint on global nuclear mass models.

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