Nuclear mass relations based on systematics of proton-neutron interactions

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The proton-neutron interaction between the last proton and the last two neutrons, $V_{1p\text{-}2n}$, and that between the last two protons and the last neutron, $V_{2p\text{-}1n}$, for nuclei with mass number $A \geqslant 60$, are extracted by using experimental binding energies of neighboring nuclei. By using a simple function to describe $V_{1p\text{-}2n}$ and $V_{2p\text{-}1n}$, we present new relations connecting the masses of neighboring nuclei with improved accuracies.

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Nuclear mass (or nuclear binding energy) is one of the fundamental properties of a nucleus. An accurate knowledge of nuclear masses is very important not only in nuclear physics but also in many other branches of science, for example, astrophysics and cosmology. Although nuclear masses near the β stability line are measured very accurately, masses of many more unstable nuclei are not yet known. Describing and predicting masses of atomic nuclei is therefore one of the key goals in nuclear structure theory.

The early efforts toward describing nuclear masses can be traced back to the Weizsäcker formula [1–3]. Nowadays there are a number of popular models of nuclear masses, for example, the Duflo-Zuker model (D-Z) [4], the finite-range droplet model (FRDM) [5], and the Skyrme-Hartree-Fock-Bogoliubov theory (SHFB) [6]. These models describe and predict masses of about 9000 nuclei, including unknown ones. The root-mean-squared (abbreviated as "rms" from now on) deviation from the experimental values for known nuclei is about 380 keV for the D-Z model and about 670 keV for the other two. There are also many efforts based on systematics of local mass relations, such as the famous Audi-Wapstra systematics [7–9], the Garvey-Kelson (G-K) mass relations [10], and others [11–13]. For a comprehensive review, see Ref. [14].

Recently, Barea and collaborators investigated the G-K mass relations from a new perspective [15–17]: For a given nucleus, there are a number of evaluations (maximally 12) based on the G-K relations, and they took the average of all available evaluations. The rms deviation σ is 76 keV with respect to the Atomic-Mass Evaluation 2003 [9], for mass number $A \geqslant 60$, if all 12 G-K relations are available.

In Ref. [18], Fu and collaborators took an exponential function to describe the residual proton-neutron (p-n) interaction between two valence protons and two valence neutrons, denoted by $V_{2p\text{-}2n}$ [19], and derived a new set of local mass formulas that are competitive with the G-K mass relations based on the systematics of p-n interactions. If all masses of the neighboring nuclei involved in maximally four local mass relations are available [18], the rms deviation from the AME2003 is 78 keV. The crucial role played by the residual p-n interaction has been long emphasized [20–22] and extensively studied. See Ref. [23] for a review. Some recent and important progress can be found in Refs. [19,24–35].

The purpose of this paper is to investigate how far we can go in constructing local mass relations based on systematics of the p-n interaction. We first show that the more appropriate quantities to apply in this construction are the p-n interaction between the last proton and the last two neutrons, $V_{1p\text{-}2n}$, and that between the last two protons and the last neutron, $V_{2p\text{-}1n}$. They are more proper than $V_{2p\text{-}2n}$ in constructing local mass relations. We use a simple function to describe the average values of $V_{1p\text{-}2n}$ and $V_{2p\text{-}1n}$ and present new relations connecting the masses of neighboring nuclei with improved accuracies.

The p-n interaction (denoted by $V_{ip\text{-}jn}$) between the last i proton(s) and the last j neutron(s) for a given nucleus was defined in Ref. [31]:

$$V_{ip\text{-}jn}(N+j, Z+i) = [B(N+j, Z+i) - B(N, Z+i)] - [B(N+j, Z) - B(N, Z)], \quad (1)$$

where $B(N, Z)$ is the negative of the nuclear binding energy for the nucleus with proton number Z and neutron number N.

In Fig. 1, we present $V_{1p\text{-}2n}(N, Z)$ and $V_{2p\text{-}1n}(N, Z)$ versus proton number Z for nuclei with $A \geqslant 60$, excluding those for which either the proton number or the neutron number is magic. The binding energies are taken from Ref. [9]. The circles and crosses correspond to $V_{2p\text{-}1n}$ and $V_{1p\text{-}2n}$, respectively. We see that both $V_{2p\text{-}1n}$ and $V_{1p\text{-}2n}$ change smoothly versus Z, despite of sizable fluctuations, and that there are no apparent differences between these two quantities in the plot. We thus take one $v(Z)$ to describe the average values for both $V_{2p\text{-}1n}$ and $V_{1p\text{-}2n}$, shown as the red solid curve in Fig. 1, where

$$v(Z) = a \times Z^b + c, \quad (2)$$

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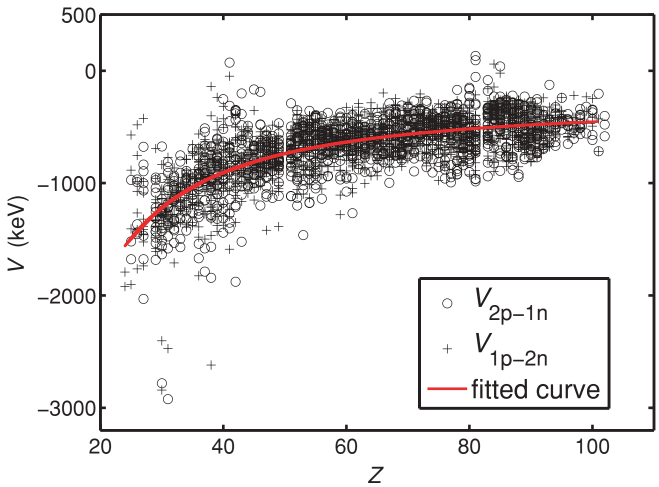

FIG. 1. (Color online) $V_{1p\text{-}2n}(N,Z)$ and $V_{2p\text{-}1n}(N,Z)$ versus Z for $A \geqslant 60$. The results are extracted by using the AME2003 database [9]. The red curve is plotted by using $v(Z)$ given in Eq. (2).

with $a = -115\,000$ keV, $b = -1.417$, and $c = -285.4$ keV. The preceding values of a, b, and c are optimized simultaneously for $V_{1p\text{-}2n}(N,Z)$ and $V_{2p\text{-}1n}(N,Z)$, with the rms deviation of 200 keV. If parameters a, b, and c are optimized separately for $V_{1p\text{-}2n}(N,Z)$ and $V_{2p\text{-}1n}(N,Z)$, the rms deviations for $V_{1p\text{-}2n}(N,Z)$ and $V_{2p\text{-}1n}(N,Z)$ from corresponding $v(Z)$ are found to be 198 and 203 keV, respectively (see Table I).

We have investigated systematics of $V_{2p\text{-}2n}$ in Ref. [18], where we used an exponential function of Z and obtained the rms deviation ($\simeq$255 keV) between V_{2p-2n} extracted from experimental data of binding energies and those determined by the optimized exponential function. Here we use $v(Z)$ [see Eq. (2)] for $V_{2p\text{-}2n}$ with parameters a, b, and c readjusted and find that the rms deviation changes very slightly (less than 1.0 keV). The rms deviations for other $V_{ip\text{-}jn}$ are also presented in Table I. One sees that the rms deviation from $v(Z)$ is the smallest for $V_{1p\text{-}2n}(N,Z)$ and $V_{2p\text{-}1n}(N,Z)$. Thus, $V_{1p\text{-}2n}(N,Z)$ and $V_{2p\text{-}1n}(N,Z)$ are expected to provide us with the best accuracy while being applied to constructing local mass relations.

Table I also presents the number (denoted by $\mathcal{N}$) of possible local mass relations for nuclei with $A \geqslant 60$ and all masses involved in Eq. (1) experimentally known for each $V_{ip\text{-}jn}$. One sees that the values of $\mathcal{N}$ are close to each other when $i \leqslant 3$ and/or $j \leqslant 3$ (not including the case where both i and j equal 3). When we construct the mass relations in this paper, we use both $V_{2p\text{-}1n}$ and $V_{1p\text{-}2n}$, for all of which the value of $\mathcal{N}$ is large. Therefore, the total number of evaluations in this paper, by using $V_{2p\text{-}1n}$ and $V_{1p\text{-}2n}$, is larger than any other $V_{ip\text{-}jn}$. Apparently, for cases with larger $\mathcal{N}$, one again expects to achieve better accuracies.

Assuming that both $V_{1p\text{-}2n}(N,Z)$ and $V_{2p\text{-}1n}(N,Z)$ are represented by $v(Z)$ in Eq. (2), we obtain

$$\begin{aligned}
B^{\rm pred}(N,Z) &= B(N-1,Z) + B(N,Z-2) \\
&\quad - B(N-1,Z-2) + v(Z),\\
B^{\rm pred}(N,Z) &= B(N+1,Z) - B(N+1,Z-2) \\
&\quad + B(N,Z-2) - v(Z),\\
B^{\rm pred}(N,Z) &= B(N,Z+2) - B(N-1,Z+2) \\
&\quad + B(N-1,Z) - v(Z+2),\\
B^{\rm pred}(N,Z) &= -B(N+1,Z+2) + B(N,Z+2) \\
&\quad + B(N+1,Z) + v(Z+2),\\
B^{\rm pred}(N,Z) &= B(N-2,Z) + B(N,Z-1) \\
&\quad - B(N-2,Z-1) + v(Z),\\
B^{\rm pred}(N,Z) &= B(N+2,Z) - B(N+2,Z-1) \\
&\quad + B(N,Z-1) - v(Z),\\
B^{\rm pred}(N,Z) &= B(N,Z+1) - B(N-2,Z+1) \\
&\quad + B(N-2,Z) - v(Z+1),\\
B^{\rm pred}(N,Z) &= -B(N+2,Z+1) + B(N,Z+1) \\
&\quad + B(N+2,Z) + v(Z+1).
\end{aligned} \tag{3}$$

Similar to procedures in Refs. [15–18], we take the average of all possible evaluations for the binding energy $B^{\rm pred}(N,Z)$ of a given nucleus.

The rms deviation (σ) of our predicted binding energies with respect to experimental results, for nuclei with $A \geqslant 60$, is summarized and compared with those by using the G-K mass relations in Ref. [16] in Table II. One sees that the deviation by using Eq. (3) is on average smaller than that by using the G-K relations, except for the case of small n (the first column).

Now let us look at the deviations of the predicted binding energies from data obtained by experiment, by using Eq. (3), and by using Eq. (6) of Ref. [18]. The latter equation is given

TABLE I. The rms deviations (denoted by σ, in keV) between $V_{ip\text{-}jn}$ extracted from the binding energies compiled in the AME2003 database [9] and optimized $v(Z)$ [using Eq. (2)] for $A \geqslant 60$, excluding those for which either the proton numbers or the neutron numbers are magic. The parameters of $v(Z)$ are optimized for each of $V_{ip\text{-}jn}$. One sees that the rms deviation between $V_{ip\text{-}jn}$ and $v(Z)$ is the smallest for $V_{1p\text{-}2n}$ and $V_{2p\text{-}1n}$ (about 200 keV). We also present the numbers of possible local mass relations (denoted by $\mathcal{N}$) involving of $V_{ip\text{-}jn}$. It is noted that the numbers of possible local mass relations are close to each other for $i \leqslant 3$ and/or $j \leqslant 3$ (not including the case where both i and j equal 3) and decrease drastically for larger i and j values.

	$V_{1p\text{-}1n}$	$V_{1p\text{-}2n}$	$V_{2p\text{-}1n}$	$V_{2p\text{-}2n}$	$V_{2p\text{-}3n}$	$V_{3p\text{-}2n}$	$V_{3p\text{-}3n}$	$V_{3p\text{-}4n}$	$V_{4p\text{-}3n}$	$V_{4p\text{-}4n}$
σ	336	198	203	255	348	335	460	489	520	617
$\mathcal{N}$	1425	1396	1351	1316	1246	1211	296	283	275	251

TABLE II. The rms deviations (in keV) of masses evaluated by using Eq. (3) of this paper (first row) from the AME2003 data and that evaluated by using the G-K relations (second row) presented in Ref. [16] for nuclei with $A \geqslant 60$. n is the number of possible evaluations for a given nucleus.

Relations	$n \geqslant 1$	$n \geqslant 4$	$n \geqslant 7$	$n \geqslant 8$	$n \geqslant 12$
Eq. (3)	123	92	73	70	–
G-K	115	98	86	–	76

here for the sake of convenience and completeness:

$$\begin{aligned} &4B(Z-1,N+1)+4B(Z+1,N-1)\\ &\quad -4B(Z-1,N-1)-4B(Z+1,N+1)\\ &\quad +B(Z+2,N+1)+B(Z+1,N+2)\\ &\quad +B(Z-2,N-1)+B(Z-1,N-2)\\ &\quad -B(Z-2,N+1)-B(Z-1,N+2)\\ &\quad -B(Z+2,N-1)-B(Z+1,N-2)=0. \end{aligned} \quad (4)$$

This is a relation involving the masses of 12 neighboring nuclei, but we focus on binding energies $B(Z-1,N+1)$, $B(Z+1,N-1)$, $B(Z-1,N-1)$, and $B(Z+1,N+1)$, as in Ref. [18]. Thus, the maximum number of possible evaluations n that we use is four. In Table III we present the rms deviation and number of nuclei (denoted by $\mathcal{N}'$) described by using Eq. (3) suggested in this paper and Eq. (4) (taken from Ref. [18]). Better local mass relations are those that describe more nuclei with smaller deviations. One sees that Eq. (3) describes more nuclei ($\mathcal{N}'$ larger) with smaller deviations. According to Table III, Eq. (3) describes 1506 nuclei with the rms deviation of 92 keV, in comparison to Eq. (4) for 1292 nuclei with the rms deviation of 110 keV. Equation (3) also presents smaller deviations (88 keV, see the third row) for those described by Eq. (4) and is thus superior to Eq. (4) in describing the nuclear masses.

We classify our predicted masses into four categories, nuclei with even values for both proton numbers Z and neutron numbers N (even-even), those with even values for Z and odd values for N (even-odd), those with odd values for Z and even values for N (odd-even), and those with odd values for both Z and N (odd-odd). In Fig. 2, we present the distribution of deviations (denoted by Δ) of our predicted masses from the AME2003 database versus Z, with $A \geqslant 60$ and $n = 8$, for even-even, even-odd, odd-even, and odd-odd nuclei. Among these four cases, the deviations in panel (a), which correspond to even-even nuclei, are the smallest, with 83% between -60 to 60 keV; the deviation for odd-odd nuclei, shown in panel (d), is the largest. The rms deviations (in keV) for even-even, even-odd, odd-even, and odd-odd nuclei, are 52, 69, 70, 86, respectively. The reason why the deviation of predicted masses for odd-odd nuclei by using the V_{in-jp} is larger than that for even-even and odd-A nuclei was argued in Ref. [31].

We perform an interesting numerical experiment, which proceeds as follows. As seen in other recent works [15–18], one usually achieves a relatively higher precision in describing

TABLE III. The rms deviations (σ) and number of nuclei (denoted by $\mathcal{N}'$) described by using Eq. (3) of this paper and Eq. (6) of Ref. [18]. The first row corresponds to results given by Eq. (3) here, and the second row corresponds to results by using Eq. (4) (taken from Eq. (6) of Ref. [18]). The third row presents the results by using Eq. (3) in this paper, but for nuclei that are described by Eq. (4). One sees that the former is superior to the latter: Eq. (3) in this work describes more nuclei with smaller deviations.

	$n \geqslant 1$		$n \geqslant 4$		$n \geqslant 8$	
	σ	$\mathcal{N}'$	σ	$\mathcal{N}'$	σ	$\mathcal{N}'$
Eq. (3), this work	123	1806	92	1506	70	815
Eq. (6), Ref. [18]	110	1292	78	435	–	–
Eq. (3), this work	88	1292	66	435	66	435

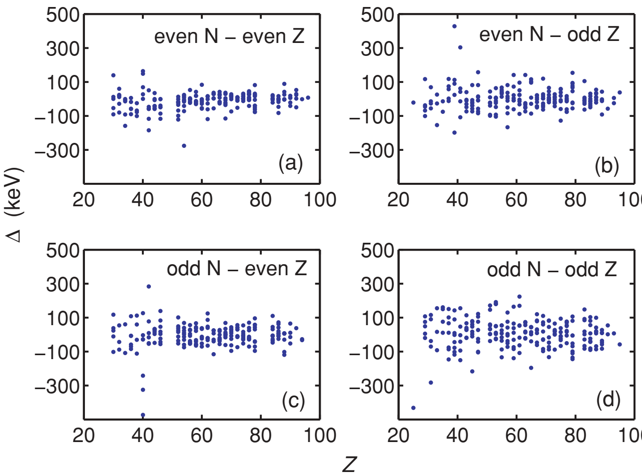

FIG. 2. (Color online) The distribution of deviations (denoted by Δ) of our predicted masses for $n = 8$ by using Eq. (3) with respect to the AME2003 database. Panels (a)–(d) correspond to the even-even, even-odd, odd-even, and odd-odd nuclei, respectively.

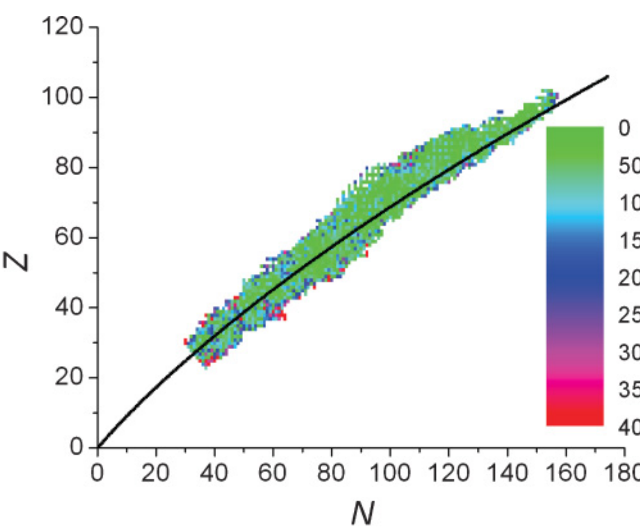

FIG. 3. (Color online) The deviations (in keV) of calculated binding energies in this paper with respect to those evaluated in the AME2003 database for nuclei with $A \geqslant 60$. The solid curve represents the β stability given in Eq. (5). One sees that large deviations arise for neutron-rich nuclei with relative small A.

TABLE IV. The rms deviations (σ) by using Eq. (3) of this work and the G-K relations for different n and d (the "distance" between a given nucleus and the β stability line) for nuclei with $A \geqslant 60$. Columns labeled (3) present the values of σ obtained by using Eq. (3) of this paper, and columns labeled G-K contain the values obtained by the G-K mass relations. One sees that σ is smaller for Eq. (3) than for G-K mass relations with few exceptions.

Region	$1 \leqslant n \leqslant 4$		$5 \leqslant n \leqslant 8$		$n = 8$		$9 \leqslant n \leqslant 12$		$n = 12$	
	(3)	G-K	(3)	G-K	(3)	G-K	(3)	G-K	(3)	G-K
$0 \leqslant d \leqslant 2$	118	131	70	98	59	94	–	73	–	73
$2 \leqslant d \leqslant 4$	118	126	83	87	80	80	–	86	–	84
$4 \leqslant d \leqslant 6$	226	254	117	160	82	116	–	97	–	79
$6 \leqslant d \leqslant 8$	208	277	98	146	57	176	–	79	–	86
$8 \leqslant d \leqslant 10$	220	166	97	91	63	67	–	118	–	50

nuclear masses when the number of possible evaluations on the mass of a given nucleus is large. To refine the accuracy of mass relations for neighboring nuclei, we combine Eq. (3) in this paper (where $n \leqslant 8$) and Eq. (4) (taken from Ref. [18]), in which $n \leqslant 4$. For $n = 12$ (=8 + 4), one obtains a considerably smaller rms deviation for *even-even* nuclei; $\sigma = 42$ keV when all 12 relations are available. However, σ for other types of nuclei (odd-A and odd-odd) does not decrease, according to our work.

We also investigate the accuracy of Eq. (3) from the stable to unstable regions. Such an investigation provides us with more detailed information on the accuracy of our local mass relations, in particular, whether or not such mass relations remain good if one goes to regions far from the β stability line. If the mass relations deteriorated for unstable nuclei, they would not be very useful for predicting the unknown masses. We take the β stability line described as follows:

$$Z = \frac{A}{1.98 + 0.0155A^{\frac{2}{3}}}. \tag{5}$$

We define d to represent the "distance" between one nucleus and the β stability line, varying from 0 to 10. The rms deviations (σ) for different n and d are summarized in Table IV, and are compared with those by using the G-K mass relations. One sees that large deviations arise for neutron-rich nuclei with relative small A. Here we notice that for $8 \leqslant d \leqslant 10$ the deviations with $n = 9$–12 and are much larger than those with $n = 12$ or $4 \leqslant n \leqslant 8$ if one uses the G-K relations. This sudden change of σ is worth pointing out, because the rms deviation becomes smaller with larger n, on average. See the last row in Table IV. From Table IV, one also sees that the rms deviations by using Eq. (3) are, in general, smaller than those of G-K relations with exceptions (for $8 \leqslant d \leqslant 10$ and/or small n).

Because we evaluate the mass of a given nucleus based on experimental masses of the neighboring nuclei, experimental uncertainties (denoted by $\sigma_{\rm exp}$) of these masses may also lead to deviations in applying Eq. (3). It is then interesting to evaluate how much of the preceding rms deviations σ might originate from the experimental uncertainties of masses for the neighboring nuclei. Here we define $\sigma_{\rm exp} = \sqrt{\sum_i (\delta_{B_i})^2}$, where δ_{B_i} is the experimental uncertainty for binding energy of ith term in Eq. (3). Comparisons between $\sigma_{\rm exp}$ and σ for different values of n are presented in Table V. Our results suggest that about 20%–60% of deviation σ might be originated from $\sigma_{\rm exp}$. One also sees that both σ and $\sigma_{\rm exp}$ are relatively small for $140 \leqslant A < 180$ and $200 \leqslant A < 260$.

To summarize, in this paper we investigate systematics of the p-n interactions (denoted by $V_{ip\text{-}jn}$) between the last i valence protons and j valence neutrons of nuclei with mass number $A \geqslant 60$, based on the masses of neighboring nuclei. We demonstrate that $V_{1p\text{-}2n}$ and $V_{2p\text{-}1n}$ are appropriate for constructing local mass relations. We use a simple function $v(Z)$ to describe $V_{1p\text{-}2n}$ and $V_{2p\text{-}1n}$ and present new relations connecting the masses of neighboring nuclei, with improved accuracies, based on systematics of $V_{1p\text{-}2n}$ and $V_{2p\text{-}1n}$. The rms deviations of our predicted values (in keV) for even-even, even-odd, odd-even, and odd-odd nuclei with $n = 8$, with respect to experimental data compiled in the AME2003 database [9], are 52, 69, 70, 86, respectively. We note that the simple function of $v(Z)$ is empirical, and that one arrives at similar rms deviations between predicted masses and experimental data, if one takes $v(N)$ or $v(A)$ ($A = Z + N$, the mass number for each nucleus) to describe $V_{1p\text{-}2n}$ and $V_{2p\text{-}1n}$. If one optimizes the parameters in $v(Z)$ separately for $V_{1p\text{-}2n}$ and $V_{2p\text{-}1n}$, the improvement is very minor (less than 1 keV).

A comparison between our results and those of previous studies [16,18] is made in detail. We tabulate the rms deviations of our predicted masses from the AME2003 database [9] with different mass regions for both the stable and unstable

TABLE V. The rms deviations σ by using Eq. (3) and $\sigma_{\rm exp}$ calculated from uncertainties of experimental data of nuclear masses for different n in various regions of A.

Region	$n \geqslant 1$		$n \geqslant 4$		$n \geqslant 8$	
	σ	$\sigma_{\rm exp}$	σ	$\sigma_{\rm exp}$	σ	$\sigma_{\rm exp}$
$60 \leqslant A < 80$	227	151	151	89	98	51
$80 \leqslant A < 100$	143	84	133	39	117	17
$100 \leqslant A < 120$	157	56	109	35	84	25
$120 \leqslant A < 140$	114	44	71	26	58	13
$140 \leqslant A < 160$	86	52	71	25	64	15
$160 \leqslant A < 180$	65	42	51	27	42	15
$180 \leqslant A < 200$	103	41	93	34	61	19
$200 \leqslant A < 220$	77	28	55	21	45	16
$220 \leqslant A < 240$	77	40	53	29	47	25
$240 \leqslant A < 260$	89	19	56	18	34	18

nuclei. The results show that there are considerably large deviations for neutron-rich nuclei with relative small A and that the deviations are relatively small for $140 \leqslant A < 180$ and $200 \leqslant A < 260$.

Note added in Proof: After this paper was accepted, we were informed by Prof. Z. X. Li of other recent efforts of evaluating the nuclear masses. In [36], Wang and collaborators improved the macroscopic-microscopic mass formula by considering the isospin effect and mirror nuclei constraint, and achieved an accuracy with rms deviation around 0.44 MeV for 2149 measured masses.

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