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Description and evaluation of nuclear masses based on residual proton-neutron interactions

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In this paper we study the residual proton-neutron interactions and make use of the systematics of these interactions to describe experimental data of nuclear masses and to predict some of the unknown masses. The odd-even effect staggering of the residual proton-neutron interaction between the last proton and the last neutron is found and argued in terms of pairing interactions. Two local mass relations, which work very accurately for masses of four neighboring nuclei, are discovered. The accuracy of our predicted masses for medium and heavy nuclei is competitive with that of the AME2003 extrapolations, with the virtue of simplicity.

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I. INTRODUCTION

Nuclear mass $M(Z,N)$, and alternatively, binding energy $B(Z,N)$, is one of the fundamental quantities for a given nucleus with proton number Z and neutron number N. The relation between $M(Z,N)$ and $B(Z,N)$ is as follows: $B(Z,N) = M(Z,N) - ZM_{\rm p} - NM_{\rm n}$, where $M_{\rm p}$ is the mass of a free proton, and $M_{\rm n}$ that of a free neutron. This quantity is of great interest not only in nuclear physics but also in astrophysics.

There have been continuous efforts toward constructing formulas to describe available databases and to predict unknown masses, since the early years of nuclear physics. Important progress (e.g., the famous Weizsäcker formula [1], the finite range droplet model [2]) has been made along this line. In recent years, the relativistic mean field model plus the BCS theory has reached an accuracy of root-mean-squared deviation (RMSD) $\sigma \simeq 2$ MeV [3], the Skyrme-Hartree-Fock-Bogoliubov theory [4,5] $\sigma \simeq 581$ keV, the Duflo-Zuker model [6] $\sigma \simeq 380$ keV, and a recent macroscopic-microscopic mass formula $\sigma \simeq 441$ keV [7]. For a comprehensive review, see Ref. [8].

Besides these microscopic and/or macroscopic models, local mass relations have also proved to be useful, for instance the application of Coulomb displacement energies of mirror nuclei in mass predictions of the neutron-deficient nuclei relevant for the astrophysical *rp* process [9]. The most often used local mass relations are probably the Garvey-Kelson formulas [10]. Applications of the Garvey-Kelson mass formulas was investigated many years ago in Refs. [11–13] and was rehabilitated by Barea *et al.* [14,15] in recent years. Very recently, Morales and Frank improved the nuclear mass predictions via iterative processes of the Garvey-Kelson mass relations, by rewriting the Garvey-Kelson mass relations in terms of one-neutron and one-proton separation energies [16]. We also note that an improved mass formula for heavy nuclei with $Z \geqslant 90$ and $N \geqslant 140$ reaches an accuracy of $\sigma \simeq 105$ keV [17].

In Refs. [18,19] we suggested several sets of local mass relations, based on the residual proton-neutron interactions. This paper is a more sophisticated approach along the same line, with the focus on prediction of unknown masses. In Sec. II we present the residual two-body interactions between the last i protons and j neutrons (denoted by $\delta V_{i{\rm p}-j{\rm n}}$) in terms of the interaction between the last proton and the last neutron. We introduce a few phenomenological corrections to refine our predictions of $\delta V_{i{\rm p}-j{\rm n}}$. In Sec. III we construct our local mass formulas by using these $\delta V_{i{\rm p}-j{\rm n}}$ and discuss the RMSDs of our predictions. We present our predicted masses by applying these mass formulas and using the experimental data compiled in the AME2003 database [20] as well as those obtained in recent measurements. In Sec. IV we discuss and summarize the results of this paper.

II. SYSTEMATICS OF THE RESIDUAL PROTON-NEUTRON INTERACTIONS

The residual proton-neutron interactions have been realized to play an important role in the evolution of collectivity, deformation, and phase transitions [21–25], and thus have been attracting considerable attention [26–38]. The proton-neutron interaction between the last i protons and j neutrons is given by

$$\delta V_{i{\rm p}-j{\rm n}}(Z,N) = B(Z,N) + B(Z-i,N-j) - B(Z,N-j) - B(Z-i,N). \quad (1)$$

It is easy to obtain

$$\begin{aligned} \delta V_{1{\rm p}-2{\rm n}}(Z,N) &= \delta V_{1{\rm p}-1{\rm n}}(Z,N) + \delta V_{1{\rm p}-1{\rm n}}(Z,N-1), \\ \delta V_{2{\rm p}-1{\rm n}}(Z,N) &= \delta V_{1{\rm p}-1{\rm n}}(Z,N) + \delta V_{1{\rm p}-1{\rm n}}(Z-1,N); \end{aligned} \quad (2)$$

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namely, $\delta V_{2\mathrm{p}-1\mathrm{n}}$ and $\delta V_{1\mathrm{p}-2\mathrm{n}}$ can be decomposed in terms of $\delta V_{1\mathrm{p}-1\mathrm{n}}$, the residual interaction between the last proton and the last neutron.

We calculate $\delta V_{1\mathrm{p}-1\mathrm{n}}$, $\delta V_{1\mathrm{p}-2\mathrm{n}}$, and $\delta V_{2\mathrm{p}-1\mathrm{n}}$, by using Eq. (1) and the experimental data compiled in Ref. [20]. Our calculated $\delta V_{i\mathrm{p}-j\mathrm{n}}$ are presented in Fig. 1, denoted by open circles. For nuclei with the same mass number A, we calculate the average value of $\delta V_{i\mathrm{p}-j\mathrm{n}}(A)$, denoted by $\overline{\delta V_{i\mathrm{p}-j\mathrm{n}}}(A)$ (see

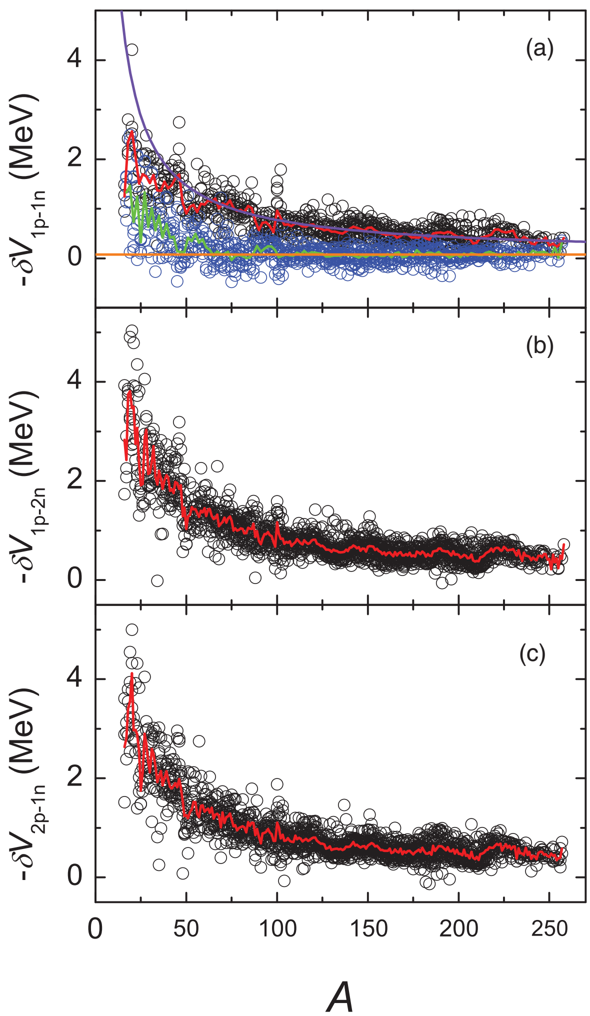

FIG. 1. (Color online) Residual proton-neutron interactions for nuclei with mass number $A \geqslant 16$. A minus sign is added to $\delta V_{i\mathrm{p}-j\mathrm{n}}$ in this figure so that most of the data are above zero, guiding our eyes more comfortably. In panel (a) we present $-\delta V_{1\mathrm{p}-1\mathrm{n}}$ separately for nuclei with even A (black circles) and odd A (blue circles), and the curve in red (green) is plotted by using the average values of $-\delta V_{1\mathrm{p}-1\mathrm{n}}$ for nuclei with mass number A even (odd). The straight line in orange is plotted according to Eq. (3): $-\delta V_{1\mathrm{p}-1\mathrm{n}}(N, Z) = 74$ keV for odd-A nuclei with $A > 100$ and the curve in violet-blue is plotted according to $-\delta V_{1\mathrm{p}-1\mathrm{n}}(N, Z) = 74 + 69\,861/A$ keV for even-A nuclei with $A \geqslant 100$. In panels (b) and (c), circles in black correspond to $-\delta V_{1\mathrm{p}-2\mathrm{n}}$ and $-\delta V_{2\mathrm{p}-1\mathrm{n}}$, respectively, and curves in red are plotted by using their average values with given A. The $-\delta V_{1\mathrm{p}-1\mathrm{n}}$ for nuclei with $Z = N$, $-\delta V_{1\mathrm{p}-2\mathrm{n}}$ for nuclei with $Z = N$ or $Z = N - 1$, or $-\delta V_{2\mathrm{p}-1\mathrm{n}}$ for nuclei with $Z = N$ or $Z = N + 1$ are not included. See the text for details.

the solid curves in red and green in Fig. 1). In Fig. 1 we did not include the results in which nuclei with $Z = N$ are involved, because $\delta V_{1\mathrm{p}-1\mathrm{n}}$ for nuclei with $Z = N$ is exceptionally large.

In Fig. 1(a), one sees that the values of $\delta V_{1\mathrm{p}-1\mathrm{n}}$ for nuclei with odd A are very different from those with even A. In order to understand the possible origin of this odd-even difference, the modified Bethe-Weizsäcker formula [7] is assumed and combined with Eq. (1) for $i = j = 1$. The pairing interaction [denoted by $V_{\mathrm{pairing}}(Z, N)$] in Refs. [7] is as follows:

$$V_{\mathrm{pairing}}(Z, N) = a_{\mathrm{pairing}} A^{-1/3} \begin{cases} 2 - I & \text{for even } Z \text{ and even } N, \\ I & \text{for odd } Z \text{ and odd } N, \\ 1 - I & \text{for odd } Z \text{ and even } N \text{ with } Z < N, \\ 1 & \text{for odd } Z \text{ and even } N \text{ with } Z > N, \\ 1 - I & \text{for even } Z \text{ and odd } N \text{ with } Z > N, \\ 1 & \text{for even } Z \text{ and odd } N \text{ with } Z < N, \end{cases}$$

where $a_{\mathrm{pairing}} = 5442.3$ keV, and $I = |N - Z|/A$. One obtains that the dominant contribution to $\delta V_{1\mathrm{p}-1\mathrm{n}}$ from the pairing interaction[1] is

$$V_{\mathrm{pairing}}(Z, N) + V_{\mathrm{pairing}}(Z-1, N-1) - V_{\mathrm{pairing}}(Z, N-1) - V_{\mathrm{pairing}}(Z, N-1) \simeq \pm a_{\mathrm{pairing}} I A^{-1/3}.$$

Its magnitude is ~164 keV for medium and heavy nuclei, and the signs + and − correspond to $A =$ odd and even, respectively. Here we assume $N > Z$ because we focus on medium and heavy nuclei. This leads to larger values of $-\delta V_{1\mathrm{p}-1\mathrm{n}}$ for nuclei with even A (open circles in black) than those with odd A (open circles in blue), with the odd-even difference about 330 keV. The odd-even difference of $\overline{\delta V_{1\mathrm{p}-1\mathrm{n}}}(A)$ in Fig. 1(a) is about 440 keV, on average. Therefore we suggest that the odd-even difference of $\delta V_{1\mathrm{p}-1\mathrm{n}}(A)$ is dominantly originated from the pairing interaction.

According to Fig. 1(a), the $\overline{\delta V_{1\mathrm{p}-1\mathrm{n}}}(A)$ (see the solid curve in green) for odd-A nuclei with $A \geqslant 100$ is almost constant [close to zero; see the solid line in orange in Fig. 1(a)]. Based on this behavior, we obtain

$$B(Z, N) + B(Z-1, N-1) - B(Z, N-1) - B(Z-1, N) \simeq \overline{\delta V_{1\mathrm{p}-1\mathrm{n}}}(A) \simeq -74 \text{ keV}, \tag{3}$$

where $N + Z = A$ is odd and $A \geqslant 100$. Numerical experiments show that the RMSD of the above relation is only 132 keV for $A \geqslant 100$. This relation is more precise than the Garvey-Kelson mass relations, the RMSD of which is 170 keV for nuclei with $A \geqslant 100$.

The $\delta V_{1\mathrm{p}-1\mathrm{n}}$ for even-A nuclei with $A \geqslant 100$ is higher (with very few exceptions) than those for their neighboring odd-A

[1]The odd-even behavior of $\delta V_{1\mathrm{p}-1\mathrm{n}}$ cannot be explained if one assumes the conventional form of the pairing interaction, e.g., $V_{\mathrm{pairing}}(Z, N) = a_{\mathrm{pair}} A^{-1/2} C$, $C = 1, 0, -1$ for even-even, odd-A, and odd-odd nuclei, respectively.

nuclei. We empirically have

$$\overline{\delta V_{1p-1n}}|_{\text{odd A}} - \overline{\delta V_{1p-1n}}|_{\text{even A}} \simeq \frac{69\,861}{A} \text{ keV},$$

as shown by using the solid curve in violet-blue in Fig. 1(a). From this relation, one obtains

$$\begin{aligned} B(Z, N) + B(Z-1, N-1) - B(Z, N-1) - B(Z-1, N) \\ \simeq \overline{\delta V_{1p-1n}}(A) \simeq -74 - \frac{69\,861}{A} \text{ keV}, \end{aligned} \tag{4}$$

where $N + Z = A$ is even and $A \geqslant 100$. The RMSD of this relation is 168 keV, very close to that of the Garvey-Kelson mass relations (170 keV).

The main advantage of relations given in Eqs. (3)–(4) is that they involve masses of only four neighboring nuclei, while the number of neighboring nuclei involved in the Garvey-Kelson mass relations is six. This is important for reliable predictions in the process of iterative extrapolations. The smaller the number of nuclei in the mass relations is, the smaller the intrinsic error associated with the extrapolations [16] is.

For δV_{1p-2n} and δV_{2p-1n}, there is no odd-even effect as for δV_{1p-1n} in Fig. 1(a). The reason is readily seen in Eq. (2): The number of δV_{1p-1n} with even A is always the same as that with odd A for any $\delta V_{ip-jn}(Z, N)$ if $ij =$ even.

Because our strategy to describe the known masses and predict the unknown masses is to apply Eq. (1), it is most important to obtain reliable predictions of δV_{ip-jn}. Toward this goal, we first take our calculated $\overline{\delta V_{1p-1n}}(A)$ as our initial values, and then introduce a few corrections which are explained as follows.

One of the corrections is called the shell correction, denoted by $\Delta_{\rm sh}$ here. The shell effect on residual proton-neutron interactions was discussed in Refs. [32,33,36], where it was shown that proton-neutron interactions are stronger if the proton fractional fillings and neutron fractional fillings are close to each other [38]. Based on this observation, we empirically obtain the $\Delta_{\rm sh}$ as follows:

$$\begin{aligned} \Delta_{\rm sh}(Z, N) = a_{\rm sh} + 2b_{\rm sh}|\delta_{\rm p}\Omega_N(N_{\rm p} - \Omega_Z) \\ - \delta_{\rm n}\Omega_Z(N_{\rm n} - \Omega_N)|, \end{aligned} \tag{5}$$

where $N_{\rm p}$ ($N_{\rm n}$) is the valence proton (neutron) number with respect to the nearest closed shell, $\delta_{\rm p}$ ($\delta_{\rm n}$) equals $+1$ if the valence protons (neutrons) are particle-like and -1 if hole-like, $\Omega_Z = \sum_{j_Z}(j_Z + \frac{1}{2})$ with j_Z representing angular momenta of single-particle levels for valence protons, and $\Omega_N = \sum_{j_N}(j_N + \frac{1}{2})$ with j_N representing angular momenta of single-particle levels for valence neutrons. $a_{\rm sh}$ and $b_{\rm sh}$ are parameters to be determined via the χ^2 fitting. This correction is the key improvement which reduces the RMSD of δV_{1p-1n} by $\sim$3 keV.

Other corrections that we introduce are enlightened by Refs. [7]. We substitute the modified Bethe-Weizsäcker formula of Refs. [7] into Eq. (1) and expand Eq. (1) in terms of $1/A$ for δV_{1p-1n}. We find that, for nuclei with $A \geqslant 100$, among various contributions to δV_{1p-1n}, the contribution from the surface energies is very small (~ -5 keV), and the contribution from the Coulomb energies is ~ -26 keV. The most important part originates from the symmetry energies, which present ~ -269 keV for $A \geqslant 100$ in δV_{1p-1n}, and the pairing interactions, which present on average 164 keV for odd-A nuclei and -164 keV for even-A nuclei. We therefore focus only on the Coulomb terms and symmetry energies. We study their expansions in terms of $1/A$ and obtain our empirical corrections. The first is called the Coulomb correction, denoted by $\Delta_{\rm C}$:

$$\begin{aligned} \Delta_{\rm C}(Z, N) \approx a_{\rm C}\bigg(-\frac{4}{9}Z^{4/3}A^{-7/3} - \frac{2}{3}ZA^{-4/3} \\ + \frac{4}{9}Z^2A^{-7/3} + \frac{4}{9}Z^{1/3}A^{-4/3}\bigg); \end{aligned} \tag{6}$$

the second is called the symmetry energy correction, denoted by $\Delta_{\rm sym}$:

$$\Delta_{\rm sym}(Z, N) = a_{\rm sym}\frac{1}{A(2 + |IA|)^3} + b_{\rm sym}A^{-1}, \tag{7}$$

where $I = (N - Z)/A$. The $a_{\rm C}$, $a_{\rm sym}$, and $b_{\rm sym}$ are parameters to be determined. The improvement of these two corrections on our predicted δV_{1p-1n} is only $\sim$1 keV. Although these two corrections are small in the present work, we believe that one will achieve important improvements along this line in future, if substantial progress is made in understanding the symmetry energy in atomic nuclei.

In Table I we present the parameters in Eqs. (5)–(7), separately for even A and odd A. We use the χ^2-fitting procedure to achieve the best agreement with the values δV_{1p-1n} extracted from experimental data of binding energies. It is interesting to note that the shell correction on δV_{1p-1n} for even-A nuclei is stronger than for odd-A nuclei (approximately by a factor of three).

Our predicted $\delta V_{ip-jn}(Z, N)$ are summarized as follows:

$$\begin{aligned} -\delta V^{\rm cal}_{1p-1n}(Z, N) &= -\overline{\delta V_{1p-1n}}(A) + \Delta_{\rm sh}(Z, N) \\ &\quad + \Delta_{\rm C}(Z, N) + \Delta_{\rm sym}(Z, N), \\ -\delta V^{\rm cal}_{1p-2n}(Z, N) &= -\overline{\delta V_{1p-2n}}(A) + \Delta_{\rm sh}(Z, N) \\ &\quad + \Delta_{\rm sh}(Z, N-1) + \Delta_{\rm C}(Z, N) \\ &\quad + \Delta_{\rm C}(Z, N-1) + \Delta_{\rm sym}(Z, N) \\ &\quad + \Delta_{\rm sym}(Z, N-1), \\ -\delta V^{\rm cal}_{2p-1n}(Z, N) &= -\overline{\delta V_{2p-1n}}(A) + \Delta_{\rm sh}(Z, N) \\ &\quad + \Delta_{\rm sh}(Z-1, N) + \Delta_{\rm C}(Z, N) \\ &\quad + \Delta_{\rm C}(Z-1, N) + \Delta_{\rm sym}(Z, N) \\ &\quad + \Delta_{\rm sym}(Z-1, N). \end{aligned} \tag{8}$$

TABLE I. The parameters used in Eqs. (5)–(7), in units of keV.

Parameter	For Even A	For Odd A
$a_{\rm sh}$	58.95	15.40
$b_{\rm sh}$	−0.1444	−0.03157
$a_{\rm C}$	−34.80	12.00
$a_{\rm sym}$	12007	22211
$b_{\rm sym}$	−179.7	−70.42

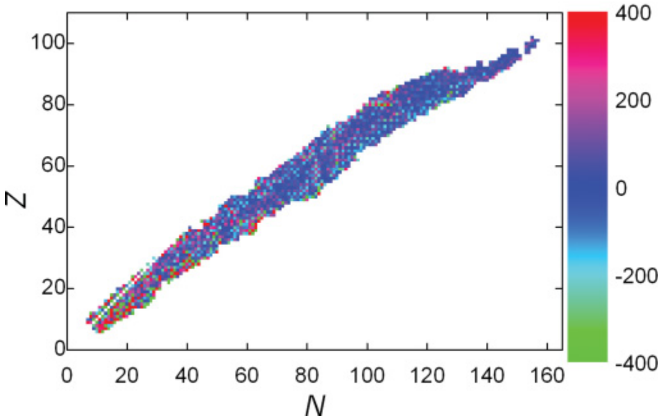

FIG. 2. (Color online) Deviations (in units of keV) of our calculated δV_{1p-1n} by using Eqs. (5)–(8) with respect to those extracted from experimental binding energies [see Eq. (1)], for the nuclei with $A \geqslant 16$.

In Fig. 2 we show deviations (in units of keV) between our calculated δV_{1p-1n} by applying Eqs. (5)–(8) and those calculated by applying Eq. (1) and experimental data of binding energies compiled in Ref. [20]. In Table II we present the RMSDs of our δV_{ip-jn} obtained by using Eqs. (5)–(8), with respect to those extracted from experimental data of binding energies [20]. One sees that the RMSDs of these δV_{ip-jn} decrease with A. The RMSD values are the smallest for δV_{1p-1n} and the largest for δV_{2p-1n}.

III. PREDICTION OF NUCLEAR MASSES

In this section we make use of $\delta V^{\rm cal}_{ip-jn}$ obtained above and predict some of the unknown masses. We replace δV_{ip-jn} by using $\delta V^{\rm cal}_{ip-jn}$ in Eq. (1), and obtain

$$\begin{aligned}
B^{\rm pred}(Z,N) &= B(Z,N-1)+B(Z-1,N)\\
&\quad -B(Z-1,N-1)+\delta V^{\rm cal}_{1p-1n}(Z,N),\\
B^{\rm pred}(Z,N) &= B(Z,N-1)+B(Z+1,N)\\
&\quad -B(Z+1,N-1)-\delta V^{\rm cal}_{1p-1n}(Z+1,N),\\
B^{\rm pred}(Z,N) &= B(Z,N+1)+B(Z+1,N)\\
&\quad -B(Z+1,N+1)+\delta V^{\rm cal}_{1p-1n}(Z+1,N+1),\\
B^{\rm pred}(Z,N) &= B(Z,N+1)+B(Z-1,N)\\
&\quad -B(Z-1,N+1)-\delta V^{\rm cal}_{1p-1n}(Z,N+1),
\end{aligned}\tag{9}$$

TABLE II. The RMSDs (in units of keV) of our calculated proton-neutron interactions by applying Eqs. (5)–(8) with respect to those extracted from experimental data of binding energies.

Region	δV_{1p-1n}	δV_{1p-2n}	δV_{2p-1n}
$A \geqslant 16$	213	235	241
$A \geqslant 60$	159	168	175
$A \geqslant 120$	124	134	142

and

$$\begin{aligned}
B^{\rm pred}(Z,N) &= B(Z,N-2)+B(Z-1,N)\\
&\quad -B(Z-1,N-2)+\delta V^{\rm cal}_{1p-2n}(Z,N),\\
B^{\rm pred}(Z,N) &= B(Z,N-2)+B(Z+1,N)\\
&\quad -B(Z+1,N-2)-\delta V^{\rm cal}_{1p-2n}(Z+1,N),\\
B^{\rm pred}(Z,N) &= B(Z,N+2)+B(Z+1,N)\\
&\quad -B(Z+1,N+2)+\delta V^{\rm cal}_{1p-2n}(Z+1,N+2),\\
B^{\rm pred}(Z,N) &= B(Z,N+2)+B(Z-1,N)\\
&\quad -B(Z-1,N+2)-\delta V^{\rm cal}_{1p-2n}(Z,N+2),\\
B^{\rm pred}(Z,N) &= B(Z,N-1)+B(Z-2,N)\\
&\quad -B(Z-2,N-1)+\delta V^{\rm cal}_{2p-1n}(Z,N),\\
B^{\rm pred}(Z,N) &= B(Z,N-1)+B(Z+2,N)\\
&\quad -B(Z+2,N-1)-\delta V^{\rm cal}_{2p-1n}(Z+2,N),\\
B^{\rm pred}(Z,N) &= B(Z,N+1)+B(Z+2,N)\\
&\quad -B(Z+2,N+1)+\delta V^{\rm cal}_{2p-1n}(Z+2,N+1),\\
B^{\rm pred}(Z,N) &= B(Z,N+1)+B(Z-2,N)\\
&\quad -B(Z-2,N+1)-\delta V^{\rm cal}_{2p-1n}(Z,N+1).
\end{aligned}\tag{10}$$

These twelve relations, together with the $\delta V^{\rm cal}_{1p-1n}$, $\delta V^{\rm cal}_{2p-1n}$, and $\delta V^{\rm cal}_{1p-2n}$ described in Eqs. (5)–(8), are key relations to predict unknown masses in this paper.

A. Error estimation

In this subsection we discuss the errors arising from our predictions. We first investigate the RMSDs of our predicted binding energies by using Eqs. (9) and (10), for nuclei whose binding energies are experimentally known. Similar to procedures in Refs. [14,15,18,19], we take the average value of predicted results by using all possible formulas for a given nucleus (the number of possible formulas is denoted by n, as in Refs. [14,15,18,19]), and calculate the deviations from experimental data. For nuclei with $A \geqslant 60$, the RMSD of Eq. (9) is 131 keV for $n \geqslant 1$; and the RMSD of Eq. (10) is 107 keV for $n \geqslant 1$. The RMSD deviation by using $\delta V_{2p-1n}(Z,N)$ and $\delta V_{1p-2n}(Z,N)$ is 123 keV in Ref. [19], and that by using the Garvey-Kelson relations is 115 keV [14]. These RMSDs show that, for nuclei whose masses are known, the RMSD by using Eq. (10) is the smallest. We note that for known masses, the number n of possible formulas to predict one of masses is usually as large as its maximum [e.g., eight for Eq. (10)]. If one focuses on the results obtained separately by *each* of the formulas, one obtains that the RMSD of Eq. (9) is 134 keV, that of Eq. (10) is 146 keV, and that of the Garvey-Kelson formulas is 157 keV for $A \geqslant 100$. This demonstrates that our formulas in Eqs. (9) and (10) are more accurate than the Garvey-Kelson relations, if the formulas are applied separately.

Below we study the deviations of our predicted masses for nuclei whose masses are unknown. There are two possible origins for deviations of our predicted masses from their true values. One is given by the uncertainties of experimental datum on the right-hand side of Eqs. (9) and (10). The second originates from the approximation in predicting the residual neutron-proton interactions, i.e., $\delta V^{\rm cal}_{\rm 1p-1n}$ in Eq. (9) or $\delta V^{\rm cal}_{\rm 1p-2n}$ and $\delta V^{\rm cal}_{\rm 2p-1n}$ in Eq. (10). We denote the errors associated with such approximations by using $\sigma_{\rm th}$. In other words, the formulas in Eqs. (9) and (10) are not exact; $\sigma_{\rm th}$ might be regarded as the RMSD value of our formulas, if all uncertainties of experimental data for binding energies were zero.

In order to "decouple" the experimental errors, we make use of the procedure described by Möller *et al.* in Ref. [2]. This procedure is based on a so-called maximum-likelihood method, which we describe it as follows. For a set of calculated results, it is assumed that the theoretical errors are Gaussian-type distributed with a standard deviation $\sigma_{\rm th}$ and centered at a mean value $\mu_{\rm th}$. For short here we denote the binding energies by B^i. i is an abbreviation of (Z, N), $i = 1, 2, \ldots, k$. k is the number of different predicted results for the selected set of nuclei. $B^i_{\rm th}$ and $B^i_{\rm exp}$ denote predicted and experimental results of binding energy of the ith nucleus, respectively. We first assume an initial value of $\sigma_{\rm th}$, say, $\sigma_{\rm th} = 100$ keV. Then we calculate the weight factor (w_i) for the ith nucleus:

$$w_i^* = \frac{1}{\left(\alpha_i{}^2 + \sigma_{\rm th}{}^{2*}\right)}, \quad i = 1, 2, \ldots, k. \tag{11}$$

Here $(\alpha_i)^2$ denotes a sum of $(\sigma_{\rm exp})^2$ of all the binding energies involved in the prediction. For example, $(\alpha_i)^2(N, Z) = (\sigma_{\rm exp})^2(Z, N-1) + (\sigma_{\rm exp})^2(Z-1, N) + (\sigma_{\rm exp})^2(Z-1, N-1)$ if one predicts the binding energies by using the first formula in Eq. (9). In this paper the superscript "$*$" of w_i and $\sigma_{\rm th}$ means that the corresponding results are not fixed and they change their values in iterations. We use these w_i^* values and calculate the mean deviation between the predicted and experimental masses for the set of data selected:

$$\mu_{\rm th}{}^* = \frac{\sum_{i=1}^k w_i^*\left(B^i_{\rm exp} - B^i_{\rm th}\right)}{\sum_{i=1}^k w_i^*}. \tag{12}$$

We use these w_i^* and $\mu_{\rm th}{}^*$ to evaluate $\sigma^*_{\rm th}$:

$$(\sigma^*_{\rm th})^2 = \frac{\sum_{i=1}^k w_i^{*2}\left[\left(B^i_{\rm exp} - B^i_{\rm th} - \mu_{\rm th}{}^*\right)^2 - \sigma^{i\ 2}_{\rm exp}\right]}{\sum_{i=1}^k w_i^{*2}}. \tag{13}$$

This new value of $\sigma_{\rm th}{}^{2*}$ is substituted into Eq. (11) to calculate another set of w_i^*, and the above process is iterated until all results are converged (the convergence is found to be extremely rapid), as mentioned in Ref. [2]. We take the converged value of $\sigma_{\rm th}{}^*$ as our evaluated $\sigma_{\rm th}$ for the selected set of nuclei. The results of $\sigma_{\rm th}$ are given for different mass regions and different n in Fig. 3. We assume $\sigma_{\rm th}$ changes smoothly with A, and take the same $\sigma_{\rm th}$ in predicting unknown binding energies in the same mass region (see the smooth curves in Fig. 3). For $A \geqslant 100$ and $n = 1$, the $\sigma_{\rm th}$ of the formulas in Eq. (9) and Eq. (10) is 113 and 127 keV, respectively. Similarly, we calculate $\sigma_{\rm th}$ of the Garvey-Kelson formulas, and the resulting $\sigma_{\rm th}$ (for individual formulas) is 138 keV for $A \geqslant 100$ and $n = 1$.

Now we exemplify the evaluation of errors (or uncertainties) for unknown masses in our predictions by two examples. In the first example, we deal with the case of $n = 1$, and we predict the unknown binding energy of a nucleus with proton number Z and neutron number N. Let us suppose we use the first formula in Eq. (9); the error $\sigma_{\rm pred}(Z, N)$ of our predicted binding energy is readily given by

$$\begin{aligned}&[\sigma_{\rm pred}(Z, N)]^2\\ &\quad = [\sigma_{\rm th}(A)]^2 + [\sigma_{\rm exp}(Z, N-1)]^2\\ &\qquad + [\sigma_{\rm exp}(Z-1, N)]^2 + [\sigma_{\rm exp}(Z-1, N-1)]^2.\end{aligned}$$

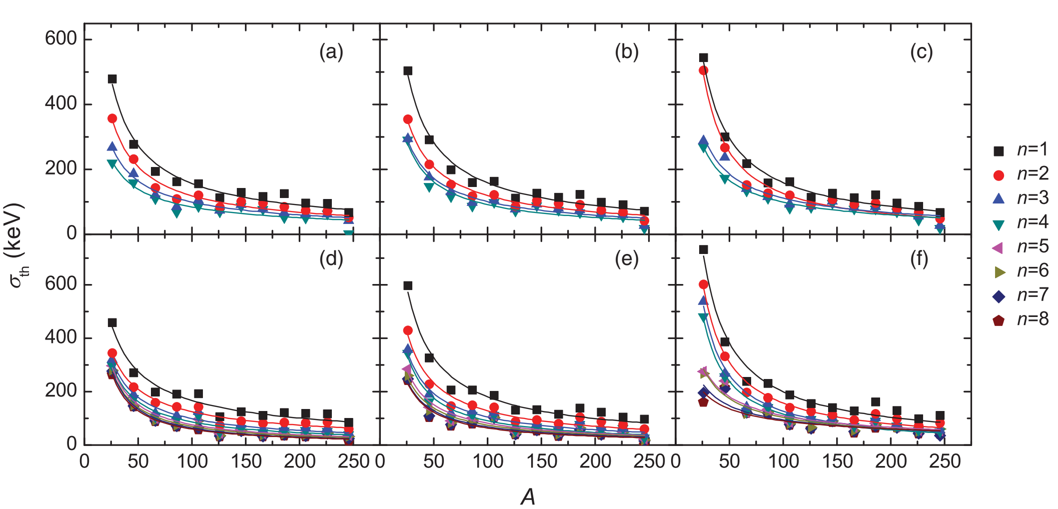

FIG. 3. (Color online) The theoretical errors ($\sigma_{\rm th}$) associated with our formulas versus mass number A. Panel (a), (b), and (c) [(d), (e), and (f)] correspond to Eq. (9) [Eq. (10)] for even-even, odd-A, and odd-odd nuclei, respectively. The results of $\sigma_{\rm th}$ are obtained for selected sets of nuclei with $n = 1$ to 4 for Eq. (9) and $n = 1$ to 8 for Eq. (10), and the smooth curves are plotted by fitting these calculated $\sigma_{\rm th}$.

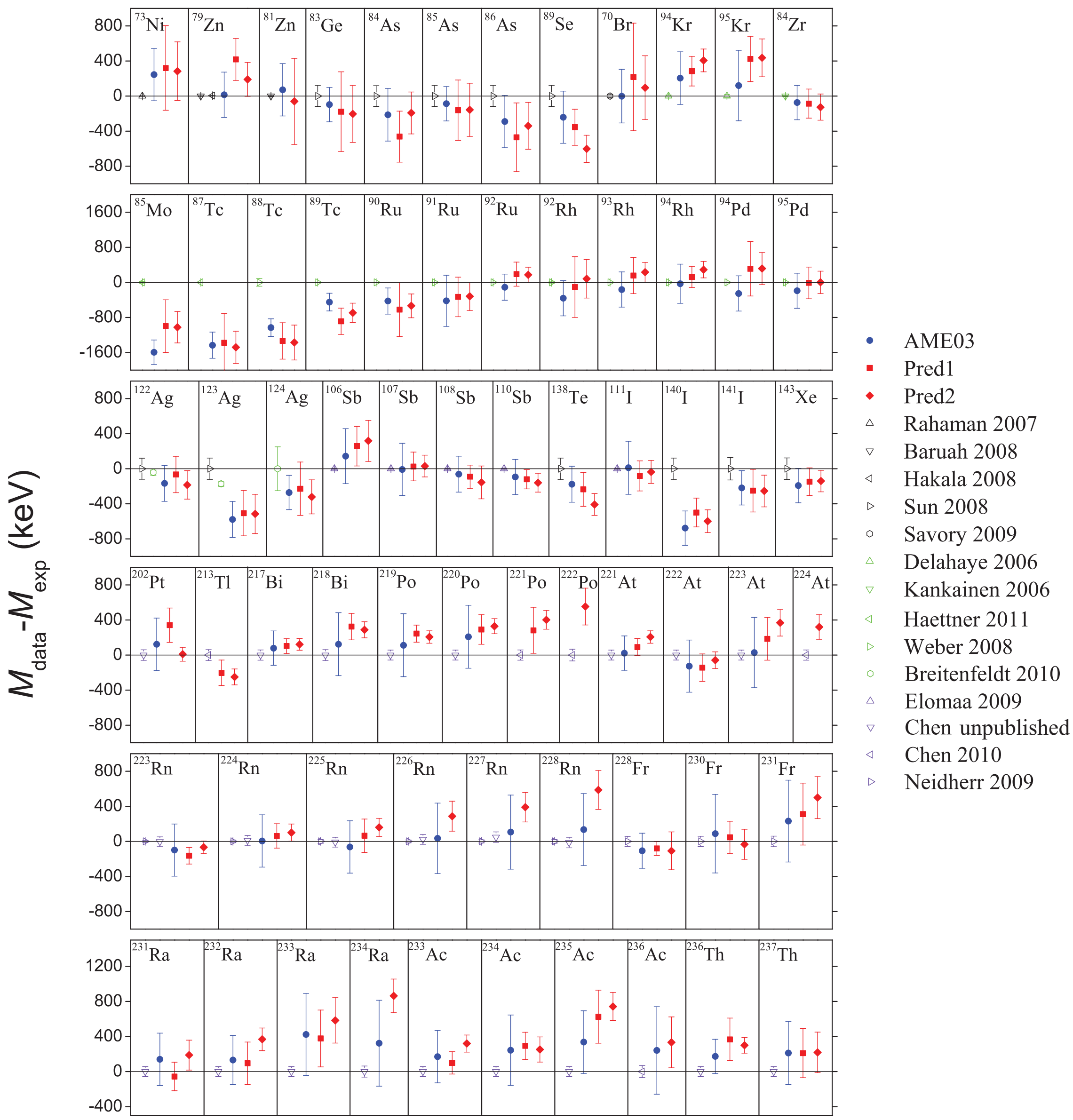

FIG. 4. (Color online) Comparison between masses (in units of keV) obtained in recent measurements, those predicted in the AME2003 extrapolations (solid circles in blue), and our new approach (solid squares and diamonds in red). The references in this figure are as follows: Rahaman 2007 [40], Baruah 2008 [41], Hakala 2008 [42], Sun 2008 [43], Savory 2009 [44], Delahaye 2006 [45], Kankainen 2006 [46], Haettner 2011 [47], Weber 2008 [48], Breitenfeldt 2010 [49], Elomaa 2009 [50], Chen unpublished [51], Chen 2010 [52], Neidherr 2009 [53].

In the second example, we deal with the case of $n = 2$. Let us suppose that we use the first and the second formulas of Eq. (9). In this case

$$\begin{aligned} B^{\mathrm{pred}}(Z,N) = {} & B(Z,N-1) + \tfrac{1}{2}B(Z-1,N) \\ & - \tfrac{1}{2}B(Z-1,N-1) + \tfrac{1}{2}B(Z+1,N) \\ & - \tfrac{1}{2}B(Z+1,N-1) + \tfrac{1}{2}\big[\delta V^{\mathrm{cal}}_{1\mathrm{p}-1\mathrm{n}}(Z,N) \\ & - \delta V^{\mathrm{cal}}_{1\mathrm{p}-1\mathrm{n}}(Z+1,N)\big], \end{aligned}$$

and $\sigma_{\mathrm{pred}}(Z,N)$ is given by

$$\begin{aligned} & [\sigma_{\mathrm{pred}}(Z,N)]^2 \\ & \quad = [\sigma_{\mathrm{exp}}(Z,N-1)]^2 + \tfrac{1}{4}[\sigma_{\mathrm{exp}}(Z-1,N)]^2 \\ & \qquad + \tfrac{1}{4}[\sigma_{\mathrm{exp}}(Z-1,N-1)]^2 + \tfrac{1}{4}[\sigma_{\mathrm{exp}}(Z+1,N)]^2 \\ & \qquad + \tfrac{1}{4}[\sigma_{\mathrm{exp}}(Z+1,N-1)]^2 + [\sigma_{\mathrm{th}}(n=2,A)]^2. \end{aligned}$$

$\sigma_{\mathrm{pred}}(Z,N)$ is calculated similarly for other cases.

If we make use of the formulas in Eqs. (9) and (10) to predict unknown masses in the second and/or the third successive extrapolations, our predicted errors are accumulated. In the second-step extrapolation one of the binding energies is based on our predictions, and in the third-step extrapolation one or two binding energies are based on predictions. The values of σ_{pred} for these nuclei are taken to be the surrogates of their σ_{exp}. Therefore the errors of our predictions increase if successive extrapolations are employed.

B. Mass predictions

We denote our predicted masses based on Eq. (9) by $M^{\mathrm{pred}(1)}$, and those based on Eq. (10) by $M^{\mathrm{pred}(2)}$. We take the experimental data of masses compiled in the AME2003 database and obtain our predicted results of 463 unknown $M^{\mathrm{pred}(1)}$ and 791 $M^{\mathrm{pred}(2)}$ by up to three successive extrapolations from known masses. These predicted results are tabulated in Ref. [39]. Without details we note that our predicted masses are, roughly speaking, very close to those predicted in the AME2003 database, in particular for those with $A \geqslant 100$.

Since the AME2003 database was published, new measurements of masses were performed [40–53]. These measurements offer us an opportunity to investigate how well our approach works in predicting unknown masses. Comparisons between new experimental data and our predictions as well as extrapolated values in the AME2003 database are made in Fig. 4. One sees that the accuracy of our predictions is competitive with that of the AME2003 extrapolations. It is interesting to note that when our predicted values are lower than experimental values, the predicted values in the AME2003 database are dominantly lower, too, and vice versa.

Now let us pay attention to a few examples for which the deviations of our predicted results from experimental data are large. (a) The nuclei ^{85}Mo, $^{87\sim89}$Tc, and ^{123}Ag. New experimental data [43,46–49] of binding energies involved in evaluations of these nuclei are very different from those compiled in the AME2003 database. By updating the data by those given in Refs. [43,46–49], our predicted results are now reasonably consistent with experimental results, as shown in Fig. 5. (b) The ^{140}I nucleus. Neither predicted results in this work nor those in the AME2003 database are very consistent with experimental data. In this paper we use ^{139}I, ^{140}Xe, and ^{141}Xe in the evaluation of mass for ^{140}I. The experimental data of masses for ^{139}I, ^{140}Xe, and ^{141}Xe are (in units of keV) $-68\,837.893 \pm 31.074$, $-72\,990.992 \pm 60.558$, and $-68\,326.902 \pm 90.613$ in the AME2003 database [20], respectively. Even if we used the new set of data given in Ref. [43], the deviation from experimental data would remain large. Improvements of predictions may be achieved if more precise measurements are made on these three masses in future. (c) ^{222}Po, $^{226-228}$Rn, $^{233-234}$Ra, ^{235}Ac. The predicted values are not very consistent with experimental data. An explanation

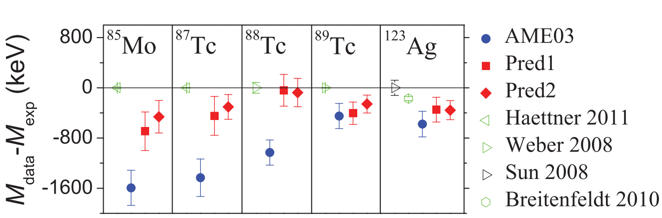

FIG. 5. (Color online) Same as Fig. 4 for ^{85}Mo, $^{87\sim89}$Tc, and ^{123}Ag, but predicted results here are recalculated based on new experimental data of masses [43,46–49] for their neighboring nuclei which are involved in Eqs. (8)–(9). One sees substantial improvement of consistency between the predicted results and experimental data. The references in this figure are as follows: Haettner 2011 [47], Weber 2008 [48], Sun 2008 [43], and Breitenfeldt 2010 [49].

is that the relevant nuclei locate along the "diagonal" line of the ($Z \geqslant 82$, $N \geqslant 126$) shell closure, where the proton fractional fillings and neutron fractional fillings are close to each other. The shell correction term is not optimized for nuclei in this region, and this deviation leads to an overestimation of $\delta V_{1\mathrm{p}-1\mathrm{n}}(A)$ values here.

By applying Eqs. (9) and (10) and by using $\delta V^{\mathrm{cal}}_{1\mathrm{p}-1\mathrm{n}}$, $\delta V^{\mathrm{cal}}_{2\mathrm{p}-1\mathrm{n}}$, and $\delta V^{\mathrm{cal}}_{1\mathrm{p}-2\mathrm{n}}$ described in Eqs. (5)–(8), as well as experimental data compiled in Ref. [20] and recent measurements in Refs. [40–77], we have predicted in total 471 $M^{\mathrm{pred}(1)}$ and 785 $M^{\mathrm{pred}(2)}$ of unknown masses by three successive extrapolations. Our predicted results are tabulated in [78].

In Table III we present a small set of selected data among our predicted results [78]. These selected masses are either important in the context of astrophysics and nuclear structure or to be measured in the near future. ^{84}Mo, ^{86}Tc, ^{88}Ru, ^{90}Rh, ^{92}Pd, and ^{94}Ag are mainly in the $N = Z$ line and thus critical to the *rp*-process simulation. ^{129}Cd, ^{135}Sn, and ^{204}Pt are possibly achieved soon in mass measurements. Our results of ^{84}Mo, ^{129}Cd, and ^{135}Sn are close to those evaluations in the AME2003 database and the mass of ^{204}Pt is not evaluated in the AME2003 database. Other results considerably deviate from the predictions in the AME2003 database. Very interestingly, however, our predicted results are quite consistent with those in the AME2011-preview evaluations [79].

IV. DISCUSSION AND CONCLUSIONS

In this paper we study systematics of the residual proton-neutron interactions, $\delta V_{i\mathrm{p}-j\mathrm{n}}$, and make use of these results in evaluating nuclear masses and predicting the unknown masses. In order to improve the accuracy of our predicted $\delta V_{i\mathrm{p}-j\mathrm{n}}$, we take the average value of $\delta V_{i\mathrm{p}-j\mathrm{n}}$ for all nuclei with given mass number A, and introduce a number of corrections. The key correction here is the shell correction.

We find an odd-even difference of $\delta V_{1\mathrm{p}-1\mathrm{n}}$ for nuclei with odd mass number A and even A. We suggest an argument on the possible origin of this odd-even difference in terms of pairing interactions. The simple behavior of $\delta V_{1\mathrm{p}-1\mathrm{n}}$ for nuclei with $A \geqslant 100$ leads to two useful formulas: $B(Z,N) + B(Z-1,N-1) - B(Z,N-1) - B(Z-1,N) = -74$ keV for odd A, the RMSD of which is only 132 keV; and $B(Z,N) + B(Z-1,N-1) - B(Z,N-1) - B(Z-1,N) = -74 - 69861/A$ keV for even A, the RMSD of which is 168 keV. The RMSD of the Garvey-Kelson mass relations is $\sim$170 keV for the same set of nuclei.

One important feature of the method in this work is that the theoretical errors associated with the formulas, σ_{th}, are smaller than those of the Garvey-Kelson relations for $n = 1$. This feature is very important, because the number of formulas n is always small for the extrapolations to unknown masses.

In predicting the unknown masses, the number of nuclei involved in each formula of the Garvey-Kelson mass relations is five, and that in each of our formulas is three (thus smaller). A smaller number of nuclei involved in local mass relations is desirable for more reliable predictions in iterative extrapolations: The smaller the number of masses in mass

TABLE III. Selected data among our predicted mass excesses (in units of keV) [78]. These unknown masses are either important in the context of astrophysics and nuclear structure or to be measured in the near future. $M^{\mathrm{pred}(1)}$ and $M^{\mathrm{pred}(2)}$ correspond to predicted results by using Eq. (9) and Eq. (10), respectively. AME2003 corresponds to predicted results in the AME2003 database, and AME2011-preview corresponds to results in tables of Ref. [79], which is a preview of the recent evaluation by Audi *et al*.

Nucleus	$M^{\mathrm{pred}(1)}$	$M^{\mathrm{pred}(2)}$	AME2003	AME2011-preview
^{84}Mo	-55687 ± 394	-55681 ± 368	-55806 ± 401	-54502 ± 401
^{86}Tc	-50969 ± 184	-51359 ± 247	-53207 ± 298	-51297 ± 298
^{88}Ru	-54277 ± 276	-54314 ± 184	-55647 ± 401	-54399 ± 298
^{90}Rh	-52378 ± 315	-52163 ± 207	-53216 ± 503	-51959 ± 401
^{92}Pd	-54962 ± 295	-54722 ± 166	-55498 ± 503	-55070 ± 503
^{94}Ag	-52719 ± 465	-52629 ± 285	-53300 ± 503	-52412 ± 641
^{129}Cd	-63500 ± 179	-63360 ± 131	-63202 ± 298	-63314 ± 196
^{135}Sn	-61017 ± 279	-61022 ± 215	-60799 ± 401	-60612 ± 401
^{204}Pt	-17955 ± 221	-17995 ± 111		-18062 ± 401

relations is, the smaller the errors associated with the process of extrapolations are [16]. This is another advantage of our approach.

We make use of our predicted values of δV_{1p-1n}, δV_{1p-2n}, δV_{2p-1n} in predicting unknown masses by using successive extrapolations of the nuclei whose masses are experimentally known [20]. Our predicted masses are compared with predictions in the AME2003 database as well as experimental values in recent measurements. It is shown that the accuracy of our predicted results is competitive with the AME2003 database, with the virtue of simplicity.

Finally, we predict unknown masses based on extrapolations of the up-to-date experimental data of binding energies, and tabulate our predicted masses in Ref. [78]. A small set of selected results, which are either important in the context of astrophysics and nuclear structure or to be measured in the near future, are presented.

We believe that the new mass relations discovered in this paper, and the simple procedures of extrapolation by using the residual proton-neutron interactions, as well as our predicted results of some unknown masses, will be very useful in future studies. More accurate predictions can be readily made if the predicted proton-neutron interactions are further refined locally.

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