Mass relations of mirror nuclei

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In this paper we revisit mass relations of mirror nuclei by considering the odd-even feature in Coulomb energy. A substantial improvement and competitive accuracy of mass relations is achieved, with root-mean-squared deviations (RMSD) of only 93 keV; for the first time one is able to construct simple mass formulas for mirror nuclei with the RMSD below 100 keV in light- and medium-mass regions (mass number $A = 20$–90) by using only four parameters. As a by-product we tabulate our predictions of masses excesses unaccessible experimentally in the Supplemental Material of this paper.

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Nuclear mass M, neutron separation energy S_n, and proton separation energy S_p are fundamental quantities in nuclear physics and astrophysics [throughout this paper we use $M(N, Z)$ to denote the mass of nucleus with neutron number N and proton number Z]. There are many theoretical models and methods to describe the atomic-mass evaluation database and to predict unknown masses [1,2]. Here we mention a few theoretical models, such as the Duflo-Zuker model [3], the finite-range droplet model (FRDM) [4,5], the Skyrme Hartree-Fock-Bogoliubov theory [6], and Weizsäcker-Skyrme (WS) model [7,8]. From another perspective, various mass relations have been proved to be useful in local mass regions, such as the Audi-Wapstra extrapolation method [9–11], the Garvey-Kelson mass relations [12,13], the mass relations based on neutron-proton interactions [14,15], and mass relations associated with mirror nuclei [16,17].

The mass relations of mirror nuclei are based on the isospin symmetry of interactions between nucleons. The empirical neutron-proton interaction of mirror nuclei was studied many years ago, with the focus of the isospin symmetry conservation [18,19]. This symmetry was exemplified recently by Zhang *et al.* [20] by the latest mass measurements. A number of generalized Garvey-Kelson mass relations of mirror nuclei were constructed by Tian *et al.*, with the resultant root-mean-square deviation (RMSD) being 0.398 MeV for 31 proton-rich nuclei [21]. By using an empirical Coulomb energy and phenomenological shell corrections, a number of simple relations between two mirror nuclei were constructed in Ref. [16], with the RMSD from 120 to 290 keV. The idea of Ref. [16] was further exploited by replacing mass differences by one-nucleon separation energies of two corresponding mirror nuclei in Ref. [17], where the RMSD were reduced to 110–130 keV. In this paper we revisit mass relations of Ref. [17] by further considering the odd-even feature in Coulomb energy. Simple mass formulas for mirror nuclei are constructed with the RMSD 93 keV for nuclei mass number A between 20 to 90, with a total of four parameters.

Let us begin with the simple Weizsäcker formula, viz.,

$$\begin{aligned} M(N,Z) &\equiv NM_n + ZM_p - B(N,Z) \\ &= NM_n + ZM_p - a_v A + a_s A^{2/3} + a_c Z^2 A^{-1/3} \\ &\quad + a_a (N-Z)^2 A^{-1} - \delta_{\rm pair}, \end{aligned} \tag{1}$$

where $A = N + Z$, M_n, and M_p represent masses of a free neutron and a free proton, respectively; a_v, a_s, a_c, a_a are the volume term, surface term, Coulomb term, and symmetry term coefficient, respectively (here we use the convention that Coulomb energy, surface energy, and symmetry energy are positive, and the volume energy and the pairing term $\delta_{\rm pair}$ are negative). From the above Weizsäcker formula, one easily derives a simple formula of mass differences between two corresponding mirror nuclei with neutron and proton numbers $(N, Z) = (K - k, K)$ and $(K, K - k)$ as follows [16]:

$$\begin{aligned} \Delta_m(K-k,K) &\equiv M(K-k,K) - M(K,K-k) \\ &= a_c k A^{2/3} + k(M_p - M_n), \end{aligned} \tag{2}$$

where $A = 2K - k$ is the mass number of corresponding mirror nuclei. In the above formula, the first term results from the Coulomb energy difference between mirror nuclei, and the second term correspond to the proton-neutron mass difference. We note that the parameter $(M_p - M_n)$ should be close to the mass difference of a free proton and a free neutron but meanwhile subtracted by the mass of an electron (i.e., 1.293–0.511 MeV = 0.782 MeV), if one adopts the mass database from the atomic mass evaluation (AME) in calculations, and this is the case in this paper. We also note here that if one further considers the parity of neutrons and protons of $\delta_{\rm pair}$ in the Weizsäcker formula, then the mass formulas of Ref. [16] are improved: Our present numerical experiments by using the AME2016 database show that, for an even value of k ($k = 2, 4$, i.e., proton number and neutron numbers of

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the mirror nuclei have the same parity), the improvement by discriminating the parity of k is relatively small (the RMSD value is reduced by about 20 keV), while for an odd value of k (i.e., $k = 1$ and 3, in these cases the parity of $K - k$ and that of K are different), the reduction of the RMSD value is large (by about 90 keV).

In this paper we report an odd-even staggering for deviations of the formulas in Ref. [17] from experimental values and make use of this feature to improve our mass formulas. According to Eqs. (15) and (16) in Ref. [17],

$$\begin{aligned}\Delta_n(K-k,K) &\equiv M(K-1-k,K) - M(K-k,K)\\ &\quad - M(K,K-k-1) + M(K,K-k)\\ &= a_c\delta_c^n + (M_p - M_n) = a_c\delta_c^n - C, \end{aligned}\qquad (3)$$

$$\begin{aligned}\Delta_p(K-k,K) &\equiv M(K-k,K-1) - M(K-k,K)\\ &\quad - M(K-1,K-k) + M(K,K-k)\\ &= a_c\delta_c^p + (M_n - M_p) = a_c\delta_c^p + C, \end{aligned}\qquad (4)$$

where Δ_n is the difference of one-neutron separation energy between the nucleus with $(N,Z) = (K-k,K)$ and one-proton separation energy of the nucleus with $(N,Z) = (K,K-k)$, and Δ_p is the difference of one-proton separation energy of the nucleus with $(N,Z) = (K-k,K)$ and one-neutron separation energy of the nucleus with $(N,Z) = (K,K-k)$. δ_c^n and δ_c^p is given by the simple Coulomb-energy term in Eq. (1). According to Eqs. (17) and (18) of Ref. [17],

$$\delta_c^n = (k+1)(A-1)^{2/3} - kA^{2/3}, \qquad (5)$$

$$\delta_c^p = (k-1)(A-1)^{2/3} - kA^{2/3}, \qquad (6)$$

with $A = 2K - k = N + Z$. The Δ_n-δ_c^n formula of Eq. (3) and the Δ_p-δ_c^p relation of Eq. (4) have been exemplified to the AME2016 database, with their RMSD equal to 113 keV and 132 keV, respectively. Clearly, both Δ_n and Δ_p are double mass differences for two successive mirror nuclei. If the isospin symmetry is conserved, then the mass difference of mirror nuclei should be interpreted in terms of Coulomb energy and neutron-proton mass difference. Yet the ambiguity in Coulomb energies of two mirror nuclei leads to an RMSD of 100–200 keV, even if one adopts pairing term individually for protons and neutrons, as discussed above. The key of the substantial improvement of mass formulas in Ref. [17] is that *the difference between Coulomb energies of two successive nuclei is small*; thus the effect of this ambiguity becomes much smaller, even if there is considerably large uncertainty in our theoretical Coulomb energy.

Let us proceed our discussion with rewriting Eqs. (3) and (4) in terms of Δ_m of Eq. (2),

$$\Delta_n(K-k,K) = \Delta_m(K-k-1,K) - \Delta_m(K-k,K),$$

$$\Delta_p(K-k,K) = \Delta_m(K-k,K-1) - \Delta_m(K-k,K).$$

From these two relations, one immediately sees that the RMSD values for both Δ_n and Δ_p are expected to exhibit an odd-even staggering. For example, $\Delta_n(K-k,K)$ involves two $\Delta_m(N,Z)$ with the same proton number $Z = K$, while the difference of their neutron numbers is 1, and therefore one of the neutron number of Δ_m involved in $\Delta_n(K-k,K)$ is odd and the other is even. The situation is similar to $\Delta_p(K-k,K)$.

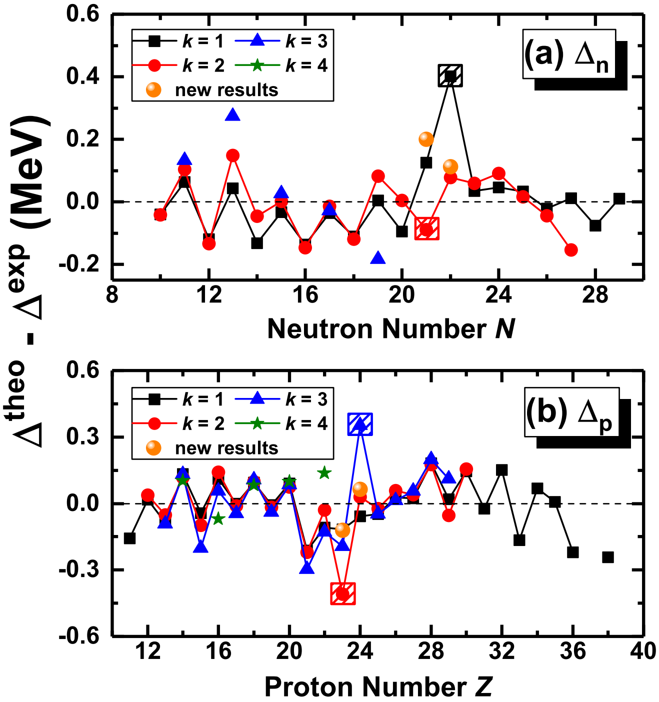

FIG. 1. Deviations (in unit of MeV) of theoretical values of mirror nuclei mass relations, i.e., Eqs. (3) and (4), from experimental data in the AME2016 [11] for $10 \leqslant Z, N \leqslant 40$. Solid squares in black, circles in red, triangles in blue, and stars in olive correspond to $k = 1, 2, 3, 4$, respectively. Panel (a) plots the Δ_n-δ_c^n relation of Eq. (3) and panel (b) plots the Δ_p-δ_c^p relation of Eq. (4). One clearly sees odd-even staggering of deviation around zero for all values of k. The results extracted from the mass excess of ^{44}V in the AME2016 database are denoted with shadows, and results of the same nuclei by recent measurement [20] are shown by solid circles in orange. One sees those large deviations are reduced substantially with results of the recent experimental measurements.

In Figs. 1(a) and 1(b), we plot the deviations of theoretical values by using Eqs. (3) and (4) from experimental data in the AME2016 database [11], where odd-even staggerings are easily seen, despite a few “anomalous” results which are denoted with open squares in shadow. These anomalies are all related to proton-rich nucleus ^{44}V whose experimental uncertainty is very large (182 keV) in the AME2016 database. As Eqs. (3) and (4) are very accurate, it is tempting to predict the mass of this nucleus by these formulas. The predicted result of the mass excess for this nucleus was −23825 (44) keV, −23716 (214) keV, and −23707 (132) keV, −23709 (113) keV, respectively (see the Supplemental Material of Ref. [17]), in comparison with −24116 (182) keV in the AME2016 database. Very interestingly, new mass measurements of this nucleus were performed recently: Its experimental mass excess was reported to be −23827 (20) keV in Ref. [20] and −23805 (80) keV in Ref. [22], both of which are very close to our predicted results enclosed in the Supplemental Material of Ref. [17]. We now replace the mass excess of the ^{44}V nucleus in the AME2016 database by the experimental mass excess reported in Ref. [20] and replot those corresponding results by using solid circles in orange. Here one sees that those anomalies almost disappear.

TABLE I. The RMSD (in keV) of Eqs. (3) and (4), the pair number of mirror nuclei involved (denoted by $\mathcal{N}$), and the values of our parameters a_c and C (in unit of keV) in Eqs. (3) and (4) optimized by using the AME2016 database [11], for nuclei with N and $Z \geqslant 10$, and with the result of ^{44}V replaced by using the result of a recent measurement [20]. The results in the last row, labeled Δ, are obtained by using the same a_c and C for different parity in Eqs. (3) and (4). RMSD′, a_c', and C' are the same results of Eqs. (3) and (4) but replacing the Coulomb term in Eq. (1) with Eq. (8). a_c and C are discriminated by their parity of proton and neutron numbers. For Δ_p with odd proton numbers and for Δ_n with odd neutron numbers, we denote the a_c and C by "odd"; for Δ_p with even proton numbers and for Δ_n with even neutron numbers, we denote the a_c and C by "even."

Δ	$\mathcal{N}$	RMSD	a_c(even, odd)	C(even, odd)	RMSD′	a_c'(even, odd)	C'(even, odd)
Δ_n	43	82	$701 \pm 8, 733 \pm 9$	$1599 \pm 84, 2043 \pm 99$	82	$690 \pm 7, 723 \pm 9$	$716 \pm 74, 1124 \pm 87$
Δ_p	68	94	$692 \pm 7, 713 \pm 7$	$1457 \pm 83, 1843 \pm 82$	94	$684 \pm 7, 704 \pm 7$	$607 \pm 74, 962 \pm 74$
Δ	111	93	$696 \pm 5, 719 \pm 5$	$1527 \pm 60, 1905 \pm 63$	92	$688 \pm 5, 710 \pm 5$	$664 \pm 54, 1011 \pm 56$

Now we make use of Eqs. (3) and (4), but with discrimination for parity of neutron number N for the Δ_n-δ_c^n formula and for parity of proton number Z in the Δ_p-δ_c^p formula, and with updated mass excess of ^{44}V by experimental data in Ref. [20]. In the first two rows of Table I we present the optimized parameters a_c and C in Eq. (3) and (4), and corresponding RMSD values and the number (denoted by $\mathcal{N}$) of mirror pairs in our calculations. There are in total eight parameters for Δ_n-δ_c^n and Δ_p-δ_c^p formulas. The resultant RMSD values are 82 keV and 94 keV for Δ_n-δ_c^n and Δ_p-δ_c^p, respectively.

From Table I, one sees that the two set of parameters, one set for Δ_n and the other set for Δ_p, well overlap with each other. Thus, unlike Ref. [17], here we assume the same values of a_c and C in Eq. (3) and (4) and present them in the third row of Table I. This unification leads minor changes of the resultant RMSD values, but the total number of parameters is reduced from 8 to 4.

By these unified notations of Δ and δ_c, we have

$$\Delta = a_c\delta_c \mp C, \tag{7}$$

where we take a $-$ sign for Δ_n and a $+$ sign for Δ_p. The Δ-δ_c plot is presented in Fig. 2, where the results for Δ_p with odd proton numbers and for Δ_n with odd neutron numbers are denoted by solid circles in red and by solid squares in black otherwise. To be compact and convenient in our figure, the plot for Δ_p is presented by using $|\Delta_p| = -\Delta_p$ and $|\delta_c^p| = -\delta_c^p$ (both Δ_p and δ_c^p are negative). One sees a clear odd-even feature of Δ_n and Δ_p for small $|\delta_c^n|$ and $|\delta_c^p|$. The resultant RMSD value of Δ-δ_c relation is 93 keV for 111 pairs of mirror nuclei.

In Table I, the values of parameters $a_c \sim 0.7$ MeV and are close to the value of treating an atomic nucleus as a uniformed charged sphere, which is equal to

$$a_c = \frac{3}{5}\frac{e^2}{4\pi\epsilon_0 r_0},$$

where r_0 is usually taken to be 1.2 fm, correspondingly $a_c \simeq$ 0.72 MeV. On the other hand, the parameter C is around 1.5 MeV for the "even" type and around 1.9 MeV for the "odd" type, both of which are much larger than the expected value of C [0.782 MeV, see the discussion below Eq. (2)]. Furthermore, the difference of parameter C between these two cases is about 0.4 MeV. Below we discuss these two issues.

Let us first come to the question why the value of C deviates from its expected value. This issue could be explained by an oversimplification of the Coulomb energy term in Eq. (1). If one assumes a more sophisticated form [23–25] instead,

$$E_c = E_c^d + E_c^e + E_c^s = a_c\frac{Z^2}{A^{1/3}} - \frac{5}{4}\left(\frac{3}{2\pi}\right)^{2/3} a_c\frac{Z^{4/3}}{A^{1/3}} - a_c\frac{Z}{A^{1/3}}, \tag{8}$$

then one obtains much complicated formulas of δ_c^n and δ_c^p, denoted by $\delta_c^{n'}$ and $\delta_c^{p'}$. In the above formula, the second term E_c^e is called the exchange term in the Fermi gas model, and the third term E_c^s is called the self-energy term which equals the total Coulomb energy of Z protons moving individually in a sphere with the same size of the nucleus in consideration. For convenience and to be compact in our discussion, we present the formulas of $\delta_c^{n'}$ and $\delta_c^{p'}$ in the Appendix.

Assuming the Coulomb energy of Eq. (8), similarly to Eqs. (3) and (4) and Eq. (7), we have

$$\Delta_n(K-k, K) = a_c'\delta_c^{n'} - C', \tag{9}$$

$$\Delta_p(K-k, K) = a_c'\delta_c^{p'} + C', \tag{10}$$

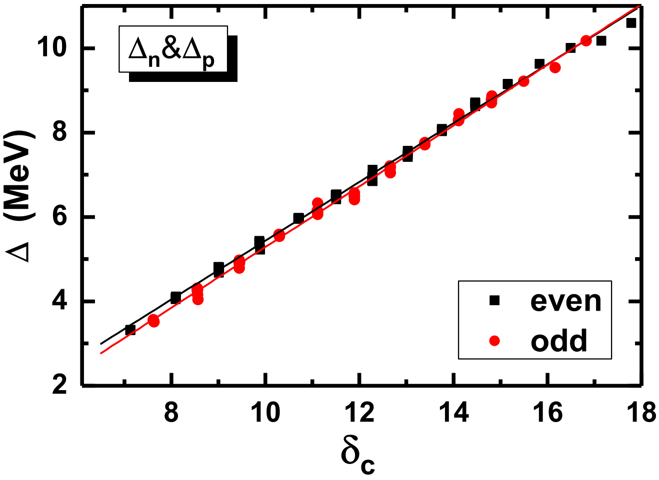

FIG. 2. Δ_n-δ_c^n and Δ_p-δ_c^p correlations for nuclei with $N, Z \geqslant 10$. Both Δ_p and δ_c^p are multiplied by -1 (see the text for details). Solid squares in black corresponds to Δ_n (Δ_p) with even neutron (proton) numbers, and circles in red corresponds to those with odd neutron (proton) numbers. The results are extracted based on the AME2016, except that the mass excess of the ^{44}V nucleus is replaced by that measured in Ref. [20]. The straight lines are plotted by using optimized parameters a_c and C listed in the last row of Table I.

The resultant values of a_c' and C' are listed in the last three columns of Table I. The average value of parameter C' in the last row is 0.838 keV, which is reasonably close to its expected value (0.782 MeV). We note that the assumption of a sophisticated Coulomb energy of Eq. (8) does account for the agreement between the average value of parameter C' and its expected value; on the other hand, the δ_c' in Eqs. (9) and (10) is more complex and the resultant RMSD values remain essentially unchanged in comparison with those in Eqs. (3) and (4) which are more favorable and convenient in numerical practices due to their simplicities.

The second issue related to the parameter C is the large difference (about 0.4 MeV) of the even and odd type of Δ-δ_c or Δ-δ_c' formulas. This puzzle is interpreted in terms of an odd-even feature in the Coulomb energy, namely a so-called pairing effect. This effect is not new and was studied extensively more than half a century ago, e.g., in Refs. [23,24,26,27]. See Ref. [25] for a comprehensive review. The general explanation is as follows. This odd-even feature in Coulomb energy results from the pairing correlation of identical protons, namely two protons have a larger probability of being found close together if their spins are oppositely directed. The Coulomb interactions between protons are far too weak to prevent pairing; on the other hand, the Coulomb energy depends on the spatial distribution of protons, and therefore its odd-even alternation is a rough measure of the pairing correlation.

It is interesting to investigate the odd-even gap of C value extracted from experimental data and present a comparison with the result in this paper (about 0.4 MeV) and previous theoretical studies. Toward that goal, we first define the empirical odd-even gap in Coulomb energy,

$$\begin{aligned}\delta_{\rm pair}(K-k,K)\\ &\equiv \tfrac{1}{2}[\Delta_m(K-k,K)+\Delta_m(K-k-2,K-2)\\ &\quad -2\Delta_m(K-k-1,K-1)],\end{aligned} \tag{11}$$

with an assumption that $\Delta_m(K-k,K)$ is given dominantly by the Coulomb energy difference and a parameter denoted by (M_p-M_n) in Eq. (2). Here the values of $\Delta_m(K-k,K)$ are evaluated by using the AME2016 database. The $\delta_{\rm pair}(K-k,K)$ values such extracted are plotted in Fig. 3 by using solid circles in black.

The theoretical odd-even gap in Coulomb energy that we extract in this paper is based on systematics demonstrated in this work. Here we rewrite Eq. (7) as follows:

$$\Delta^{(\rm odd)} = a_c^{(\rm odd)}\delta^{(\rm odd)} + C^{(\rm odd)},$$
$$\Delta^{(\rm even)} = a_c^{(\rm even)}\delta^{(\rm even)} - C^{(\rm even)},$$

where $\Delta^{(\rm odd)}$ and $\delta^{(\rm odd)}$ correspond to Δ_n and δ_c^n with odd neutron numbers or Δ_c^p and δ_c^p with odd proton numbers and $\Delta^{(\rm even)}$ and $\delta^{(\rm even)}$ correspond to Δ_n and δ_c^n with even neutron numbers or Δ_c^p and δ_c^p with even proton numbers. Our odd-even gap is then the difference between $\Delta^{(\rm odd)}$ and $\Delta^{(\rm even)}$,

$$\delta_{\rm pair} = (a_c^{(\rm odd)} - a_c^{(\rm even)})|\delta_c| + (C^{\rm odd} - C^{\rm even}). \tag{12}$$

The results of $\delta_{\rm pair}$ such obtained are plotted by using a solid line in red in Fig. 3.

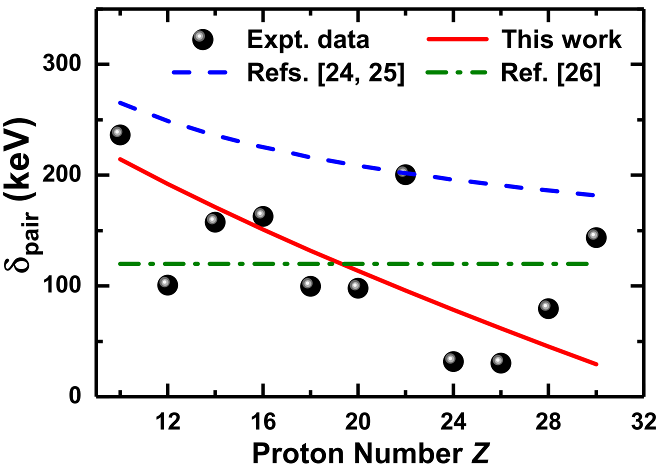

FIG. 3. The pairing gap of Coulomb energy $\delta_{\rm pair}$ for mirror nuclei, with $k=1$ and $Z \geqslant 10$. The solid circles in black correspond to empirical values of $\delta_{\rm pair}$ defined in Eq. (11) and extracted by using the AME2016 database with experimental uncertainty less than 50 keV. The solid line in red correspond to $\delta_{\rm pair}$ values defined in Eq. (12), and the dotted lines in blue and green correspond to $\delta_{\rm pair}$ taken from Refs. [24,25] and Ref. [26], respectively.

In Refs. [23–27], the odd-even fluctuation of Coulomb energy is treated as an additional term in $\Delta_m(K-k,K)$,

$$\begin{aligned}\Delta_m(K-k,K) &\equiv M(K-k,K) - M(K,K-k)\\ &= a_c k A^{2/3} + \delta_{\rm pair}^c + k(M_p - M_n).\end{aligned} \tag{13}$$

$\delta_{\rm pair}^c = (-1)^K a_c/(2A^{1/3})\,$keV in Refs. [24,25] and $\delta_{\rm pair}^c = 60[1+(-1)^K]\,$keV in Ref. [26] for $k=1$. Thus theoretical odd-even gap of Coulomb energy is $\delta_{\rm pair} = a_c/A^{1/3}\,$keV according to Refs. [24,25] and $\delta_{\rm pair} = 120\,$keV according to Ref. [26]. These two $\delta_{\rm pair}$ are plotted in Fig. 3 by using dotted lines in blue and green, respectively.

In general the four odd-even gaps in Coulomb energy, summarized in Fig. 3, are reasonably consistent, except that the values of $\delta_{\rm pair}$ used in Refs. [24,25] are systematically larger than empirical values which are extracted from experimental data of atomic masses. The large fluctuations of empirical values of $\delta_{\rm pair}$ might result from various underlying physics (for example, the shell effect). The picture based on pairing correlation between like particles [26] yields a rather constant value of $\delta_{\rm pair}$. The odd-even gap from systematics studied in this paper exhibits a tendency of decrease with proton number. The difference of these three results is warranted for further studies in future.

Finally, the nice agreement of Δ-δ_c relations encourage us to predict nuclear mass excesses which are not accessible experimentally. We make use of Eq. (7) and the parameters in the last row in Table I in our predictions. For cases with two predicted results for a given nucleus, our predicted results are taken to be their average, with the weight of uncertainty, as in Ref. [17]. We predict 68 unknown mass excesses of proton-rich nuclei with A from 26 to 90 and $Z-N \leqslant 4$. Our predicted results are tabulated in the Supplemental Material [28] of this paper.

To summarize, in this paper we revisit mass relations of mirror nuclei and focus on an odd-even feature of the Coulomb energy, with which we construct new (and simple) mass formulas, with the resultant RMSD value 93 keV. For the first time one has simple mass formulas for mirror nuclei with the RMSD below 100 keV for light- and medium-mass nuclei in a considerably large region. The values of parameters in these formulas are discussed in considerable detail. In the Supplemental Material [28] we present our predictions of 68 mass excesses which are not yet accessible in the atomic mass evaluation database, with A from 26 to 90 and $Z - N \leqslant 4$.

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APPENDIX: FORMULAS OF δ_c'

We begin our discussion with the form of Eq. (8) for Coulomb energy of atomic nuclei. The difference of the direct term in Eq. (8) for mirror nuclei is given by the first term on the right hand side of Eq. (2). The difference of Coulomb energy relate to the exchange term for mirror nuclei is given by

$$\frac{5}{4}\left(\frac{3}{2\pi}\right)^{2/3} a_c \frac{(K-k)^{4/3}}{A^{1/3}} - \frac{5}{4}\left(\frac{3}{2\pi}\right)^{2/3} a_c \frac{K^{4/3}}{A^{1/3}} \simeq -\frac{5}{2}\left(\frac{1}{3\pi^2}\right)^{1/3} a_c k \sim -0.808 a_c k,$$

where we make the approximation $k \ll K$. The difference of Coulomb energy related to the self-energy term for mirror nuclei is given by

$$-a_c \frac{K-k}{A^{1/3}} + a_c \frac{K}{A^{1/3}} = -a_c k A^{-1/3}.$$

From the above results, we obtain

$$\Delta_m(K-k, K) \equiv M(K-k, K) - M(K, K-k) = a_c k (A^{2/3} - A^{-1/3} - 0.808) + k(M_p - M_n). \tag{A1}$$

We substitute this result into the definition of $\Delta_n(K-k, K)$ and $\Delta_p(K-k, K)$ and obtain

$$\Delta_n(K-k, K) = a_c' \delta_c^{n'} - C', \quad \Delta_p(K-k, K) = a_c' \delta_c^{p'} + C',$$

where

$$\delta_c^{n'} = (k+1)(A-2)(A-1)^{-1/3} - k(A-1)A^{-1/3} - 0.808, \tag{A2}$$

$$\delta_c^{p'} = (k-1)(A-2)(A-1)^{-1/3} - k(A-1)A^{-1/3} + 0.808. \tag{A3}$$

We note that a_c' and C' are the same for $\Delta_n(K-k, K)$ with odd (even) numbers of $(K-k)$ and $\Delta_p(K-k, K)$ with odd (even) numbers of K, in the last row of Table I.

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