Mass relations of mirror nuclei in terms of Coulomb energies based on relativistic continuum Hartree-Bogoliubov calculations

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(Received 2 September 2020; revised 11 March 2021; accepted 28 April 2021; published 28 May 2021)

In this paper we study mass relations of mirror nuclei in terms of Coulomb energies calculated by the microscopic relativistic continuum Hartree-Bogoliubov theory. An additional term corresponding to the Nolen-Schiffer anomaly is assumed to take the same form as the well-known empirical formula. The resultant root-mean-square deviations of these mass relations are typically less than 100 keV. Based on these relations, 61 unknown proton-rich nuclear masses are predicted for $18 \leqslant A \leqslant 87$ with positive two-proton separation energies and are tabulated in the Supplemental Material of this paper.

DOI: 10.1103/PhysRevC.103.054326

I. INTRODUCTION

Nuclear mass $M(N, Z)$ (where N is the neutron number and Z is the proton number) is one of the most fundamental quantities in both nuclear physics and astrophysics [1,2]. Many theoretical models and approaches are developed to describe the state-of-the-art atomic-mass evaluation database and to predict unknown masses. One of the main types are called global models, such as Duflo-Zuker model [3], the finite-range droplet model (FRDM) [4,5], the improved Weizsäcker mass formula [6], and the covariant density-functional theory [7–9].

Besides these theoretical efforts, various mass relations have also been investigated, and one of the most accurate types is the relations of mirror nuclei [10–16], based on the isospin symmetry of the nucleon-nucleon interaction. With this assumption, the mass difference between two mirror nuclei is dominated by the Coulomb-energy difference [17–20], denoted by

$$\delta_m(K-k, K) \equiv E_c(K-k, K) - E_c(K, K-k), \qquad (1)$$

and the neutron-proton difference in atomic mass, viz.,

$$k\delta M_{np} \equiv k(m_n - m_p - m_e) = 0.7823k \text{ MeV}. \qquad (2)$$

In Eq. (1), $E_c(K-k, K)$ represents the Coulomb energy of the nucleus with $K-k$ neutrons and K protons, and k represents the difference of proton number (or neutron number, equivalently) for the mirror nuclei. m_n, m_p, and m_e are the neutron, proton and electron masses, respectively. Note that the electron mass is included in δM_{np} because the database of nuclear masses is tabulated by using atomic masses, and a neutral atom with a nucleus of K protons and $K-k$ neutrons has additionally k electrons more than a neutral atom with a nucleus of $K-k$ protons and K neutrons. We define the mass difference between two mirror nuclei as

$$\Delta_m(K-k, K) \equiv M(K-k, K) - M(K, K-k). \qquad (3)$$

By assuming isospin symmetry, we obtain

$$\Delta_m(K-k, K) = \delta_m(K-k, K) - k\delta M_{np}. \qquad (4)$$

In recent years, we studied the patterns exhibited by mass differences of mirror nuclei. In Ref. [13], the relation of Eq. (4) was exploited with the simple assumption that the Coulomb energy of a nucleus could be well represented by a uniformly charged sphere, with the corresponding Coulomb energy given by

$$E_c(K-k, K) = a_c K^2 A^{-1/3}, \qquad (5)$$

where $A = 2K - k$ is the mass number of the nucleus, and a_c ($\approx$0.72 MeV) is the strength parameter of the Coulomb energy. By using Eq. (1) and the empirical Coulomb energy in Eq. (5), the mass difference between two mirror nuclei is reduced to

$$\Delta_m(K-k, K) = a_c k A^{2/3} - k\delta M_{np}. \qquad (6)$$

By using a_c and δM_{np} as adjustable parameters, the resultant root-mean-square deviation (RMSD) values are 126, 221, 289, and 237 keV for $k = 1$–4, respectively. On the other hand, the optimized value of the parameter δM_{np} is close to 1.5 MeV, which is much larger than its expected value (0.782 MeV) in Eq. (2). This anomaly is well remedied by considering the

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self-energy and exchange terms [denoted $E_c^{(\rm self)}$ and $E_c^{(\rm exc)}$, respectively] in the Coulomb energy [15,20],

$$E_c^{(\rm self)} = a_c K A^{-1/3},\ E_c^{(\rm exc)} = \frac{5}{4}\left(\frac{3}{2\pi}\right)^{\frac{2}{3}} a_c \frac{K^{\frac{4}{3}}}{A^{\frac{1}{3}}}. \quad (7)$$

Accordingly, we obtain a more sophisticated formula for Coulomb energy,

$$E_c(K-k,K) = a_c \frac{K(K-1)}{A^{\frac{1}{3}}} - \frac{5}{4}\left(\frac{3}{2\pi}\right)^{\frac{2}{3}} a_c \frac{K^{\frac{4}{3}}}{A^{\frac{1}{3}}}. \quad (8)$$

Substituting the above Coulomb energy into Eq. (1), one obtains

$$\begin{aligned}\delta_m(K-k,K) &= a_c A^{-\frac{1}{3}}[K(K-1)-(K-k)(K-k-1)] \\ &\quad -\frac{5}{4}\left(\frac{3}{2\pi}\right)^{\frac{2}{3}} a_c A^{-\frac{1}{3}}\left[K^{\frac{4}{3}}-(K-k)^{\frac{4}{3}}\right] \\ &\approx a_c k(A-1)A^{-\frac{1}{3}} - \frac{5}{3}\left(\frac{3}{2\pi}\right)^{\frac{2}{3}} a_c k (K/A)^{\frac{1}{3}}.\end{aligned}$$

To facilitate our discussion, in this paper we denote the value of δ_m such obtained by $\delta_m^{(\rm emp)}$, and denote the corresponding results based on $\delta_m^{(\rm emp)}$ by using the subscript "(emp)." In the last step of the above relation for $\delta_m^{(\rm emp)}$, we present the Taylor expansion to the first order of k/K. Because $K/A \approx 1/2$ for small k, the second term equals approximately

$$\frac{5}{3}\left(\frac{3}{2\pi}\right)^{\frac{2}{3}} (1/2)^{\frac{1}{3}} a_c k \equiv Ck, \quad C = 0.808 a_c.$$

The form of δ_m defined in Eq. (1) is replaced by

$$\delta_m^{(\rm emp)}(K-k,K) = a_c k (A-1) A^{-\frac{1}{3}} - Ck, \quad (9)$$

and accordingly the mass relation of two mirror nuclei is given by

$$\Delta_m^{(\rm emp)}(K-k,K) = a_c k (A-1) A^{-\frac{1}{3}} - (C+\delta M_{np})k. \quad (10)$$

Thus one sees that consideration of the exchange term for protons leads to a constant C, with $C = 0.808 a_c = 0.808 \times 0.72 = 0.582$ MeV, which well accounts for the large disagreement between the optimized δM_{np} in Ref. [13] and its expectation value in Eq. (2). By optimizing a_c and C with respect to the Atomic Mass Evaluation (AME2016) database [21] (with the exception of mass for the ^{44}V nucleus which was recently reexamined in Refs. [22,23]), one obtains a RMSD of 151 keV for nuclei with proton number larger than eight. The optimized a_c is ≈700 keV, which is slightly smaller than and yet close to its conventional value, 720 keV; and the optimized value of C is ≈650 keV, which is slightly larger than (but reasonably consistent with) its expected value, 582 keV.

In Refs. [14,15], the mass relations of two mirror nuclei were improved by associating two pairs of mirror nuclei. We define

$$\begin{aligned}\Delta_n(K-k,K) &\equiv M(K-k,K) - M(K-k+1,K) \\ &\quad - M(K,K-k) + M(K,K-k+1), \quad (11)\end{aligned}$$

$$\begin{aligned}\Delta_p(K-k,K) &\equiv M(K-k,K) - M(K-k,K-1) \\ &\quad - M(K,K-k) + M(K-1,K-k). \quad (12)\end{aligned}$$

Clearly, one has

$$\Delta_n(K-k,K) = \delta_n(K-k,K) - \delta M_{np}, \quad (13)$$

$$\Delta_p(K-k,K) = \delta_p(K-k,K) - \delta M_{np}, \quad (14)$$

where

$$\delta_n(K-k,K) \equiv \delta_m(K-k,K) - \delta_m(K-k+1,K), \quad (15)$$

$$\delta_p(K-k,K) \equiv \delta_m(K-k,K) - \delta_m(K-k,K-1). \quad (16)$$

Assuming $\delta_m^{(\rm emp)}$ in Eq. (9), one has

$$\begin{aligned}&\Delta_n^{(\rm emp)}(K-k,K) \\ &= a_c\left[k(A-1)A^{-\frac{1}{3}} - (k-1)A(A+1)^{-\frac{1}{3}}\right] \\ &\quad - (C+\delta M_{np}), \quad (17)\end{aligned}$$

$$\begin{aligned}&\Delta_p^{(\rm emp)}(K-k,K) \\ &= a_c\left[k(A-1)A^{-\frac{1}{3}} - (k-1)(A-2)(A-1)^{-\frac{1}{3}}\right] \\ &\quad - (C+\delta M_{np}). \quad (18)\end{aligned}$$

The main advantage of these two mass relations (17) and (18) in comparison with the Δ_m relation in Eq. (10) is that the magnitudes of Coulomb-energy differences, $\delta_n(K-k,K)$ and $\delta_p(K-k,K)$, are much smaller than $\delta_m(K-k,K)$ in the Δ_m relation. This substantially reduces the uncertainties of the Coulomb energy which is calculated based on empirical formulas. The Δ_n and Δ_p relations in Eqs. (17) and (18) were exemplified by using the AME2016 database [21]. The χ^2 fitting of parameters a_c and C for these two relations yielded the RMSDs of 112 and 116 keV, respectively, for nuclei with proton number K larger than 8. If a subtle odd-even staggering of the Coulomb energy originated from the nuclear pairing correlation is considered, the RMSD values are reduced to 82 and 94 keV, respectively [15]. In Ref. [16] the mass relations are further improved by employing the so-called correlation correction, which considers both the pairing and shell effects; and the RMSD values of such improved Δ_n and Δ_p relations are reduced to 51 keV.

The efforts in Refs. [13–16] are all based on Eq. (5) or Eq. (8), which are the empirical Coulomb energies. It is therefore the purpose of this paper to examine our mass relations of mirror nuclei by employing more sophisticated and microscopically evaluated Coulomb energies. Here we adopt the results from the state-of-the-art relativistic continuum Hartree-Bogoliubov (RCHB) calculations [9]. Based on the covariant density functional, the RCHB approach solves the relativistic Hartree-Bogoliubov equations in the coordinate representation in the presence of the continuum [24]. In the RCHB mass table calculations [9], one of the most successful relativistic energy density functionals, PC-PK1 [25], was adopted. For the particle-particle channel, the density-dependent zero-range force is used and the pairing strength is fixed to be $V_0 = -342.5$ MeV fm^3 for both neutron and proton. The box size $R_{\rm box} = 20$ fm, the mesh size $\Delta r = 0.1$ fm, and the angular-momentum cutoff $J_{\rm max} = 19/2\hbar$, which can guarantee a good convergence, are adopted, respectively.

This paper is organized as follows. In Sec. II, we perform a systematic study of the RCHB-based Coulomb energies in terms of the Δ_m, Δ_n and Δ_p relations; in Sec. III, we investigate the predictive power of the RCHB-based mass relations through extrapolations from a previous AME database to the current AME2016 database, and compare the theoretical predictions in this article with our former results. Our summary and conclusion are given in Sec. IV.

II. MASS RELATIONS WITH RCHB-BASED COULOMB ENERGIES

The Coulomb-energy differences between two mirror nuclei, δ_m, defined in Eq. (1), and those among four mirror nuclei, δ_n and δ_p, defined in Eqs. (15) and (16), are calculated by using the RCHB Coulomb energies. Based on these results and the constant δM_{np}, as in Eqs. (4), (13), and (14), we evaluate Δ_m, Δ_n, and Δ_p values for $1 \leqslant k \leqslant 4$ and $K \geqslant 8 + k$ and plot them in Fig. 1 by using solid symbols. As a comparison, we extract Δ_m, Δ_n, and Δ_p values based on their definitions, i.e., Eqs. (3), (11), and (12) and the AME2016 database and plot them by using open symbols in Fig. 1.

From Fig. 1, one sees that the evolution tendency of the Δ_m, Δ_n, and Δ_p based on the RCHB calculations agree very well with those extracted by using Eqs. (3), (11), and (12) and the AME2016 database, and that, on the other hand, the RCHB results are systematically lower than those extracted from experimental data by 9.3%, 9.6%, and 9.6% for Δ_m, Δ_n, and Δ_p, respectively. In Fig. 1 we also plot the theoretical $\Delta_m^{(\mathrm{emp})}$, $\Delta_n^{(\mathrm{emp})}$, and $\Delta_p^{(\mathrm{emp})}$ calculated based on empirical Coulomb energies, i.e., Eqs. (10), (17), and (18), by using solid lines in black; one sees that these empirical values agree very well with those extracted from experimental data.

It is interesting to look at whether the difference of Δ_m, Δ_n, and Δ_p based on the RCHB calculations from those extracted from experimental data is related to the Nolen-Schiffer anomaly. Toward this end, we evaluate relative deviations between RCHB-based nuclear charge radii [9] and corresponding experimental values compiled in Ref. [26],

$$\delta R = \frac{|R_{\mathrm{expt}} - R_{\mathrm{th}}|}{R_{\mathrm{expt}}}.$$

The resultant δR for nuclei with $Z \leqslant 50$ is only 0.53%. Therefore, the RCHB calculations reproduce nuclear charge radii very well, and meanwhile the Coulomb energies are sizably underestimated. This pattern is usually attributed to the Nolen-Schiffer anomaly [20,27] and was studied in terms of isospin-nonconserving interactions [28,29].

We now note on the advantage of using the RCHB-based Coulomb energy instead of empirical Coulomb energy in the mass relations of mirror nuclei. In Fig. 2, we plot $\Delta_m(K-k, K) - \Delta_m(K-1-k, K-1)$ extracted from the experimental data (with $k = 1$) versus K by solid balls in black. The results calculated by using empirical Δ_m [Eq. (10)] are plotted by using dotted lines in green, and those extracted from the RCHB calculations are plotted by using solid squares in blue. According to our calculations shown in Fig. 2, the results extracted from experimental data exhibit odd-even features with fluctuations, which originate from pairing and shell effects. The RCHB calculation could properly describe such

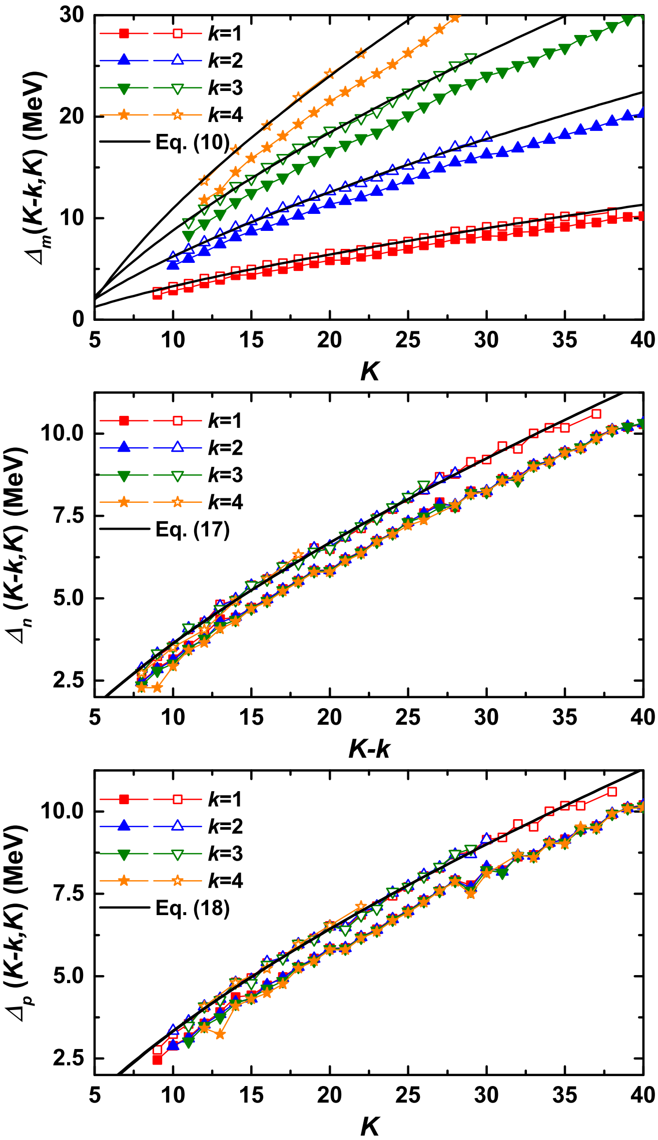

FIG. 1. The values of Δ_m and Δ_p (in units of MeV) versus proton number K, and Δ_n (in units of MeV) versus neutron number $K-k$. $\Delta_m = \delta_m(K-k, K) - k\delta M_{np}$, $\Delta_n = \delta_n(K-k, K) - \delta M_{np}$, and $\Delta_p = \delta_p(K-k, K) - \delta M_{np}$, where $\delta_m(K-k, K) \equiv E_c(K-k, K) - E_c(K, K-k)$. Solid symbols are based on the theoretical E_c values of the RCHB calculations, and the hollow symbols are based on Eq. (3), in which the masses are taken from the AME2016 database. The solid line in black are calculated by using Eqs. (10), (17), and (18).

features except slight discrepancies at $K = 16$–20 and $K = 29$–30. The results extracted from the empirical Coulomb energy cannot reproduce this subtle pattern. To make good use of this advantage, we introduce an additional term which assumes the same form of the empirical Coulomb energy formula (but a much smaller value of a_c, denoted a_c' for discrimination) to compensate for the systematic deviations of the RCHB-calculated Δ_m, Δ_n, and Δ_p from experimental

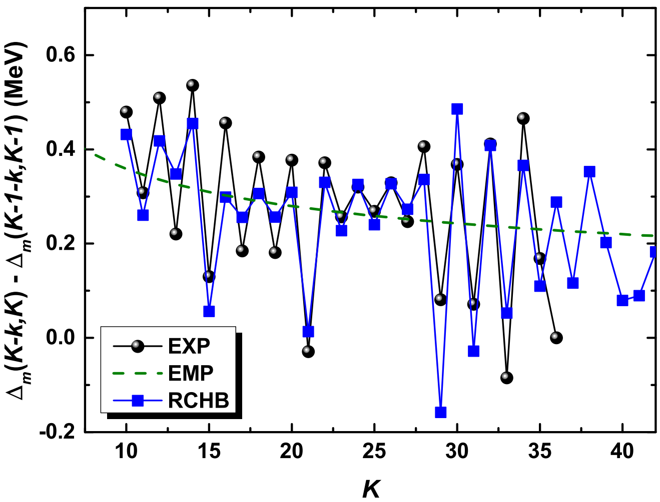

FIG. 2. Difference between $\Delta_m(K-k, K)$ and its neighbor with same k and adjacent K, i.e., $\Delta_m(K-1-k, K-1)$, for $k=1$ case. Results extracted from experimental masses are denoted by solid balls in black. The green line and blue squares are calculated by using empirical formula of Eq. (10), and RCHB-based Coulomb energy of Eq. (19), respectively.

data, namely,

$$\Delta_m(K-k, K) = E_c'(K-k, K) - E_c'(K, K-k) + a_c' k(A-1)A^{-1/3} - C'k, \quad (19)$$

$$\Delta_n(K-k, K) = E_c'(K-k, K) - E_c'(K-k+1, K) - E_c'(K, K-k) + E_c'(K, K-k+1) + a_c'\left[k(A-1)A^{-\frac{1}{3}} - (k-1)A(A+1)^{-\frac{1}{3}}\right] - C', \quad (20)$$

$$\Delta_p(K-k, K) = E_c'(K-k, K) - E_c'(K-k, K-1) - E_c'(K, K-k) + E_c'(K-1, K-k) + a_c'[k(A-1)A^{-\frac{1}{3}} - (k-1)(A-2)(A-1)^{-\frac{1}{3}}] - C'. \quad (21)$$

In Eqs. (19)–(21), E_c' represents the RCHB-based Coulomb energy [9], and a_c' and C' are adjustable parameters corresponding to a_c and $(C+\delta M_{np})$ in Eqs. (3), (9), and (18), respectively. The values of a_c' and C' are optimized by a χ^2 fitting of the AME2016 database [21] for Δ_m, Δ_n, and Δ_p relations; the resultant RMSD values for the relations of (19)–(21) are 109, 88, and 105 keV, respectively. In Fig. 3 we present deviations of these calculated Δ_m, Δ_n, and Δ_p results from those extracted from experimental data. One sees that most of the deviations are below 200 keV, albeit with a number of exceptions, among which $\Delta_m(26, 29)$, $\Delta_m(35, 36)$, $\Delta_m(37, 38)$, $\Delta_n(35, 36)$, $\Delta_n(37, 38)$, $\Delta_p(18, 22)$, $\Delta_p(26, 29)$, $\Delta_p(35, 36)$, and $\Delta_p(37, 38)$ have large uncertainties originating from experimental uncertainties for $^{40}_{22}\mathrm{Ti}_{18}$, $^{55}_{29}\mathrm{Cu}_{26}$, $^{71}_{36}\mathrm{Kr}_{35}$, and $^{75}_{38}\mathrm{Sr}_{37}$, whose experimental uncertainties are 160, 156, 129, and 220 keV, respectively.

If one examines the results with large deviations, one sees systematic and large deviation at the proton shell $Z = 28$. More specifically, large deviations arise for all Δ_m with proton number from 28 to 29, for all Δ_n with proton number from 27 to 28 and for all Δ_p with proton number from 28 to 29. These Δ values involve mirror nuclei for which the proton-rich nu-

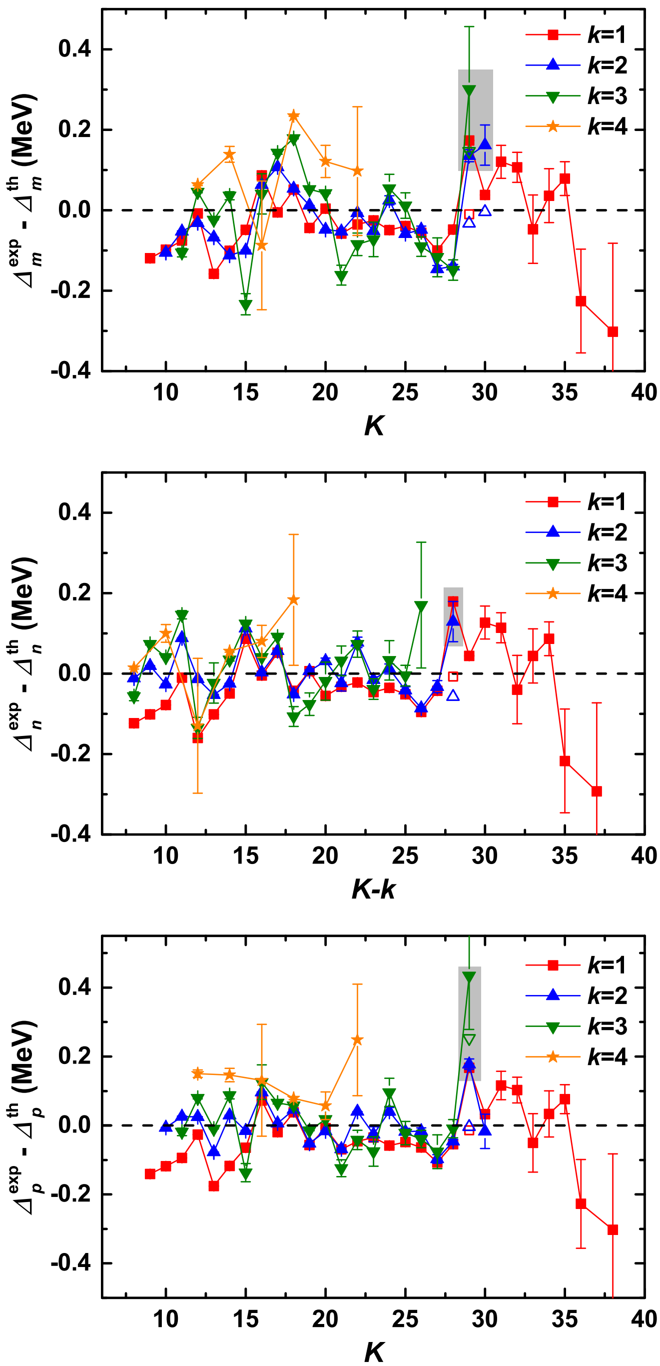

FIG. 3. Deviations (in units of MeV) of our theoretical Δ_m, Δ_n, and Δ_p in Eqs. (19)–(21) from those extracted from the AME2016 database [21] by using Eqs. (3), (11), and (12), except that the mass of ^{44}V is taken from Ref. [22]. The error bars corresponds to uncertainties in experimental data. The results affected by the anomaly of RCHB-calculated Coulomb energies at proton numbers $K = 28$ are denoted by using gray shadows and the corresponding results with the shell correction are plotted by using open squares and triangles.

TABLE I. Optimized parameters in Eqs. (19)–(21) and the corresponding RMSD values for nuclei $N, Z \geqslant 8$. $\mathcal{N}$ is the number of Δ. a'_c, C' are parameters in Eqs. (19)–(21). The RMSD value of Δ_m, Δ_n, and Δ_p corresponds to σ_m in Eq. (25), σ_n in Eq. (26), and σ_p in Eq. (27), respectively. 200 keV is added to the RCHB-calculated Coulomb energies E'_c of nuclei with proton number $Z > 28$ as an additional shell effect at $Z = 28$ (see text). The AME2016 [21] database (except that the mass of ^{44}V is taken from Ref. [22]) is used in the χ^2 fitting.

Type	$\mathcal{N}$	a'_c (MeV)	C' (MeV)	RMSD (MeV)
Δ_m	75	0.047(2)	0.641(23)	0.097
Δ_n	75	0.046(3)	0.637(38)	0.084
Δ_p	75	0.045(4)	0.606(46)	0.092

cleus has proton number larger than 28 and neutron number $\leqslant$28, and the corresponding neutron-rich nucleus has proton number $\leqslant$28 and neutron number >28; namely, the last proton of the proton-rich partner is in the pf shell, and that of the proton-deficient partner is in the $f_{\frac{7}{2}}$ shell, while the last neutron of the proton-rich partner is in the $f_{\frac{7}{2}}$ shell while that of the proton-deficient partner is in the pf shell. For these cases, theoretical values of Δ_m with proton number $K > 28$ and neutron number $K - k \leqslant 28$, Δ_n with $K - k = 28$, and Δ_p with $K = 29$, are systematically smaller than corresponding results extracted from experimental data, by about 130–430 keV. The relevant results are plotted in shadows in Fig. 3. One observes a consistent pattern if one uses the RCHB-calculated masses in Ref. [9] and extracts the Δ_m, Δ_n, and Δ_p, which yield deviations from 310 to 720 keV for nuclei in the same region, in comparison with those extracted from experimental data. To compensate for this systematic deviation for these nuclei, we add an artificial constant (200 keV) to the RCHB Coulomb energies E'_c with $Z > 28$. The deviations with this revision of these corresponding Δ from those extracted from experimental data are plotted in Fig. 3 (denoted by using open symbols). The optimized a'_c, C'_i as well as the resultant RMSD values are given in Table I. One sees that the three sets of a'_c and C'_i are very close to each other (except that the C' in the Δ_p relation is slightly smaller). All of these three relations yield RMSD less than 100 keV and are competitive with the precision in Ref. [15].

In this work we have also studied the relations of mirror nuclei based on a few other calculations. Both the resultant parameters and the RMSD values of those for other theoretical efforts are close to the results based on the RCHB calculations (yet the RMSD values are slightly larger than the RCHB calculations [9]) adopted in this paper. By using the direct term of Coulomb energy from the RCHB calculations, the optimized $a'_c = 43$ keV, $C' = 980$ keV, and RMSD values range from 93 to 113 keV; by using the Coulomb energy extracted from the FRDM2012 database [5], we obtain $a'_c = 45$ keV, and $C' = 1030$ keV, and RMSD values vary between 139 and 149 keV; by using Coulomb energies extracted from the Gogny-Hartree-Fock-Bogoliubov method (named the AMEDEE database) [30], $a'_c = 15$ keV, $C' = 600$ keV, and RMSD values range from 116 to 150 keV.

III. PREDICTIVE POWER OF RCHB-BASED MASS RELATIONS

The predictive power of the mass relations for mirror nuclei is demonstrated by numerical experiments of extrapolation from the AME2003 database [31] to the AME2016 database. The procedure of our extrapolation is as follows: First, we optimize the Δ_m, Δ_n, and Δ_p relations by using the AME2003 database, and obtain optimal parameters a'_c and C', as well as the RMSD values, for Eqs. (19)–(21). For short, we denote the unknown mass (to be predicted) of proton-rich nucleus with K protons and $K - k$ neutrons by using $M^{(m)}{}_{k,K}, M^{(p)}{}_{k,K}$, and $M^{(n)}{}_{k,K}$, based on Eqs. (19)–(21). The predicted mass of proton-rich nucleus with K protons and $K - k$ neutrons is given by

$$M^{(m)}_{k,K} = M(K, K-k) + \Delta_m, \tag{22}$$

$$M^{(n)}_{k,K} = M(K, K-k) + M(K-k+1, K) - M(K, K-k+1) + \Delta_n, \tag{23}$$

$$M^{(p)}_{k,K} = M(K, K-k) + M(K-k, K-1) - M(K-1, K-k) + \Delta_p, \tag{24}$$

where $M(N, Z)$ is experimental mass of nucleus with N neutrons and Z protons in the AME2003; however, if the experimental uncertainty is larger than our theoretical uncertainty, $M(N, Z)$ is replaced by the corresponding theoretical value. Corresponding to Eqs. (22)–(24), theoretical uncertainties of our predicted mass with proton number K and neutron number $K - k$, denoted by $\sigma^{(m)}_{k,K}$, $\sigma^{(n)}_{k,K}$, and $\sigma^{(p)}_{k,K}$, are defined, respectively, as follows:

$$\left(\sigma^{(m)}_{k,K}\right)^2 = \sigma^2(K, K-k) + \sigma^2_m, \tag{25}$$

$$\left(\sigma^{(n)}_{k,K}\right)^2 = \sigma^2(K, K-k) + \sigma^2(K-k+1, K) + \sigma^2(K, K-k+1) + \sigma^2_n, \tag{26}$$

$$\left(\sigma^{(p)}_{k,K}\right)^2 = \sigma^2(K, K-k) + \sigma^2(K-k, K-1) + \sigma^2(K-1, K-k) + \sigma^2_p, \tag{27}$$

where $\sigma(N, Z)$ on the right-hand side in the above definitions corresponds to the uncertainty of $M(N, Z)$ (which is available), σ_m, σ_n, and σ_p are the RMSD values of the Δ_m, Δ_n, and Δ_p relations obtained in the optimization process in the first step.

Our numerical experiment of extrapolation from the AME2003 database is carried out by recursive application of the above process. In this proton-rich region, there are thirteen masses not accessible in the AME2003 database but compiled in the AME2016 database. The RMSD of our predicted masses from experimental data in the AME2016 database for these thirteen nuclei is 107, 88, and 83 keV, individually for $M^{(m)}$, $M^{(n)}$, and $M^{(p)}$, respectively; one sees that the latter two approaches is more accurate than those in previous extrapolations: for the same set of nuclei, the RMSD is 351 keV in Ref. [13], 102 keV in Ref. [14], and 112 keV in Ref. [15]. One sees the advantage of the extrapolations in this work because the predicted $M^{(n)}$ and $M^{(p)}$ in terms of Eqs. (19)–(21)

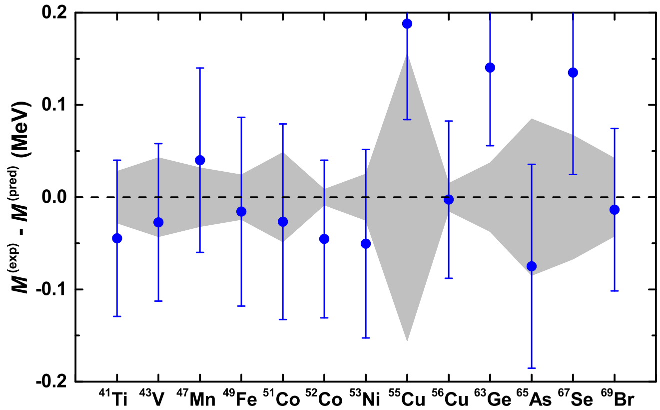

FIG. 4. Deviations (in unit of MeV) of masses extrapolated based on the AME2003 database [31], from those compiled in the AME2016 database [21]. The uncertainty of experimental database are denoted by using shadows, and theoretical uncertainties of our extrapolated masses are plotted by using error bars.

are more consistent with experimental data than previous predictions.

Because the RMSD values of predicted $M^{(n)}$ and $M^{(p)}$ are considerably smaller than that of $M^{(m)}$, our final predicted value of the mass for the nucleus with proton number K and neutron number $K-k$ is taken to be the statistical average of $M^{(n)}$ and $M^{(p)}$, viz.,

$$M_{k,K}^{(\mathrm{pred})} = \frac{\left(\frac{1}{\sigma_{k,K}^{(n)}}\right)^2 M_{k,K}^{(n)} + \left(\frac{1}{\sigma_{k,K}^{(p)}}\right)^2 M_{k,K}^{(p)}}{\left(\frac{1}{\sigma_{k,K}^{(n)}}\right)^2 + \left(\frac{1}{\sigma_{k,K}^{(p)}}\right)^2}, \tag{28}$$

and theoretical uncertainty of our predicted mass of the nucleus with proton number K and neutron number $K-k$ is correspondingly given by

$$\sigma_{k,K}^{(\mathrm{pred})2} = \frac{1}{\left(\frac{1}{\sigma_{k,K}^{(n)}}\right)^2 + \left(\frac{1}{\sigma_{k,K}^{(p)}}\right)^2}. \tag{29}$$

The deviation of our predicted results for nuclear masses which were not available in the AME2003 database, from those compiled in the AME2016 database, is plotted in Fig. 4. One sees that most deviations of our predicted masses from experimental data are well below 100 keV, except for $^{55}_{29}\mathrm{Cu}_{26}$, $^{63}_{32}\mathrm{Ge}_{31}$, and $^{67}_{34}\mathrm{Se}_{33}$. The final RMSD value of our predicted masses for these thirteen nuclei is 83 keV from those in the AME2016 database.

Because Eqs. (19)–(21) are remarkably accurate and, furthermore, preferable in extrapolations, it is of interest to make use of these formulas to extrapolate the AME2016 database and to predict unknown masses of proton-rich nuclei with $Z > N$. According to our extrapolated masses, sixty-one nuclei with $18 \leqslant A \leqslant 87$, $Z > N$, and masses not accessible in the AME2016 database, are predicted to have positive two-proton separation energies. We present our predicted masses in the Supplemental Material of this paper [32].

Finally, we present a comparison of the predicted masses in this work with those in Ref. [15]. In Fig. 5(a), we plot

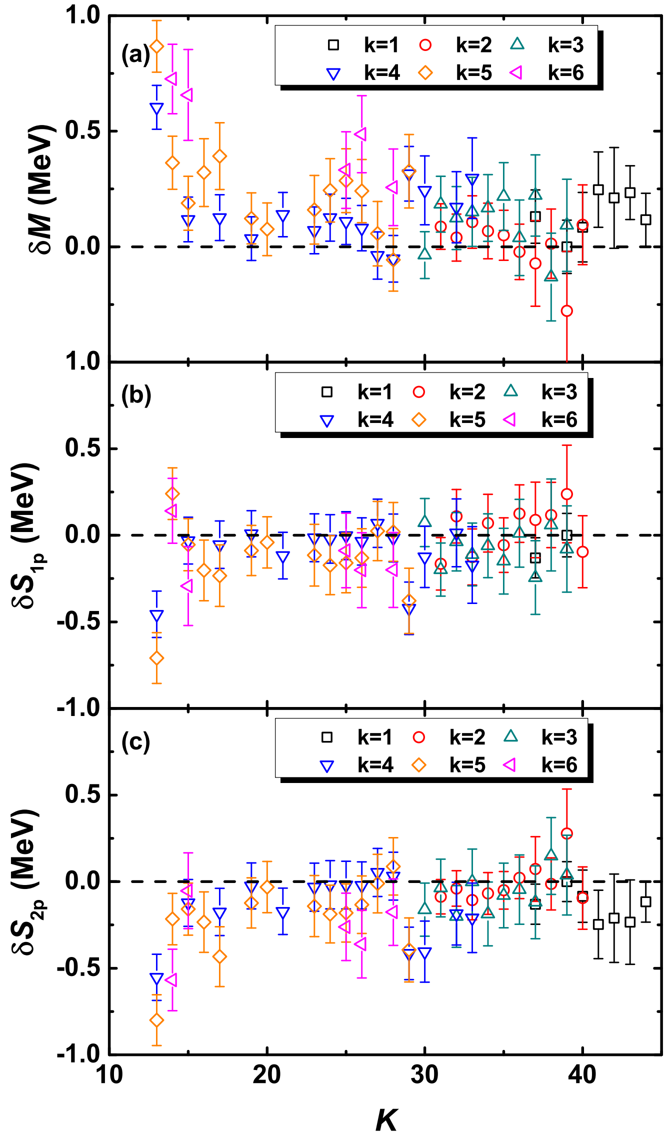

FIG. 5. Deviations (in units of MeV) of our predicted results from those predicted in Ref. [15]. (a) Nuclear masses, (b) single-proton separation energies, and (c) two-proton separation energies. The vertical axis corresponds predicted results of Ref. [15] subtracted by those predicted in this paper, with the uncertainty (error bar) taken to be the root of the squared sum of two theoretical uncertainties, one from this work and the other from Ref. [15]. One sees that the consistence between two predictions are good; one also sees that binding energies predicted in this work are very slightly larger [see panel (a)] than those in Ref. [15].

the deviations of masses predicted in this work from those in Ref. [15], namely, $M(K-k, K)$ predicted in Ref. [15] subtracted by the above $M_{k,K}^{(\mathrm{pred})}$ in this article. One sees that most deviations are well below 500 keV, except for $^{21}_{13}\mathrm{Al}_8$, $^{22}_{13}\mathrm{Al}_9$, $^{22}_{14}\mathrm{Si}_8$, and $^{24}_{15}\mathrm{P}_9$, for which the number $Z-N$ is 4–6 and the mass number is ≈20 for which case the mean-field approach is not best applicable. The average deviation of the predicted results from those in Ref. [15] is 170 keV; and if we exclude these four nuclei with relatively small mass number, the average deviation is 135 keV. On the other hand, one sees that predicted masses in this work are lower, on average, than those in Ref. [15]. In Fig. 5, we also present a comparison of our predicted one-proton with two-proton separation energies with those based on Ref. [15]. Here the one-proton separation energy

$$S_{1p}(K-k,K) = M(K-k,K-1) + M_H - M(K-k,K)$$

and the two-proton separation energy

$$S_{2p}(K-k,K) = M(K-k,K-2) + 2M_H - M(K-k,K),$$

where M_H is the mass of the hydrogen atom. In Figs. 5(b) and 5(c), we present the predicted S_{1p} and S_{2p} based on Ref. [15], subtracted by those predicted in this work. The deviations are ≈80 and ≈140 keV, on average, for S_{1p} and S_{2p}, respectively.

IV. SUMMARY

To summarize, in this paper we study mass relations of mirror nuclei in terms of Coulomb energies calculated by the microscopic relativistic continuum Hartree-Bogoliubov (RCHB) theory. Systematic underestimations of mass differences between two mirror nuclei are pointed out for RCHB-based masses, and such systematic deviations are compensated by using the same form of empirical Coulomb energy terms. The advantage of the RCHB-calculated Coulomb energy is that the odd-even feature and shell effect of Coulomb energy, which is not considered in empirical Coulomb energy formulas are reasonably reproduced. The RMSD values in this work are sizably below 100 keV. Numerical experiments of an extrapolation from the AME2003 database to the AME2016 database demonstrates the competitive predictive power of the mass relations in this paper.

Based on these mass relations, we tabulate 61 unknown masses, one-proton and two-proton separation energies, of proton-rich nuclei with mass number $18 \leqslant A \leqslant 87$, in the Supplemental Material of this paper. The theoretical predictions in this work are in general entirely consistent with the predicted result in Ref. [15]. On the other hand, predicted binding energies in this paper are very slightly larger, on average, than those in previous work [15] (by 135 keV if a very few cases with small mass number are excluded). Further consideration of this deviation is warranted.

ACKNOWLEDGMENTS

We thank the National Natural Science Foundation of China (Grants No. 11975151 and No. 11961141003) and the MOE Key Lab for Particle Physics, Astrophysics and Cosmology for financial support.

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[32] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevC.103.054326 for predicted mass excesses for 61 proton-rich nuclei whose masses are experimentally unaccessible at present, for mass number $17 \leqslant A \leqslant 101$ and $1 \leqslant k \leqslant 4$.