New extrapolation method for predicting nuclear masses

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(Received 9 September 2019; revised manuscript received 21 January 2020; accepted 9 March 2020; published 21 April 2020)

In this paper, a practical extrapolation method is proposed to predict nuclear masses which are not experimentally accessible. Our new method is based on the Garvey-Kelson mass relations and Jänecke formulas. We demonstrate that the predictive power of this method is very competitive in comparison with other previous models in the market; the root-mean-squared deviations of our extrapolated results are typically below 200 keV for mass number A larger than 120, if one predicts nuclear masses within four or five steps beyond the borders of the Atomic Mass Evaluation (AME) databases.

DOI: 10.1103/PhysRevC.101.045204

I. INTRODUCTION

Nuclear mass (or binding energy) is one of the most fundamental quantities in nuclear physics as well as astrophysics. In addition to great efforts devoted to mass measurements in nuclear science facilities worldwide, various theoretical models and methods have been proposed to predict masses which are not yet accessible experimentally [1,2]. The theoretical efforts could be classified into two types. The first type is called global mass models, such as the finite-range droplet model (FRDM) [3,4], the Skyrme Hartree-Fock-Bogoliubov (HFB) theory [5], the Koura-Tachibana-Uno-Yamada (KTUY) formula constructed by Koura and collaborators [6], and a series of the Weizsäcker-Skyrme model [7–10]. The global mass models adopt a number of parameters which reflect various phenomenologies related to nuclear masses, e.g., volume energy, symmetry energy, surface energy, Coulomb energy, Wigner energy, shell effect, pairing, deformation, exotic structure, and so on. The parameters are fixed by using experimentally accessible masses and are adopted in predictions. The other type is called local mass relations, such as the Garvey-Kelson relations (GKs) [11–18], the Audi-Wapstra (AW) extrapolation [19–21], Jänecke formulas [22–27], and the local mass relations associated with proton-neutron interactions [28–30]. Local mass relations focus on systematics and correlations between nuclear masses of neighboring nuclei and are shown to be more accurate in the extrapolation of nuclear masses close to the known borders of an experimental database in comparison with global models, which are generally believed to be more reliable in long-range extrapolations of experimentally unknown masses.

Among the 7000 or perhaps even 10 000 nuclei throughout the full nuclear chart, only about 3000 nuclear masses have been compiled in the Atomic Mass Evaluation (AME) database [21]. One therefore has to resort to theoretical predictions if one needs inputs of nuclear masses which are beyond the AME2016 database. On the other hand, the predicted results based on different models and approaches are very different as one goes far from experimentally accessible borders [2], and thus the theoretical study of nuclear masses remains a challenge in nuclear structure physics, despite numerous efforts in previous studies. It is therefore the purpose of this paper to suggest a new extrapolation method, which is demonstrated to be very competitive in comparison with other previous mass models.

This paper is organized as follows. In Sec. II, we present a short introduction of the Garvey-Kelson relations and Jänecke formulas, and then describe our new method. In Sec. III, we investigate the predictive power of our method by using numerical experiments, i.e., extrapolations from previous AME databases to the current AME2016 database. Our summary and conclusion are given in Sec. IV.

II. DESCRIPTION OF THE NEW METHOD

Let us begin the discussion with the famous Garvey-Kelson mass relations [11], viz.,

$$\begin{aligned} D_L = {} & M(N+1,Z+1)+M(N-1,Z) \\ & +M(N,Z-1)-M(N,Z+1)-M(N+1,Z) \\ & -M(N-1,Z-1)\sim 0, \end{aligned} \tag{1}$$

$$\begin{aligned} D_T = {} & M(N+1,Z-1)+M(N-1,Z) \\ & +M(N,Z+1)-M(N,Z-1)-M(N+1,Z) \\ & -M(N-1,Z+1)\sim 0, \end{aligned} \tag{2}$$

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where $M(N,Z)$ represents the nuclear mass with given neutron number N and proton number Z. Equation (1) is called the longitudinal Garvey-Kelson relation (GKL) and Eq. (2) the transverse (GKT). Such relations are not exact, and D_L, D_T are used to denote the corresponding deviations from zero. For a given nucleus, they are also regarded as deviation of atomic mass, predicted by using experimental values of its neighboring five masses, in comparison with its experimental value. For mass number $A = N + Z \geqslant 120$, the root-mean-squared deviations (RMSD) derived from the Atomic Mass Evaluation database (AME2012) [20] are 148 and 158 keV for GKL and GKT, respectively [16,17]. As for the AME2016 database [21], the RMSD values of these two relations are, respectively, 148.8 and 158.2 keV. For $A < 120$, the Garvey-Kelson relations become less accurate; this is not unexpected, as the GK relations is equivalent to identities of proton-neutron interaction between the last proton and neutron, usually denoted by $\delta V_{\rm np}$, for nuclei with neutron number and proton number (N,Z) and $(N-1,Z-1)$, or (N,Z) and $(N+1,Z-1)$, while $\delta V_{\rm np}$ exhibits irregularities for nuclei with smaller A [29].

From another perspective, the GKL and GKT are rewritten as follows:

$$\Delta^{1,-1}\Delta^{1,0}\Delta^{0,1}M(N,Z) = 0, \tag{3}$$

$$\Delta^{1,1}\Delta^{1,0}\Delta^{0,1}M(N,Z) = 0, \tag{4}$$

where operators $\Delta^{i,j}$, introduced by Jänecke *et al.* [24,25], are defined below,

$$\Delta^{i,j}M(N,Z) = M(N,Z) - M(N-i,Z-j).$$

Suppose that both Eqs. (3) and (4) hold mathematically. One has

$$\Delta^{1,0}\Delta^{0,1}M(N,Z) = \begin{cases} C_1, & A \text{ odd}, \\ C_2, & A \text{ even}. \end{cases} \tag{5}$$

The general solution of $M(N,Z)$ is

$$M(N,Z) = h_1(N) + h_2(Z) + \lambda NZ + \mu\frac{1-(-1)^{NZ}}{2}, \tag{6}$$

where h_i are arbitrary point functions and λ, μ are constants [11]; they are determined by χ^2 fitting of the available mass data. Unfortunately, Eq. (6) does not satisfactorily describe the AME database; in the case of AME2016, the RMSD of Eq. (6) is as large as $\sim$2 MeV.

Two improvements of Eq. (6) have been developed. The first improvement is to introduce so-called inhomogeneous terms into the original formula [22–25], by either adding phenomenological terms or combining the formula with other models. For example, if a phenomenological term $\lambda' NZ/A$ is introduced in Eq. (6), similar to the $1/A$ behavior of $\delta V_{\rm np}(N,Z)$ [29], the RMSD is reduced to about 0.7 MeV. Recently, an improved Jänecke mass formula has been proposed by He *et al.* [26]. In their work, two additional point functions $h_3(A = N+Z)$ and $h_4(E = N-Z)$ are considered in Eq. (6), and pairing energy is adopted to be a refined form of Mendoza-Temis [31]. Without further explanation, we quote the formula by He *et al.* [26],

$$M(N,Z) = h_1(N) + h_2(Z) + h_3(A) + h_4(E) + E_p. \tag{7}$$

Another type of improvement is to treat neutron-rich and proton-rich nuclei separately in the process of fitting to experimental data [27]. This separation is useful to reduce systematic errors of masses in extrapolation.

Along the same line of [27], in this paper we suggest a new and practical method to predict unknown nuclear masses by extrapolation. We adopt the same form of Eq. (6), and assume that this formula does not hold globally, but *locally instead*. The adjective word "local" means that for each nucleus, we make use of experimental mass values for only neighboring nuclei in order to determine point functions and corresponding parameters in Eq. (6). The distance between these neighboring nuclei and the nucleus to be predicted is optimized by a χ^2 fitting procedure, explained below.

Below we add subscript 0 to denote quantities of the nucleus that we describe or predict by our formulas (for instance, the proton and neutron numbers of the nucleus that we study are denoted by Z_0 and N_0, respectively). Suppose that we predict $M(N_0,Z_0)$ by using its neighboring experimental masses $M(N,Z)$. Our "locality" constraint is given by

$$\begin{aligned} |A - A_0| \leqslant R, \quad |E - E_0| \leqslant R, \\ A \neq A_0, \quad E \neq E_0, \end{aligned} \tag{8}$$

where R is neither a large number (because the GKs hold in local regions) nor a very small number [e.g., for $R = 1$, one has maximally 4 inputs which are not sufficient to fix 5 parameters in Eq. (6); for $R = 3$, one has maximally 24 inputs to fix 15 parameters in Eq. (6)]. Furthermore, we do not assume R is a constant throughout the nuclide chart; for cases in which the nucleus in our consideration is far from the region with compiled experimental data, one needs a larger R in order to have enough inputs to fix all parameters.

Our calculation is performed using a similar procedure as in Ref. [3]. For a given value of $\sigma_{\rm th}$, we calculate

$$\sum_j \frac{M^j_{\rm exp} - M^j_{\rm th}}{\sigma^{j2}_{\rm exp} + \sigma^2_{\rm th}}\frac{\partial M^j_{\rm th}}{\partial p_i} = 0, \tag{9}$$

$$\sigma^2_{\rm th} = \frac{\sum_j \left(\sigma^{j2}_{\rm exp} + \sigma^2_{\rm th}\right)^{-1}\left[\left(M^j_{\rm exp} - M^j_{\rm th}\right)^2 - \sigma^{j2}_{\rm exp}\right]}{\sum_j \left(\sigma^{j2}_{\rm exp} + \sigma^2_{\rm th}\right)^{-1}}, \tag{10}$$

with $i = 1, 2, \ldots, m$ and $j = 1, 2, \ldots, n$. Here, m is the number of parameters and n is the number of inputs. $M^i_{\rm exp}$ and $M^i_{\rm th}$ represent the experimental and theoretical masses of the ith nucleus. $\sigma^i_{\rm exp}$ is the experimental uncertainty of the ith nucleus. p_i stand for the parameters, namely, $h_1(N)$, $h_2(Z)$, λ, and μ, in Eq. (6). Calculations of these two formulas are performed iteratively until the value of $\sigma_{\rm th}$ converges. For details of the calculation, one may refer to Appendix. Eventually, we adopt the value of R which yields the minimal $\sigma_{\rm th}$ in this process for the prediction of $M(N_0,Z_0)$.

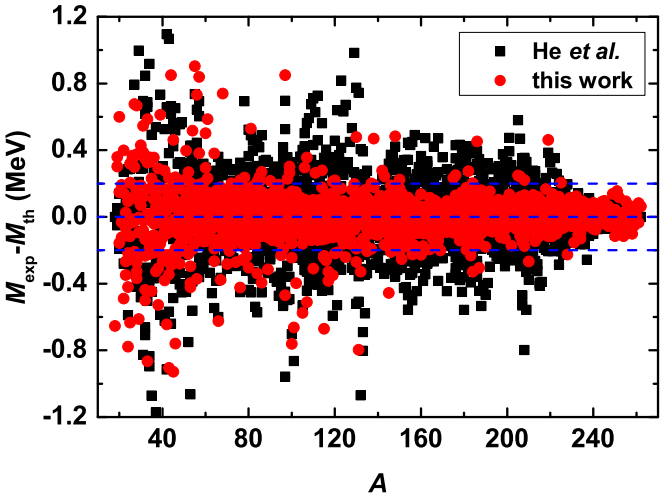

FIG. 1. Deviations (in MeV) from experimental masses in AME2016 for Eq. (7) and this work, respectively.

	124	125	126	127	128
Po	748982	768462	1123569	1527513	1636736
	764754	796244	1172234	1610969	1752651
	-149	-154	-224	-306	-330
	-89	-125	-215	-241	-295
Bi	828499	897246	1258234	1447640	1534212
	865919	949059	1342449	1565889	1684554
	-166	-181	-254	-294	-314
	-104	-175	-220	-141	-240
Pb	1270084	1423629	1267602	1343413	1272676
	1343288	1470104	1331528	1432109	1379242
	-255	-282	-254	-271	-259
	-206	-235	-61	-217	-235
Ti	1740980	1647004	1491622	1169939	911832
	1877270	1735672	1539350	1230612	978720
	-352	-329	-295	-234	-185
	-216	-135	-188	-244	-131
Hg	1804695	1803533	1387084	1216520	986574
	1915819	1944102	1464759	1286903	1024874
	-362	-365	-278	-244	-197
	-291	-115	-300	-284	-103

FIG. 2. Parameters $h_1(126)$, $h_2(82)$, λ, and μ for nuclei adjacent to the $^{208}_{82}Pb_{126}$ nucleus. For instance, the optimized $h_1(126)$, $h_2(82)$ are 1 270 084 keV and 1 343 288 keV for ^{206}Pb, and are 1 740 980 keV and 1 877 270 keV for ^{205}Ti, respectively. The values of λ and μ are also related to N_0 and Z_0, but independent of N and Z of neighboring nuclei. For example, when one describes or predicts the mass of ^{206}Pb, $\lambda = -255$ keV and $\mu = -206$ keV for all neighboring nuclei; and when one comes to the mass of ^{205}Ti, $\lambda = -352$ keV and $\mu = -216$ keV. One sees that the "local" parameters in Eq. (6) evolve with N_0 and Z_0.

III. PREDICTIVE POWER OF THE NEW METHOD

In this section, we discuss the predictive power of our method by numerical experiments, i.e., by extrapolations from the Atomic Mass Evaluation 2003 (AME2003) [19], the AME2012 database [20] to the AME2016 database [21]. As mentioned above, our method is based on the GKs whereas, due to the existence of the Wigner effect [32], the GKs are not well applicable to $Z > N$ or $Z = N =$ odd [11], and therefore those nuclei are excluded from our numerical experiments.

Before going to extrapolations, it is also interesting to remark on the description of the AME2016 for our method. We have studied this description by comparing our theoretical masses using χ^2 fitting of their nearby available data with the compiled experimental values. For 2308 nuclei in $8 \leqslant Z < 106$, $N \geqslant 10$, the resultant RMSD is 143 keV, and in $A \geqslant 120$, the RMSD is 80 keV, the accuracy of which is clearly superior to the original GKs. We note that Eq. (7) is indeed an improvement of Eq. (6), and this can be seen from the RMSD value (231 keV) of Eq. (7) for the same 2308 nuclei in the AME2016 database [in comparison, the RMSD value of Eq. (6) is about 2 MeV]. From Fig. 1, one also sees the substantial improvement of our method in comparison with Eq. (7), for $A \geqslant 60$.

Here we remark on the point functions h_1, h_2, λ, and μ in Eq. (6). These parameters change with (N_0, Z_0), and are optimized individually. In Fig. 2, we present some of the parameters [$h_1(126)$, $h_2(82)$, λ and μ] for nuclei adjacent to the ^{208}Pb nucleus. In that figure, each block corresponds to the nucleus with given (N_0, Z_0). For example, according to Fig. 2, $h_1(126)$ is 1 343 413 keV for ^{209}Pb and is 1 272 676 keV for ^{210}Pb.

Now let us first come to the extrapolation from the AME2003 database to the AME2016 database for $8 \leqslant Z, N \geqslant 10$. In Fig. 3, we show the RMSD values for $A \geqslant 60$ and $A \geqslant 120$, respectively, corresponding to 202 and 115 nuclear masses which are inaccessible in the AME2003 database, but compiled in the AME2016 database. As comparisons, we plot the RMSD values of the Audi-Wapstra extrapolation [19], the FRDM12 model [4], the HFB-17 model [5], the KTUY model [6], and the WS [7], WS3 [8], and WS3 + RBF [9] models. In addition, we also show the results of Jiang's work [30] based on the AME2003 database. Here one sees that our method works quite well in the extrapolation for $A \geqslant 60$; in particular,

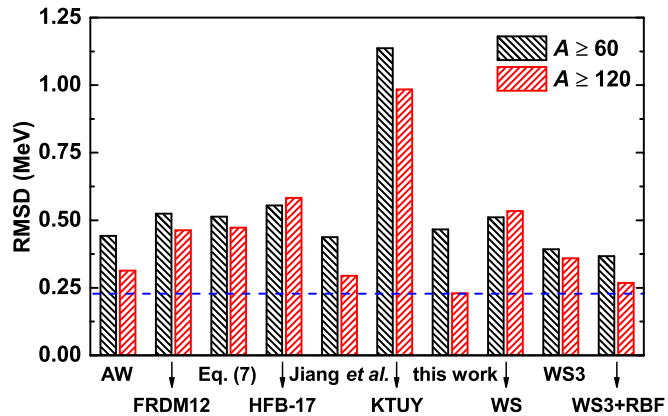

FIG. 3. Histogram of the RMSD values by extrapolations from the AME2003 database to the AME2016 database for our new method and some previous works, which include the Audi-Wapstra (AW) extrapolation [19], Eq. (7), FRDM12 [4], HFB-17 [5], KTUY [6], Jiang's work [30], this work, WS [7], WS3 [8], and WS3 + RBF [9]. The black slashed bars correspond to $A \geqslant 60$ and the red slashed bars correspond to $A \geqslant 120$, respectively. The blue dashed horizontal line denotes the RMSD of this work for $A \geqslant 120$.

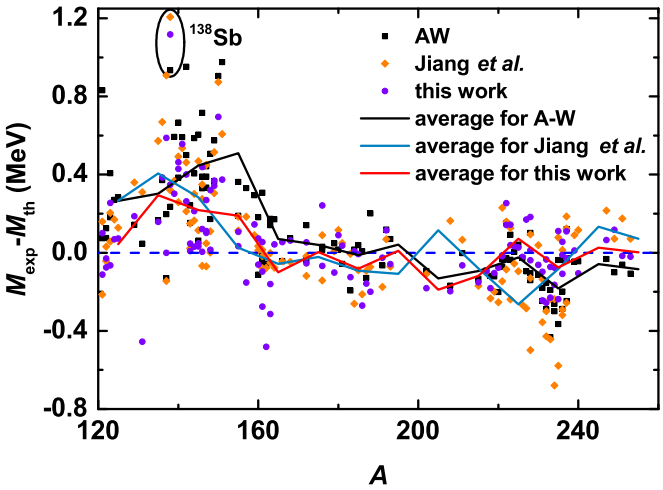

FIG. 4. Differences between predicted masses based on the AME2003 database and the values in the AME2016 database, for the AW extrapolation [19], Jiang's method [30], and this work. The deviations from the experimental mass of ^{138}Sb by these three methods are marked due to the very large experimental mass uncertainty for this nucleus.

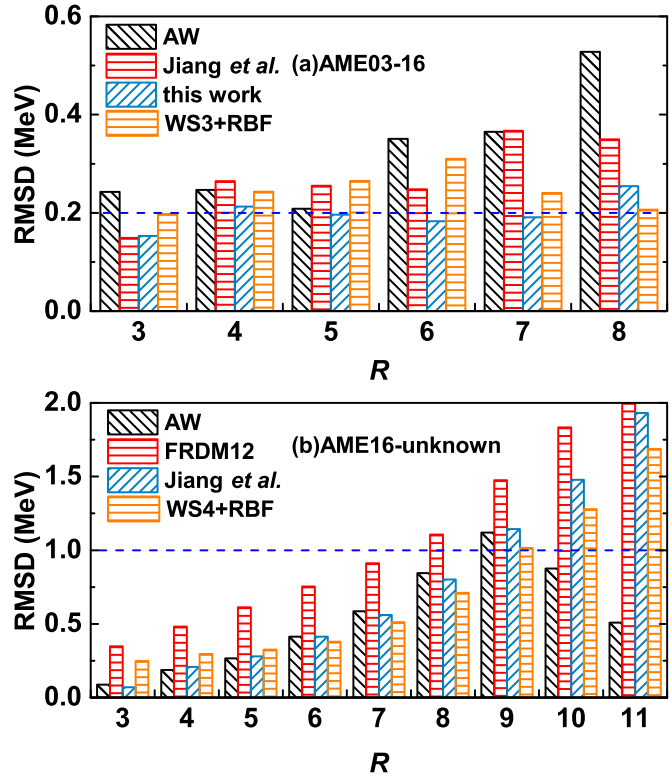

FIG. 5. (a) The RMSD of extrapolations from the AME2003 to the AME2016 for the Audi-Wapstra (AW) extrapolation [19], the approach of Jiang *et al.* [30], our approach, and WS3 + RBF [9] with respect to different numbers of parameter R, for $A \geqslant 120$. (b) The same as (a), but from the AME2016 to unknown nuclei for the AW extrapolation [21], FRDM12 [4], the approach of Jiang *et al.* [30], and WS4 + RBF [10], with reference to our predicted results.

this method is best applicable to cases with $A \geqslant 120$. For $A \geqslant 60$, the RMSD is 466 keV, and for $A \geqslant 120$, it is only 230 keV; for the same extrapolated mass values with $A \geqslant 120$, the RMSD of the Audi-Wapstra extrapolation is 314 keV, that of Ref. [30] is 295 keV, and the global WS3 with radial basis function correction is 268 keV.

Let us look at deviations between extrapolated results based on theoretical models and experimental data compiled in the AME2016 database, but not in the AME2003 database, in more detail. In Fig. 4, we present the deviations of such predicted masses (totaling 115 nuclei) from the experimental values in the AME2016 database, for our method and two local mass relations, i.e., the Audi-Wapstra extrapolation [19] and the systematics of neutron-proton interaction [30], as well as the average deviations (with an interval $\Delta A = 10$) of all three sets of extrapolations. One sees that the Audi-Wapstra extrapolation generally underestimates masses for nuclei with $120 \leqslant A \leqslant 160$, but overestimates the masses in $A \geqslant 220$. For Ref. [30], the underestimation in Ref. [19] for $120 \leqslant A \leqslant 160$ is improved, but deviations are large for $A \simeq 230$. For the results of our method, the deviations of both $120 \leqslant A \leqslant 160$ and $A \simeq 230$ are relatively small. Here we note ^{138}Sb, whose uncertainty of atomic mass compiled in the AME2016 is 1.064 MeV. In Fig. 4, we have put the deviation of the extrapolated atomic mass for ^{138}Sb inside a circle in black; in case this deviation is excluded, the RMSD values of the Audi-Wapstra extrapolation, Ref. [30], and this work become 303, 274, and 206 keV, respectively.

Our numerical experiments are also exemplified by extrapolation from the AME2012 database to the AME2016 database. For $A \geqslant 120$, the extrapolation has only 29 nuclei and we present predicted results by using our new method in Table I. For comparison, the results of the Audi-Wapstra extrapolation [20], Bao *et al.* [18] based on GKs, and WS4 + RBF [10] are also listed. According to the table, mass(es) of one nucleus or more nuclei are not accessible by the Audi-Wapstra extrapolation [20], Bao *et al.* [18], or Jiang *et al.* [30]. In Table I, 21 among the 29 nuclei are evaluated using those five methods, and the RMSD values of these 21 nuclei are 175, 169, 216, 215, and 158 keV (see the last row of Table I), respectively. Once again, if we exclude the result of ^{138}Sb, the RMSD values are reduced to 164, 160, 209, 212, and 130 keV, respectively. According to this comparison, Ref. [18] yields comparably good predictions with the Audi-Wapstra extrapolation, and the RMSD value of Jiang *et al.* [30] is very close to that of WS4 + RBF [10]; still, our method is superior to all previous predictions for $A \geqslant 120$. It is also worthwhile to point out that the theoretical uncertainties of our extrapolated masses are in general smaller than other previous methods, as shown in Table I.

The above success of extrapolation encourages us to discuss the advantages of our new method in comparison with other local mass relations. In our method, we begin with the general solution of the GKs, but remove specific combinations in the GKs. In the GKs, one needs the inputs of neighboring nuclei with specific N and Z, while in our present method, one could make use of *all* available data of neighboring nuclei. For instance, in the case of extrapolation from the AEM2003 to the AME2016, the average number of nuclei whose masses

TABLE I. Predicted mass excesses and their uncertainties (in keV) predicted by Audi-Wapstra (AW) extrapolation [20], Bao *et al.* [18], Jiang *et al.* [30], WS4+RBF [10], and this work, respectively, for the nuclei with $A \geqslant 120$, from the AME2012 database [20] to the AME2016 database [21]. The last row presents the RMSD (in keV) of the 21 calculated masses in this table with and without consideration of ^{138}Sb, given outside and inside the parentheses, respectively.

Element	AME2016	AW	Bao *et al.*	Jiang *et al.*	WS4+RBF	This work
^{121}Rh	−56250 ± 619	−56430 ± 298	−56390 ± 190	−56325 ± 144	−55859	−56325 ± 149
^{123}Pd	−60430 ± 789	−60417 ± 196	−60322 ± 199	−60531 ± 192	−60391	−60276 ± 128
^{129}Cd	−63058 ± 17	−63509 ± 196	−63569 ± 124	−63638 ± 96	−63646	−63338 ± 194
^{131}Cd	−55219 ± 102	−55331 ± 196	−54984 ± 159	−55822 ± 170	−55385	−54954 ± 363
^{138}Sb	−54220 ± 1064	−54539 ± 298	−54521 ± 157	−54552 ± 117	−54493	−54653 ± 65
^{141}I	−59927 ± 16	−59904 ± 196	−59951 ± 135	−59930 ± 100	−59882	−59943 ± 78
^{149}Ba	−53120 ± 438	−53021 ± 196	−53171 ± 149	−52947 ± 395	−53069	−53153 ± 154
^{150}La	−56130 ± 435	−56383 ± 196	−56432 ± 136	−56337 ± 174	−56299	−56450 ± 144
^{151}La	−53310 ± 435	−53729 ± 196	−53472 ± 224	−53275 ± 153	−53701	−53238 ± 121
^{137}Eu	−60146 ± 4	−60119 ± 196	−60100 ± 94	−59998 ± 94	−60147	−60145 ± 96
^{190}Ti	−24372 ± 8	−24379 ± 50	−24416 ± 83	−24410 ± 56	−24431	−24376 ± 111
^{215}Pb	4342 ± 52	4416 ± 101	4466 ± 114	4499 ± 66	4328	4456 ± 68
^{194}Bi	−16029 ± 6	−16036 ± 51	−15958 ± 85	−15957 ± 56	−16167	−15957 ± 62
^{198}At	−6715 ± 6	−6721 ± 51	−6659 ± 87	−6636 ± 60	−6872	−6715 ± 69
^{197}Fr	10254 ± 54		10488 ± 145	10441 ± 117	10282	10334 ± 60
^{198}Fr	9574 ± 32		9613 ± 105	9597 ± 90	9184	9514 ± 84
^{202}Fr	3096 ± 7	3092 ± 51	3140 ± 91	3123 ± 69	2876	3057 ± 41
^{232}Fr	46073 ± 14	45986 ± 155	45984 ± 114	46091 ± 71	46030	45941 ± 57
^{233}Fr	48920 ± 20	49034 ± 298	48894 ± 132	48907 ± 107	49062	48898 ± 48
^{201}Ra	11937 ± 20	11841 ± 106	11950 ± 94	12033 ± 100	11820	11970 ± 73
^{205}Ac	14107 ± 51		13940 ± 105	14049 ± 119	13973	14032 ± 62
^{206}Ac	13479 ± 50	13462 ± 71	13446 ± 103	13392 ± 94	13250	13376 ± 82
^{215}U	24923 ± 88		24917 ± 154	25184 ± 128	25212	24817 ± 62
^{216}U	23066 ± 28		23191 ± 123	23283 ± 130	23118	23072 ± 56
^{221}U	24520 ± 51	24483 ± 102	24498 ± 111	24468 ± 88	24546	24541 ± 107
^{222}U	24273 ± 52	24222 ± 101	24204 ± 98	24292 ± 89	24321	24236 ± 96
^{219}Np	29457 ± 88	29277 ± 196		29606 ± 249	29316	29115 ± 154
^{229}Am	42150 ± 87		41891 ± 199	41912 ± 170	42148	42168 ± 170
^{259}No	94079 ± 7	94111 ± 100	94107 ± 93		93995	94121 ± 60
RMSD (keV)		175 (164)	169 (160)	216 (209)	215 (212)	158 (130)

were used to predict 115 unknown masses is about 31. This value is larger than the GKs (which are 14) to predict an unknown mass of nucleus. The second advantage is that we adopt experimental data by different weights according to their experimental uncertainties, namely, experimental data with large uncertainties are taken with smaller weight factors, as shown in Eqs. (9) and (A7). The third advantage is that we have a procedure to optimize the number of R which leads to the smallest theoretical error $\sigma_{\rm th}$; e.g., the selected numbers are $R = 5$ and $R = 6$ for ^{202}Fr and ^{222}U, respectively, but not the smallest numbers $R = 4$ and $R = 5$, whose predictions, 3030 and 24 235 keV, are further away from the experimental values.

It is interesting to survey how far our extrapolation method can go from the borders of the available experimental data. First, we investigate the numerical experiment in Fig. 3 in more detail. The three most accurate methods, i.e., AW extrapolation, Jiang *et al.*, and WS3 + RBF, as well as our method are compared with respect to the range number R. The RMSD results for $A \geqslant 120$ (^{138}Sb is expelled) are illustrated in Fig. 5(a). Apart from $R = 4$ and $R = 8$, our method yields RMSD lower than 200 keV. One sees visible improvements in accuracy of our method compared with other convincing mass predictions, from $R = 3$ to $R = 7$. For $R = 8$, our method yields a slightly large deviation compared with WS3 + RBF, whereas it is still better than AW and Jiang's extrapolation. There are no available data in the $R \geqslant 9$ cases. As an extension of this investigation, we apply both our method and the extrapolation method of Jiang *et al.* [30] to the AME2016 database. In Ref. [30], the systematics of the neutron-proton interaction versus A and the subtle shell effects are considered, and therefore it is expected to be reliable even for extrapolation rather far from the borders of the AME database in the nuclear chart. In Fig. 5(b), we plot the deviation of predictions between the approach of Jiang *et al.* [30] and this work using the same diagram as Fig. 5(a). We also include the comparison of predictions in this work with those in the FRDM12, WS4 + RBF, and Audi-Wapstra models. One sees that, in general, the deviations between this work and other models increase with R. We should note here that the abnormal decreases of the RMSD from $R = 9$ to $R = 10$ and $R = 11$ for the Audi-Wapstra extrapolations are essentially originated from the fact that there are very few results in the AME2016 database which correspond to $R \geqslant 9$: For $R = 10$,

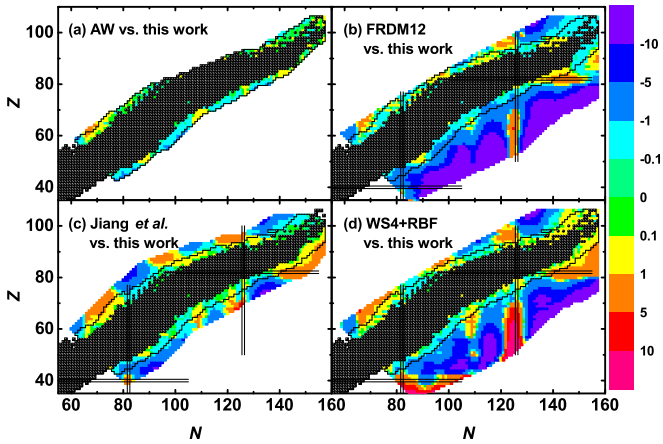

FIG. 6. Deviations of theoretically predicted masses for previous efforts with respect to predictions of this work by using the AME2016, with the constraint of $A \geqslant 120$, vs neutron number N and proton number Z. Deviations are denoted in different colors according to the magnitude of the deviations. (a) Audi-Wapstra (AW) extrapolation [21]; (b) FRDM12 [4]; (c) Jiang *et al.* by using the systematics of proton-neutron interactions and the AME2016 database [30]; and (d) the WS4 + RBF method by Wang *et al.* [10]. The black contours correspond to the region with $R \leqslant 8$ in this paper, and the dots in black correspond to nuclei whose experimental masses compiled in the AME2016. (b)–(d) The magic numbers $N = 82$ and 126 and $Z = 40$ and 82 are sandwiched by solid lines in orange.

there are only six predictions, and for $R = 11$, there is only one predicted mass, in the Audi-Wapstra systematics [21].

In Fig. 6, we plot the deviations of the above four models with respect to this work versus N and Z with $A \geqslant 120$. In Fig. 6(a), one sees that deviations of the AW extrapolation from the predictions in this work are very small, and most of the masses in the AW extrapolation are able to be evaluated in this work (if the $R \leqslant 8$ constraint is used). In Figs. 6(b)–6(d), one sees that the systematic differences between the predictions in our work and the predictions in the other three works, i.e., the FRDM12 by Moller *et al.*, the systematics of the neutron-proton interactions by Jiang *et al.* [30], and the WS4 + RBF model by Wang *et al.* [10], are larger than 1 Mev for $R > 8$. In addition, one sees from Figs. 6(b)–6(d) that the approach in this work generally overestimates the nuclear masses when $R \geqslant 9$; meanwhile, it underestimates the masses near the $N = 82$, $N = 126$, $Z = 82$ (and probably $Z = 40$ for WS4 + RBF) neutron-rich shells. This means that this approach is not able to take the shell effect into account properly in long-range extrapolations.

We tabulate our predicted nuclear masses based on the AME2016 database [21] for $A \geqslant 120$ in the Supplemental Material [34], where we have excluded results for which theoretical uncertainties are larger than 1 MeV or $R > 8$. The results of Ref. [30] based on the AME2016 database and the experimental data (as well as the estimated values) in the AME2016 database are also listed therein for convenience. In addition, the fitted parameters for each prediction over the whole nuclide chart are provided in another material.

IV. SUMMARY

To summarize, in this paper we suggest a new and practical method to predict nuclear masses which are inaccessible experimentally. This method is based on the Garvey-Kelson mass relations and Jännecke mass formula. We have demonstrated, by extrapolations from the AME2003 and AME2012 databases to the AME2016 database, that the predictive power of our new method is very competitive. For mass number A larger than 120, our extrapolated results have the smallest root-mean-squared deviations from the latest experimental results. With the practice of other popular approaches, we put a constraint on our method: our extrapolation should be within six steps (namely, $R \leqslant 8$) from the borders of the AME database.

We enclose our predicted atomic masses for about 600 nuclei, whose masses are not yet experimentally accessible according to the AME2016 database, in the Supplemental Material [34]. As this new method is highly accurate in extrapolation, our predictions are hopefully useful in theoretical studies and future experimental measurements.

ACKNOWLEDGMENTS

This work was partly supported by the National Natural Science Foundation of China under Grants No. 11675101, No. 11975151, No. 11961141003, No. 11905130, No. 11875070, and No. 11711540016, Shanghai Sailing Program (Grant No. 19YF1434200), the Natural Science Foundation of Anhui Province under Grant No. 1708085QA10, Shanghai Key Laboratory (Grant No. 11DZ2260700), Open Foundation of Shanghai Key Laboratory of Particle Physics and Cosmology (Grant No. 18DZ2271500-3) and the Open Fund for Discipline Construction, Institute of Physical Science and Information Technology, Anhui University.

APPENDIX: DETAILS OF FITTING PROCEDURE

In Sec. II, we have mentioned that the prediction of mass $M(N_0, Z_0)$ and the corresponding theoretical error $\sigma_{\rm th}$ are derived by convergence of Eqs. (9) and (10). Here we begin from the equation used to predict $M(N_0, Z_0)$ as

$$M(N_0, Z_0) = \sum_{i=1}^{k} h_1(N_i')\delta_{N_0,N_i'} + \sum_{j=1}^{l} h_2(Z_j')\delta_{Z_0,Z_j'} + \lambda N_0 Z_0 + \mu \frac{1-(-1)^{N_0 Z_0}}{2}, \quad \text{(A1)}$$

where the prime in N_i' and Z_i' is used to discriminate respectively from N_i and Z_i in the fitting procedure, and k, l represent the size of the region of nuclei whose masses are going to be fitted. In our present approach, Eq. (6) holds "locally," which means k and l cannot be very large numbers. To be more specific, we introduce another parameter, R, in Eq. (8). The relation between k, l, and R is as follows: $k, l <= 2R + 1$, where R gives the upper limit for the difference between A and A_0, E and E_0, for nuclei used to optimize our parameters. It is different from the "global" use of Eq. (6), in which one changes k and l as flexibly as one wishes. $\delta_{N_0,N_i'}$ and $\delta_{Z_0,Z_j'}$ are Kronecker δ functions. Here we note that there is collinearity

as

$$\sum_{j=1}^{k} \delta_{N_i,N'_j} = \sum_{j=1}^{l} \delta_{Z_i,Z'_j}(=1) \tag{A2}$$

holding for arbitrary input (N_i, Z_i). Thus one of these δ inputs should be replaced with the others and disappear from Eq. (A1). For convenience, we exclude the δ_{Z_i,Z'_1} and construct the matrices as

$$X = \begin{pmatrix} \delta_{N_1,N'_1} & \cdots & \delta_{N_1,N'_k} & \delta_{Z_1,Z'_2} & \cdots & \delta_{Z_1,Z'_l} & N_1Z_1 & \frac{1-(-1)^{N_1Z_1}}{2} \\ \delta_{N_2,N'_1} & \cdots & \delta_{N_2,N'_k} & \delta_{Z_2,Z'_2} & \cdots & \delta_{Z_2,Z'_l} & N_2Z_2 & \frac{1-(-1)^{N_2Z_2}}{2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \delta_{N_n,N'_1} & \cdots & \delta_{N_n,N'_k} & \delta_{Z_n,Z'_2} & \cdots & \delta_{Z_n,Z'_l} & N_nZ_n & \frac{1-(-1)^{N_nZ_n}}{2} \end{pmatrix}$$

and

$$Y_{\text{exp}} = (M_{\text{exp}}(N_1, Z_1)\, M_{\text{exp}}(N_2, Z_2) \ldots M_{\text{exp}}(N_n, Z_n))^T, \tag{A3}$$

where M_{exp} represents the experimental mass value used in the fitting procedure,

$$W = \begin{pmatrix} \sigma_1^{-1} & 0 & \cdots & 0 \\ 0 & \sigma_2^{-1} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma_n^{-1} \end{pmatrix}, \tag{A4}$$

in which $\sigma_i = (\sigma_{\text{exp}}^{i2} + \sigma_{\text{th}}^2)^{1/2}$ and the matrix of parameters

$$\beta = (h_1(N'_1), \ldots, h_1(N'_k), h_2(Z'_2), \ldots, h_2(Z'_l), \lambda, \mu)^T. \tag{A5}$$

Here, X, Y_{exp}, W, and β are $n \times m\,(m = l + k + 1), n \times 1, n \times n$, and $m \times 1$ matrices, respectively. n is the number of inputs and m is the number of parameters. Once the β is determined, the theoretical masses M_{th}^i of the fitted subset are given as

$$Y_{\text{th}} = \left(M_{\text{th}}^1\, M_{\text{th}}^2\, \ldots\, M_{\text{th}}^n\right)^T = X\beta. \tag{A6}$$

To solve Eq. (9), we mention that it is equivalent to minimizing S^2 with respect to β [3], where

$$\begin{aligned} S^2 &= (Y_{\text{exp}} - Y_{\text{th}})^T W^2 (Y_{\text{exp}} - Y_{\text{th}}) \\ &= (Y_{\text{exp}} - X\beta)^T W^2 (Y_{\text{exp}} - X\beta). \end{aligned} \tag{A7}$$

Therefore,

$$\begin{aligned} \frac{\partial S^2}{\partial \beta} &= 2\frac{\partial (Y_{\text{exp}} - X\beta)^T}{\partial \beta} W^2 (Y_{\text{exp}} - X\beta) \\ &= -2X^T W^2 (Y_{\text{exp}} - X\beta) = 0 \end{aligned} \tag{A8}$$

yields [33]

$$\beta = (X^T W^2 X)^{-1} X^T W^2 Y_{\text{exp}}. \tag{A9}$$

According to β, the theoretical value $M_{\text{th}}^i(Y_{\text{th}})$ is derived by Eq. (A6). Here it is better to note that in our application, the number of parameters is always smaller than that of the fitted data, leading X to be a nonsquare matrix, which has no well-defined inverse matric. $(X^T W^2 X)^{-1}$ cannot be decomposed as $X^{-1} W^{2^{-1}} X^{T^{-1}}$ and would not result in $Y_{\text{th}} = Y_{\text{exp}}$. Then, Y_{th} are used in Eq. (10) to iterate σ_{th} until the value of σ_{th} converges. The prediction of $M(N_0, Z_0)$ is

$$M_{\text{th}}(N_0, Z_0) = x_0\beta, \text{ where}$$

$$x_0 = \left(\delta_{N_0,N'_1} \ \ldots\ \delta_{N_0,N'_k},\ \delta_{Z_0,Z'_2} \ \ldots\ \delta_{Z_0,Z'_l}\ N_0Z_0\ \frac{1-(-1)^{N_0Z_0}}{2}\right). \tag{A10}$$

Our theoretical uncertainty is given by

$$t\frac{S}{\sqrt{n-m}}\sqrt{\sigma_{\text{th}}^2 + x_0(X^T W^2 X)^{-1} x_0^T}, \tag{A11}$$

where the value of t is fixed by an integral as follows [33]:

$$\int_{-t}^{t} \frac{\Gamma\left(\frac{n-m+1}{2}\right)}{\sqrt{\pi(n-m)}\,\Gamma\left(\frac{n-m}{2}\right)} \left[1 + \frac{z^2}{n-m}\right]^{-\frac{n-m+1}{2}} dz = 0.6826.$$

Here, $\Gamma(x)$ is the usual Γ function, $\Gamma(x) = (x-1)!$, $x! = x(x-1)!$, with $\Gamma(1)! = 1$ and $\Gamma(\frac{3}{2})! = \sqrt{\pi}$.

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