

Nuclear mass predictions with a radial basis function approach

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With the help of the radial basis function (RBF) and the Garvey-Kelson relation, the accuracy and predictive power of some global nuclear mass models are significantly improved. The rms deviation between predictions from four models and 2149 known masses falls to ~ 200 keV. The AME95-03 and AME03-Border tests show that the RBF approach is a very useful tool for further improving the reliability of mass models. Simultaneously, the differences from different model predictions for unknown masses are remarkably reduced and the isospin symmetry is better represented when the RBF extrapolation is combined.

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Nuclear mass predictions and evaluations are of great importance, not only for various applications, but also for the testing and development of nuclear theory. The unmeasured masses are usually predicted by using some global nuclear mass models in which some physics are considered and the model parameters are determined by the known masses [1,2] or by adopting some local mass relations based on the measured masses of its neighbors. Some global nuclear mass models such as the finite-range droplet model (FRDM) [3], the Weizsäcker-Skyrme (WS) mass model [4–6], the Hartree-Fock-Bogoliubov (HFB) model [7], and the Duflo-Zuker (DZ) mass model [8], successfully reproduce the measured masses with accuracy at the level of 300–600 keV. However, the divergence for describing the masses of the extremely neutron-rich nuclei from these different global mass models indicates that more physics and more information about nuclear force should be considered in the models. The uncertainty in nuclear force and the limiting of computational resources cause great difficulties for further improving these available global nuclear mass models. On the other hand, one could use the local mass relations such as the isobaric multiplet mass equation (IMME) [9], the Garvey-Kelson (GK) relations [10], and the residual proton-neutron interactions [11–13] to give predictions of unmeasured masses. It is found that when these local mass relations are used to predict the masses of nuclei in an iterative fashion, the intrinsic error grows rapidly [14] due to the following: (1) The local mass relations are just approximately satisfied in known masses and (2) the previously predicted masses are used on each new iteration and a systematic error accumulates (see Table I in Ref. [14] and the expressions σ_{pred} in Ref. [13]). To improve the accuracy of nuclear mass predictions, the systematics of the nuclear mass surface is analyzed in the image reconstruction techniques [15,16] based on the Fourier transform (CLEAN algorithm) by combining some global nuclear mass models. Compared with other local mass relations mentioned previously, the image reconstruction techniques predict the mass of a unmeasured nucleus by using many more known masses rather than just the masses of its neighbors. Therefore, more information from the experimental data could be involved for the mass predictions.

It is found that important improvements in the predictions given by the different models were obtained with the CLEAN reconstruction.

In this Rapid Communication, we attempt to propose a more efficient systematic method based on the radial basis function approach [17,18], together with the available nuclear mass models, for further improving the nuclear mass predictions. The mass predictions for unmeasured nuclei can be treated as a problem of mass surface extrapolation from the scattered experimental data. The most prominent global interpolation and extrapolation scheme is the radial basis function (RBF) approach that originates from Hardy's multiquadric interpolation [17]. As a powerful solution to the problem of scattered data fitting, the radial basis function is widely applied in surface reconstruction. The simplest form of the RBF solution is written as $S(\mathbf{x}) = \sum_{i=1}^m w_i \phi(\|\mathbf{x} - \mathbf{x}_i\|)$, where \mathbf{x}_i denotes the points from measurement, w_i is the weight of center \mathbf{x}_i , ϕ is the basis function, $\|\mathbf{x}\|$ is the Euclidean norm, and m is the number of the scattered data to be fitted. Given m samples (\mathbf{x}_i, f_i) , one wishes to reconstruct the smooth function $S(\mathbf{x})$ with $S(\mathbf{x}_i) = f_i$. The RBF weights w_i are determined by the solution of the linear system resulting from the interpolation condition. Standard basis functions include the following: spline, $\phi(r) = r$, or $\phi(r) = r^2 \log(r)$; Gaussian, $\phi(r) = \exp(-cr^2)$, with $c > 0$; multiquadric, $\phi(r) = \sqrt{r^2 + c^2}$; and inverse multiquadric, $\phi(r) = 1/\sqrt{r^2 + c^2}$.

With the RBF approach, the difference $R(N, Z) = M_{\text{exp}} - M_{\text{th}}$ between the calculated masses M_{th} with global nuclear mass models and the experimental data M_{exp} could be reconstructed. Once the reconstructed function $S(N, Z)$ is obtained, the revised masses for unmeasured nuclei are given by $M_{\text{th}}^{\text{RBF}} = M_{\text{th}} + S$. Here we perform three tests for each mass model, and for all tests we only consider nuclei with neutron number $N \geq 8$ and proton number $Z \geq 8$. The first one is that we reconstruct the function $S(N, Z)$ for a selected known nucleus based on other known masses, together with a certain global mass model. In other words, we take the 2148 known masses of nuclei for training the RBF ($m = 2148$) and use the remaining one nucleus from the 2149 nuclei in the atomic mass evaluation of 2003 (AME2003) [2] as a test. The corresponding results from this kind of cross validation will be shown in Fig. 1 and Table I. The second one is that we take the masses in AME1995 [1] for training the RBF ($m = 1760$)

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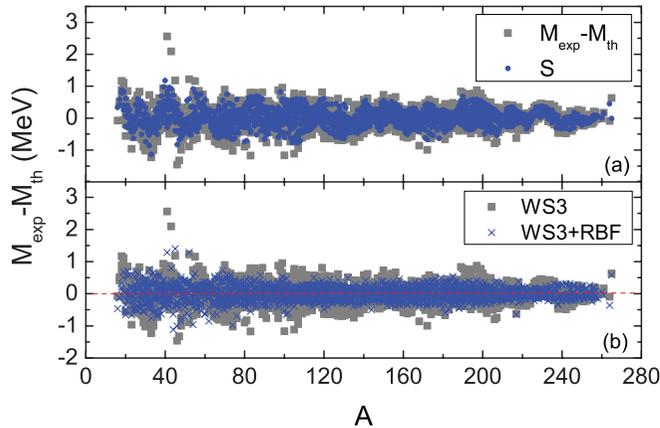


FIG. 1. (Color online) Difference between predicted masses with the WS3 model and the experimental data. The solid circles in (a) denote the reconstructed function $S(N, Z)$ from the radial basis function with $\phi = r$. The crosses in (b) denote the corresponding deviations from data when the function S is added to the masses with WS3.

and predict the 389 “new” masses in AME2003, and the corresponding results will be listed in Table II. The third one is that we take the masses of nuclei near the β -stability line (nuclei with neutron separation energy of $5 \leq S_n \leq 12$ MeV) for training the RBF ($m = 1700$) and predict the remaining 449 masses of nuclei approaching drip lines, and the results will be shown in Table III. We find that the mass deviation $R(N, Z)$ can be reconstructed relatively better with $\phi(r) = r$, i.e., a natural spline function. Therefore, we adopt the basis function $\phi(r) = r$ in the calculations.

In Fig. 1(a), we show the differences between the calculated masses with the WS3 model [6] and the experimental data [2] (gray squares). The reconstructed function S (solid circles) is also shown for comparison. One sees that the RBF reproduces the differences $M_{\text{exp}} - M_{\text{th}}$ with high quality and has good approximation properties. With the approximating function $S(N, Z)$, the differences between the predicted masses and the experimental data are dramatically reduced [see the crosses in Fig. 1(b)]. In Table I, we list the rms deviations between the 2149 know masses [2] and predictions from five mass models: WS3 [6], DZ28 [8], FRDM [3], HFB17 [7], and WS* [5]. The column Model+RBF means the reconstructed function S with the RBF approach is added to the calculated masses with the five models. The column Model+RBF+GK12

TABLE I. rms σ deviations between 2149 know masses [2] and predictions of five models (in keV). Here, to predict the mass of a nucleus in AME2003, we take the remaining 2148 known masses for training the RBF ($m = 2148$)—see the text for details.

	Model	Model+RBF	Model+RBF+GK12
WS3 [6]	336	223	184
DZ28 [8]	360	227	187
FRDM [3]	656	283	216
HFB17 [7]	581	390	313
WS* [5]	441	256	217

TABLE II. rms deviations with respect to 389 “new” masses in AME2003 based on the mass models and the measured masses in AME1995 ($m = 1760$) for training the RBF (in keV).

	Model	Model+RBF
WS3	378	311
DZ28	430	341
FRDM	536	351
HFB17	519	380
WS*	517	358

denotes that the Garvey-Kelson relation [10], which contains 12 estimates for a nucleus with the corresponding values of its 21 neighbors, is also adopted for further improving the smoothness of the function $S(N, Z)$. With the help of the RBF and the GK relation, the rms deviations from the 2149 nuclei are reduced sharply for all five models, and the results from four models reach ~ 200 keV. In Fig. 2, we show the rms deviations obtained with the first test for WS3 but as a function of average neutron-separation energy of nuclei. With the RBF approach, the rms deviations are reduced obviously, especially for nuclei approaching the drip lines.

The second test, i.e., AME95-03 test, is usually used to check the predictive power of mass models. The crosses in Fig. 3 denote the positions of nuclei to be predicted in the AME95-03 test. Table II lists the rms deviations with respect to 389 “new” masses in AME2003 based on the five mass models and the measured masses in AME1995 for training. The reduction of rms deviation is 18% for the WS3 model, 21% for the DZ28 model, 35% for the FRDM, 27% for the HFB17 model, and 31% for the WS* model, respectively, when the RBF approach is combined. We note that the reduction of the rms deviation ($N, Z \geq 8$) is $\sim 12\%$ with the CLEAN reconstruction [16] combining the 31-parameter Duflo-Zuker (DZ31) mass model [19] in this test. The corresponding result with the RBF approach remarkably reaches $\sim 23\%$. Combining the liquid drop model (LDM) mentioned in Ref. [15], the rms reduction in the AME95-03 test reaches $\sim 54\%$ with the CLEAN reconstruction and $\sim 72\%$ with the RBF approach, respectively. It seems that the radial basis function approach is a more efficient tool for improving the accuracy of nuclear mass predictions. Furthermore, in the CLEAN algorithm one needs to perform a series of iterations until a given stopping criteria ($\sigma = 100$ keV, for example) which is not required in the RBF approach. In the RBF approach, one just

TABLE III. rms deviations (in keV) from 449 masses of nuclei approaching AME03-Border based on the mass models and the known masses of nuclei with a neutron separation energy of $5 \leq S_n \leq 12$ MeV ($m = 1700$) for training the RBF.

	Model	Model+RBF
WS3	423	367
DZ28	491	392
FRDM	855	582
HFB17	730	575
WS*	591	417

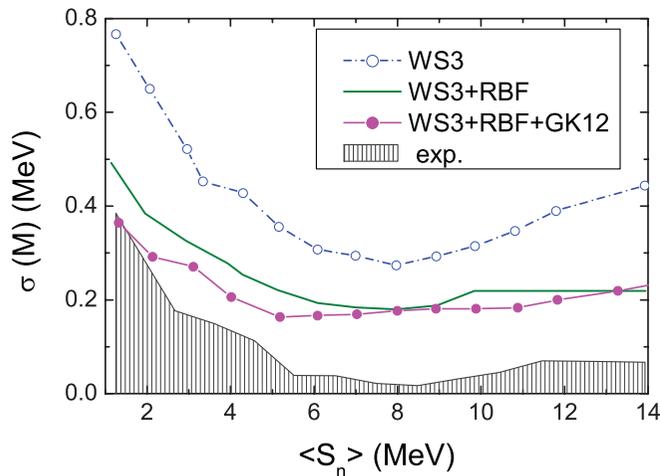


FIG. 2. (Color online) rms deviation with respect to the masses as a function of average neutron-separation energy of nuclei. The shades present the average standard deviation errors of the measured masses [2].

needs to calculate the weights w_i , which can be estimated using the matrix methods of linear least squares, because the approximating function $S(N, Z)$ is linear in the weights.

In Table III, we list the rms deviations with respect to the 449 masses of nuclei approaching AME03-Border based on the five models and the known masses of nuclei with a neutron separation energy of $5 \leq S_n \leq 12$ MeV in AME2003 for training. The definition of the AME03-Border test here is slightly different from that in Ref. [16] (see the squares in Fig. 3). The rms deviation is reduced by 20% for the DZ28 model, 21% for the HFB17 model, 29% for the WS* model, and 32% for the FRDM, respectively. For the WS3 model, we obtain a reduction of 13%. These calculations indicate that the reliability of the available mass models can be significantly improved by combining the RBF approach. With the GK relation, the results in Tables II and III can be further improved as do those in Table I, because the GK relation is also well

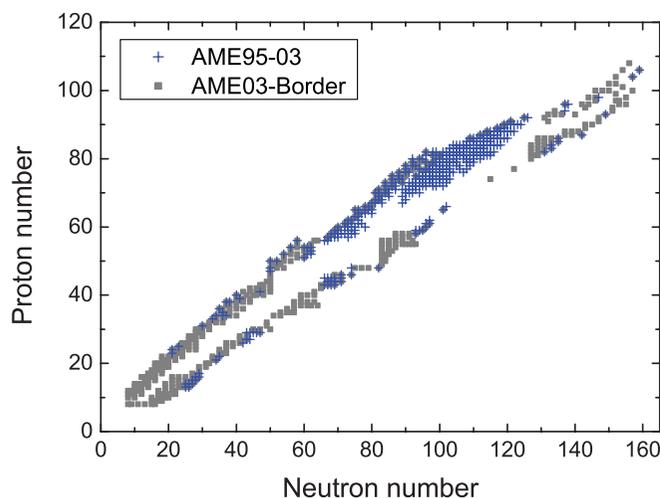


FIG. 3. (Color online) Positions of nuclei predicted in the AME95-03 test (crosses) and the AME03-Border test (squares).

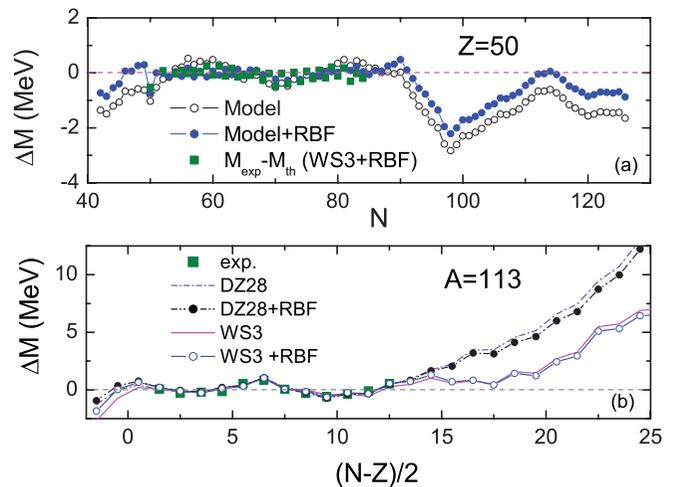


FIG. 4. (Color online) (a) Difference between the calculated masses with the mass model WS3 and those with DZ28 for Sn isotopes. The solid circles denote the corresponding results when the RBF approach is combined. (b) Difference of the calculated masses with the mass models from the results through fitting the experimental masses with a parabola for isobaric nuclei of $A = 113$. The squares denote the deviations from the experimental data, i.e., $M_{\text{exp}} - M_{\text{fit}}$. The solid and the dashed-dotted curve denote the results with WS3 and DZ28, respectively.

satisfied at the mass region with nuclei far from the β -stability line [10].

In addition, we study the predictions from these mass models for unmeasured nuclei. It is known that the predictions from different models toward the neutron-drip line tend to diverge. As an example, the difference $\Delta M = M(\text{DZ28}) - M(\text{WS3})$ between the calculated masses with the DZ28 model and those with the WS3 model for Sn isotopes is shown in Fig. 4(a) (open circles) as a function of neutron numbers. For known nuclei, the differences between the calculated masses from the two models are small. However, the deviations reach a few MeV for nuclei approaching the drip lines. The solid circles in Fig. 4(a) denote the corresponding results when the RBF approach is combined. The differences between the predicted masses from the two models are reduced by ~ 1 MeV. Simultaneously, we

TABLE IV. rms deviations (in MeV) with respect to the evaluated masses in AME2003 [2] (marked by #) and those in Ref. [13] for nuclei with $Z \leq 102$ based on the residual proton-neutron interactions. Here the RBF approach ($m = 2149$) and the GK relation are involved in the mass predictions with the five models. n_1 and n_2 denote the number of evaluated masses taken from AME2003 and Ref. [13] for the rms calculations, respectively.

	n_1	AME2003 [2]	n_2	δV_{1p1n} [13]
WS3	935	0.629	459	0.479
DZ28	935	1.058	459	0.470
FRDM	935	0.784	459	0.597
HFB17	892	0.743	459	0.706
WS*	935	0.626	459	0.498

list in Table IV the rms deviations with respect to the evaluated masses in AME2003 [2] (marked by #) and those in Ref. [13] based on the residual proton-neutron interactions. We find that when the RBF approach ($m = 2149$) and the GK relation are involved in the mass predictions, the rms deviations with respect to the evaluated masses in AME2003 are remarkably reduced. The rms reductions reach 23% for the WS3 model, 34% for the DZ28 model, 38% for the FRDM, 23% for the HFB17 model, and 31% for the WS* model, respectively. The rms deviations from the evaluated masses based on the residual proton-neutron interactions [13] are also significantly reduced, with a rms reduction of 38% for the WS3 model, 42% for the DZ28 model, 44% for the FRDM, 33% for the HFB17 model, and 46% for the WS* model, respectively. These calculations also demonstrate that the differences from these different models can be remarkably reduced when the RBF approach and the GK relation are applied.

In Fig. 4(b) we show the difference $\Delta M = M_{\text{th}} - M_{\text{fit}}$ between the predicted masses with models and the results by fitting the known masses with a parabola for a series of isobaric nuclei with $A = 113$. According to the isobaric multiplet mass equation (IMME), which is a basic prediction leading from the isospin concept, the masses of isobaric nuclei can be expressed as $M_{\text{fit}}(A, T_z) = a + bT_z + cT_z^2$, with $T_z = (N - Z)/2$. One sees from Fig. 4(b) that the deviation $M_{\text{th}} - M_{\text{fit}}$ is quite large for nuclei approaching the neutron drip line. When the RBF approach is combined, the deviations are slightly reduced, which indicates that the isospin symmetry is relatively better represented with the help of the RBF extrapolation. Simultaneously, we study the b coefficients in the IMME with different models. The b coefficients in the

IMME for nuclei can be extracted from the binding energies of pairs of mirror nuclei $b = \frac{BE(T=T_z) - BE(T=-T_z)}{2T}$ with the isospin $T = |N - Z|/2$. We calculate rms deviations between the experimental b coefficients in the IMME for 62 pairs of mirror nuclei and the predicted ones with the models. When the RBF approach and the GK relation are used, the rms deviations from the experimental b coefficients are significantly reduced from 159 to 97 keV for the WS3 model, from 274 to 144 keV for the FRDM, and from 180 to 91 keV for the WS* model, respectively. It implies that the isospin symmetry is an important concept for constraining the nuclear mass models.

In summary, we proposed an efficient systematic method based on the radial basis function (RBF) approach for improving the accuracy and predictive power of global nuclear mass models. With the help of the RBF and the Garvey-Kelson relation, the rms deviation between the predictions from four mass models and the 2149 known masses falls to ~ 200 keV. The AME95-03 and AME03-Border tests show that the RBF approach provides us with a very useful tool, which is even more efficient than the CLEAN algorithm, for further reducing the rms deviation from the experimental data. In addition, with the RBF extrapolation, the divergence from different model predictions for unknown masses is remarkably improved, and the isospin symmetry is better represented.

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