An improved nuclear mass formula: WS3

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Abstract. We introduce a global nuclear mass formula which is based on the macroscopic-microscopic method, the Skyrme energy-density functional and the isospin symmetry in nuclear physics. The rms deviation with respect to 2149 known nuclear masses falls to 336 keV, and the rms deviations from 1988 neutron separation energies and α-decay energies of 46 super-heavy nuclei are significantly reduced to 286 and 248 keV, respectively. The predictive power of the mass formula for describing new measured masses in GSI and those in AME2011 is excellent. In addition, we introduce an efficient and powerful systematic method, radial basis function approach, for further improving the accuracy and predictive power of global nuclear mass models.

1. Introduction
It is known that nuclear masses are of great importance for the study of super-heavy nuclei [1, 2, 3, 4], nuclear symmetry energy [5] and nuclear astrophysics [6, 7, 8]. For the synthesis of super-heavy nuclei (SHN), a reliable nuclear mass formula is required for providing some valuable information on the central position of the “island of stability”, the position of proton drip line and the properties of SHN at their ground states. In addition, most of masses for nuclei along the r-process path have not yet been measured. Accurate predictions for the masses of these extremely neutron-rich nuclei play a key role for the study of nuclear astrophysics. Available nuclear mass formulas include some global and local formulas. For the global formulas, the model parameters are usually determined by all measured masses and the masses of almost all bound nuclei can be calculated. Some global nuclear mass models have been successfully established, such as the finite range droplet model (FRDM) [9] which is based on the macroscopic-microscopic method, the Hartree-Fock-Bogliubov (HFB) model [10], the Duflo-Zuker formula [11, 12] and the Weizsäcker-Skyrme formula [13, 14, 15]. These models can reproduce the measured masses with accuracy at the level of 600 to 300 keV. The local mass formulas are generally based on algebraic or systematic approaches. They predict the masses of unknown nuclei from the masses of known neighboring nuclei, such as the Garvey-Kelson relations [16], the isobaric multiplet mass equation, the residual proton-neutron interactions [17, 18] and the image reconstruction technique (like the CLEAN algorithm [19] and the radial basis function method [20]). The main difficult of the local mass formulas is that the model errors rapidly increase for nuclei far from the measured nuclei. For neutron drip line nuclei and super-heavy nuclei, the differences between the calculated masses from these different models are quite large. It is therefore necessary to check the reliability and predictive power of the nuclear mass formulas.
2. Weizsäcker-Skyrme mass formula

In Ref. [15] an improved nuclear mass formula, Weizsäcker-Skyrme mass formula, was proposed. The total energy of a nucleus is written as a sum of the liquid-drop energy, the Strutinsky shell correction $\Delta E$ and the residual correction $\Delta_{\text{res}}$

$$E(A, Z, \beta) = E_{\text{LD}}(A, Z) \prod_{k \geq 2} \left(1 + b_k \beta_k^2\right) + \Delta E(A, Z, \beta) + \Delta_{\text{res}}.$$  \hfill (1)

The liquid-drop energy of a spherical nucleus $E_{\text{LD}}(A, Z)$ is described by a modified Bethe-Weizsäcker mass formula,

$$E_{\text{LD}}(A, Z) = a_v A + a_s A^{2/3} + E_C + a_{\text{sym}} I^2 A + a_{\text{pair}} A^{-1/3} \delta_{np} + \Delta_W$$  \hfill (2)

with the isospin asymmetry $I = (N - Z)/A$ and the Coulomb energy,

$$E_C = a_c \frac{Z^2}{A^{1/3}} \left(1 - 0.76 Z^{-2/3}\right).$$  \hfill (3)

In the original Bethe-Weizsäcker formula, the symmetry energy coefficient $a_{\text{sym}}$ is simply written as a constant. To consider the surface-symmetry energy of finite nuclei, the mass-dependence of the $a_{\text{sym}}$ was proposed in Refs. [21, 22]. To check the mass-dependence of $a_{\text{sym}}$, we have studied the symmetry energy coefficients of finite nuclei based on the experimental data for masses [23]. The liquid-drop energy which is a function of mass number $A$ and charge number $Z$ can also be expressed as a function of $A$ and the isospin asymmetry $I$. By performing a partial derivative of the liquid-drop energy per particle with respect to $I$, the symmetry energy coefficients of finite nuclei can be extracted. In addition to the mass-dependence of $a_{\text{sym}}$, the isospin dependence of the symmetry energy coefficients of finite nuclei can also be clearly observed. To consider the isospin dependence of $a_{\text{sym}}$, we proposed a new form for the symmetry energy coefficient

$$a_{\text{sym}} = c_{\text{sym}} \left[1 - \frac{\kappa}{A^{1/3}} + \frac{2 - |I|}{2 + |I|A}\right],$$  \hfill (4)

with which the mass- and isospin-dependence of $a_{\text{sym}}$ can be reproduced reasonably well. The $|I|$ term in $a_{\text{sym}}$ represents the traditional Wigner effect [23]. With the proposed form for $a_{\text{sym}}$, we found that the accuracy of the liquid-drop formula can be improved by $\sim 5\%$ and the value of $c_{\text{sym}}$ which represents the nuclear symmetry energy at normal density goes up to about 30 MeV (very close to the extracted value from other approaches). Furthermore, it was found that the model parameters in the liquid-drop formula with the proposed form of $a_{\text{sym}}$ are quite stable for different mass region [24].

The $a_{\text{pair}}$ term empirically describes the pairing effect with

$$\delta_{np} = \begin{cases} 
2 - |I| & : N \text{ and } Z \text{ even} \\
|I| & : N \text{ and } Z \text{ odd} \\
1 - |I| & : N \text{ even, } Z \text{ odd, and } N > Z \\
1 - |I| & : N \text{ odd, } Z \text{ even, and } N < Z \\
1 & : N \text{ even, } Z \text{ odd, and } N < Z \\
1 & : N \text{ odd, } Z \text{ even, and } N > Z
\end{cases}$$  \hfill (5)

The influence of nuclear deformations on the liquid-drop energy is considered based on a parabolic approximation. We studied the variation of the energy of a nucleus as a function of $\beta_2$ and $\beta_4$ by using the Skyrme energy-density functional plus the extended Thomas-Fermi
approach [25], and found that the parabolic approximation is applicable for small deformations. The terms with $b_k$ in Eq. (1) describe the contribution of nuclear deformation (including $\beta_2$, $\beta_4$ and $\beta_6$) to the macroscopic energy. Mass dependence of the curvatures $b_k$ is written as [13],

$$b_k = \left(\frac{k}{2}\right) g_1 A^{1/3} + \left(\frac{k}{2}\right)^2 g_2 A^{-1/3},$$

(6)

according to the Skyrme energy-density functional, which greatly reduces the computation time for the calculation of deformed nuclei.

The microscopic shell correction

$$\Delta E = c_1 E_{sh} + |I| E'_{sh}$$

(7)

is obtained with the traditional Strutinsky procedure by setting the order $p = 6$ of the Gauss-Hermite polynomials and the smoothing parameter $\gamma = 1.2 \hbar \omega_0$ with $\hbar \omega_0 = 41 A^{-1/3}$ MeV. $E_{sh}$ and $E'_{sh}$ denote the shell energy of a nucleus and of its mirror nucleus, respectively. The $|I|$ term in $\Delta E$ is to take into account the mirror nuclei constraint [14] from the isospin symmetry, with which the accuracy of the mass model can be significantly improved by 10% without introducing any new model parameters. The charge-symmetry and charge-independence of nuclear force implies the energies of a pair of mirror nuclei should be close to each other if removing the Coulomb term. Combining the macro-micro method, one finds that the difference of the shell correction for mirror nuclei should be close to each other. The experimental data also support this point. From the traditional Strutinsky shell correction calculations, we note that the difference of the shell correction reaches a few MeV for some nuclei. The new expression for the shell correction in which the shell energy of the mirror nucleus is also involved, is proposed to consider the mirror effect.

In the calculations of the shell corrections, the single-particle levels are obtained under an axially deformed Woods-Saxon potential [26]. Simultaneously, the isospin-dependent spin-orbit strength is adopted based on the Skyrme energy-density functional,

$$\lambda = \lambda_0 \left(1 + \frac{N_i}{A}\right)$$

(8)

with $N_i = Z$ for protons and $N_i = N$ for neutrons, which strongly affects the shell structure of neutron-rich nuclei and super-heavy nuclei.

In this formula, we also consider the Wigner effect of heavy nuclei coming from the approximate symmetry between valence protons and neutrons. We found that some heavy doubly magic nuclei, such as $^{132}$Sn, $^{208}$Pb and $^{270}$Hs, lie along a straight line $N = 1.37Z + 13.5$. The shell corrections of nuclei are approximately symmetric along this straight line. The Wigner effect of heavy nuclei causes the nuclei along this line are more bound. The term $\Delta W$ is to consider this effect and reduces the rms error by $\sim 5\%$ (see Ref.[15] for details).

Finally, we would like to introduce a very efficient and powerful systematic correction to the global nuclear mass formulas - radial basis function (RBF) correction [20]. The RBF approach is a prominent global interpolation and extrapolation scheme for scattered data fitting. It is widely used in surface reconstruction. Based on a global nuclear mass formula and known masses, the differences between model calculation and experimental data are analyzed. The aim of the RBF approach is to find a smooth function $S(N, Z)$ to describe the differences $M_{\text{exp}} - M_{\text{th}}$. Once the reconstructed function $S$ is obtained, the revised masses for unmeasured nuclei are given by $M_{\text{th}}^{\text{RBF}} = M_{\text{th}} + S$. Here, $M_{\text{th}}$ denotes the calculated mass from a global nuclear mass model. We find that the RBF correction can improve the accuracy of a global mass formula by $\sim 10\%$ to $40\%$ without introducing any new model parameters.
Table 1. rms deviations between data AME2003 [27] and predictions of some models (in keV). The line $\sigma(M)$ refers to all the 2149 measured masses, the line $\sigma(S_n)$ to the 1988 measured neutron separation energies $S_n$, the line $\sigma(Q_{\alpha})$ to the $\alpha$-decay energies of 46 super-heavy nuclei.

|       | FRDM | HFB-17 | DZ10 | WS  | WS* | DZ31 | DZ28 | WS3 |
|-------|------|--------|------|-----|-----|------|------|-----|
| $\sigma(M)$ | 656  | 581    | 561  | 516 | 441 | 362  | 360  | 336 |
| $\sigma(S_n)$ | 399  | 506    | 342  | 346 | 332 | 299  | 306  | 286 |
| $\sigma(Q_{\alpha})$ | 566  | –      | 916  | 284 | 263 | 1052 | 936  | 248 |
| Reference | [9]  | [10]   | [11] | [13] | [14] | [11] | [12] | [15] |

3. Results

The rms deviations between the 2149 experimental masses AME2003 [27] and predictions of some models are calculated,

$$\sigma(M) = \left[ \frac{1}{m} \sum (M_{\text{exp}}^{(i)} - M_{\text{th}}^{(i)})^2 \right]^{1/2}.$$  \hspace{1cm} (9)

We show in Table 1 the calculated rms deviations $\sigma(M)$ (in keV). $\sigma(S_n)$ denotes the rms deviation to the 1988 measured neutron separation energies $S_n$. $\sigma(Q_{\alpha})$ denotes the rms deviation with respect to the $\alpha$-decay energies of 46 super-heavy nuclei ($Z \geq 106$) [14]. FRDM and HFB-17 denote the finite-range droplet model [9] and the latest Hartree-Fock-Bogoliubov (HFB) model with the improved Skyrme energy-density functional [10], respectively. DZ10, DZ28 and DZ31
denote the Duflo-Zuker mass models with 10, 28 and 31 parameters, respectively [11, 12]. The rms deviation from the 2149 masses with WS3 is remarkably reduced to 336 keV, much smaller than the results from the FRDM and the latest HFB-17 calculations, even lower than that achieved with the best of the Duflo-Zuker models. The rms deviation with respect to the 1988 neutron separation energies is reduced to 286 keV, and the rms deviation to the α-decay energies of 46 super-heavy nuclei is reduced to 248 keV, much smaller than the result of Duflo-Zuker formula (which is about one MeV). Fig. 1 (a) shows the difference between the experimental data AME2003 and the calculated masses with the WS3 formula [15] \( (M_{\text{exp}} - M_{\text{th}}) \). One sees that most of nuclei can be described remarkably well and the deviations for some semi-magic nuclei are slightly large.

Table 2. rms deviations with respect to 154 new masses in AME2011 [28] and those to 53 new measured masses in GSI [29] from four mass models (in keV).

|              | FRDM | HFB17 | DZ28 | WS3 |
|--------------|------|-------|------|-----|
| 154 new masses in AME2011 | 723  | 693   | 622  | 433 |
| 53 new masses in GSI       | 600  | 582   | 504  | 360 |

Table 3. The same as Table 2, but the radial basis function (RBF) corrections are involved.

|              | FRDM | HFB17 | DZ28 | WS3 |
|--------------|------|-------|------|-----|
| 154 new masses in AME2011 | 475  | 596   | 442  | 397 |
| 53 new masses in GSI       | 193  | 250   | 287  | 229 |

Here, we also check the predictive power of different mass formulas for description of new masses. The crosses in Fig. 1(b) denote the available masses in AME2003. After 2003, 154 new measured data have been collected by Audi and Wang (blue squares) in the interim AME2011 [28] and 53 new masses are measured in GSI [29] (red squares). The rms deviations with respect to these new data are listed in Table 2. For the new masses in AME2011, the corresponding results of FRDM and HFB are about 700 keV and the result of DZ28 model is more than 600 keV. The result of WS3 is only 433 keV. For the 53 new data in GSI, the result from WS3 is also the smallest one (only 360 keV).

Combining the radial basis function correction, we find that the accuracy of global mass formulas can be significantly improved. With the RBF corrections (see Table 3), the rms error to the new data in AME2011 is reduced from 723 keV to 475 keV and the rms error to the new data in GSI is reduced from 600 keV to about 200 keV based on the FRDM calculations. For other models, the improvement is also remarkable. Fig. 2 shows the difference between different model predictions and experimental data for the new masses measured in GSI [29]. The solid circles denote the results when the RBF corrections are involved. For these global nuclear mass models, especially the FRDM and HFB17 models, the RBF approach plays an important role for improving the systematic errors. Here, the measured masses in AME2003 are adopted for training the RBF [to obtain the function \( S(N, Z) \)] based on the leave-one-out cross-validation.


Figure 2. (Color online) Difference between model predictions and the experimental data for the new measured masses in GSI.

Figure 3. (Color online) Radial basis function corrections for different global nuclear mass models. The dashed lines show the magic numbers.
method. Simultaneously, the Garvey-Kelson relation [16], 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 $S(N, Z)$. For unmeasured nuclei, the masses are predicted by using $M_{\text{th}}^{\text{RBF}} = M_{\text{th}} + S$ with the calculated mass $M_{\text{th}}$ from a global nuclear mass model. Fig. 3 shows the RBF corrections for different global nuclear mass models. For the super-heavy nuclei region, the RBF corrections are large for the FRDM and DZ28 model. For the DZ28 model, one can see from Table 1 that the rms deviation with respect to the known masses is only 360 keV, however, the rms deviation $\sigma(Q_\alpha)$ with respect to the $\alpha$-decay energies of 46 super-heavy nuclei goes up to 936 keV, which also implies that the systematic errors for the masses of super-heavy nuclei could be large in this model.

It is known that the $\alpha$-decay energies of super-heavy nuclei have been measured with a high precision, which provides us with useful data for testing mass models. Fig. 4 shows the difference between model predictions and the experimental data for the $\alpha$-decay energies of SHN. Comparing with the FRDM, the $\alpha$-decay energies of the super-heavy nuclei are much better reproduced with the WS3 model. The difference is within $\Delta Q_\alpha = \pm 0.5$ MeV for SHN with the WS3 formula. The corresponding result from the FRDM is $\pm 1.0$ MeV. Here, we would like to emphasize that the description for the $\alpha$-decay energies of SHN is also a useful tool to test the predictive power of the mass models because the measured $\alpha$-decay energies are not involved in the fit for the model parameters.

Based on the WS3 formula, the shell corrections and the surface of the $\alpha$-decay energies of super-heavy nuclei have been studied simultaneously. In Fig. 5, we show the calculated shell corrections $\Delta E$ of nuclei. There are two islands in the super-heavy mass region. One is located at $N = 162, Z = 108$ and the other is located around $N = 178, Z = 118$. The triangles denote the synthesized SHN in Dubna through fusion reactions by using $^{48}$Ca bombarding on actinide targets. The calculated deformations of nuclei demonstrate that the nuclei with $N = 184$ are (nearly) spherical in shape. However, the maximum of the shell corrections occurs at around $N = 178$ instead of $N = 184$. The shell corrections (in absolute value) for nuclei with $Z = 126$ are smaller than that for nucleus ($N = 178, Z = 118$) by more than one MeV. Furthermore,
Figure 5. Shell corrections of nuclei in super-heavy region from WS3 calculations. The black squares denote the nuclei with spherical shapes and the triangles denote the synthesized SHN in Dubna. The dark gray zigzag line denotes the calculated proton drip line. The dashed lines show the possible magic numbers.

nuclei with $Z = 126$ and $N \leq 184$ locate beyond the calculated proton drip line, which indicates that the probability to synthesize nuclei with $Z = 126$ would be much smaller than that of produced super-heavy nuclei already. Fig. 6 shows the predicted $\alpha$-decay energies of super-heavy nuclei. The thick and thin curves denote the results for even-$Z$ and odd-$Z$ nuclei, respectively. The two dashed lines show neutron numbers $N = 162$ and 184, and the solid line show the position of $N = 178$.

Figure 6. Predicted (ground state to ground state) $\alpha$-decay energies of super-heavy nuclei. One can also see the valley at $N = 178$. For SHN with $Z = 116 \sim 118$, the $\alpha$-decay energies for nuclei with $N = 178$ are smaller than those for nuclei with $N = 184$.

4. Summary

In this talk, we introduced a global nuclear mass formula, Weizsäcker-Skyrme mass formula, which is based on the Skyrme energy-density functional, the macroscopic-microscopic method and the isospin symmetry in nuclear physics. The rms deviations from 2149 measured masses and 1988 neutron separation energies are significantly reduced to 336 and 286 keV, respectively. As a test of the extrapolation of the mass model, the $\alpha$-decay energies of 46 super-heavy nuclei have been systematically studied. The rms deviation with the proposed model falls to 248 keV, much smaller than the result 936 keV from the DZ28 model. Shell effect and isospin effect, especially isospin symmetry play a crucial role for improving the nuclear mass formula. For further testing the predictive power of the nuclear mass models, 154 new measured data in AME2011 and 53 new masses measured in GSI have been studied. The Weizsäcker-Skyrme mass formula can reproduce these new data remarkably well. We also introduced an efficient and powerful systematic method, radial basis function (RBF) approach, for further improving the accuracy and predictive power of global nuclear mass models. With the proposed mass formula, the shell corrections and $\alpha$-decay energies of super-heavy nuclei have been studied simultaneously. The calculated shell corrections and $\alpha$-decay energies of super-heavy nuclei imply that the shell gap at $N = 178$ also influences the central position of the "island of stability" for SHN.
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