A statistical view on nuclear mass formula based on liquid drop model

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The statistical method can be used to verify whether a theory is improved or not. As an example, a statistical study is applied to the error of the nuclear binding energy between the observed values and the theoretical values from the mass formula based on the liquid drop model (LDM). A new shell correction term is introduced to the traditional LDM. With such improvement, the error shows smaller standard deviation, better normality, reduced systematic part, and less dependent on the shell effect. The inclusion of the shell effect can be concluded to be an improvement purely from a statistical view. The present eight-parameter mass formula including shell effect gives standard deviation $\sigma = 1.4$ MeV for 2350 observed binding energies from AME2012.

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LDM is an empirical model describing the binding energy and other bulk properties of nuclei in a most easily way. Some microscopic approaches, such as the energy density functional theory and the Hartree-Fock-Bogoliubov method, describe the binding energy of most nuclei under a fine accuracy. Some other microscopic approaches, such as the nuclear shell model, concentrate on the light and medium mass nuclei. Our previous works show that the shell model can give a precise description on light nuclei from stability line to both neutron and proton drip line.

Here we first go back to the original LDM mass formula:

$$BE(A, Z)_{LDM5} = a_c A - a_s A^{2/3} - a_v Z (Z - 1) A^{-1/3} + a_\sigma^p (A - 2 Z)^2 / A + \delta a_p A^{-1/2}, \quad (1)$$

where $\delta = 1, 0, -1$ for even-even, odd-even, and odd-odd nuclei, respectively. The five terms in Eq. (1) are the volume energy, the surface energy, the Coulomb energy, the pairing energy. Here and after we label Eq. (1) as LDM5 because of its five parameters. These five parameters are considered to be the most important terms for nuclear binding in a macroscopic view and reproduce experimental binding energies, generally speaking, within the precision of 1%. Recently, it is shown that the volume energy and surface energy share the same physical origin.

Based on the original formula (1), many additional terms are introduced considering more physical reasons. Such as, the contribution of surface energy from proton-neutron asymmetry is introduced in the LDM mass formula (2):

$$BE(A, Z)_{LDM6} = a_c A - a_s A^{2/3} - a_v Z (Z - 1) A^{-1/3} + a_\sigma^p (A - 2 Z)^2 / A + a_\sigma^n (A - 2 Z)^2 / A^{4/3} + \delta a_p A^{-1/2}, \quad (2)$$

where $a_\sigma^p$ is the coefficient of the surface term of proton-neutron asymmetry energy. The Eq. (2) is labeled as...
LDM in the later discussion. It should be noted that there are several forms of this term when introducing to LDM \[10\].

To introduce the shell effect in the LDM, Strutinsky procedure is the standard method \[3\]. Recently, a shell correction term is presented as the function of the number of the valence nucleons respected to the nearest closed shell \[11\]:

\[
BE(N_p, N_n)_{\text{shell}} = a_1 F_{\text{max}} + a_2 F_{\text{max}}^2, \tag{3}
\]

where \( F_{\text{max}} = (N_p + N_n)/2 \) with \( N_{(p)} \) is the number of valence neutron (proton) respected to the nearest closed shell. It is obvious that the shell correction is related to the number of valence nucleons. Here, we suggest a new function for shell correction:

\[
BE(Z, N)_{\text{shell}} = (Z + N) \sum_{Z_0, N_0} V_{Z_0, N_0} e^{-\frac{(Z-Z_0)^2+(N-N_0)^2}{\sigma_0^2}}, \tag{4}
\]

where \( Z_0 \) and \( N_0 \) are the spin-orbit magic numbers, 28, 50, 82 for both proton and neutron, and 126 for neutron. The function considers the shell effect in a phenomenological way that the nuclei around doubly magic nuclei get extra binding energy, with \( V_{Z_0, N_0} \) the strength of the shell correction. The shell correction decreases when nuclei go far away from the doubly magic nuclei, with \( \sigma_0^2 \) the scale of the distance. The exclusion of the magic number 20 is because the LDM5 and LDM6 do not show the systematic necessity of the extra binding energy for the nuclei around \( Z = N = 20 \). The possible reason is that the LDM works insufficiently in the light region.

With the shell correction term \[11\], the LDM mass formula can be written as:

\[
BE(A, Z)_{\text{LDM8}} = a_v A - a_s A^{2/3} - a_e Z(Z - 1) A^{-1/3} + a_v^2 (A - 2Z)^2 / A + a_e^2 (A - 2Z)^2 / A^{4/3} + BE(A, Z)_{\text{shell}} + \delta a_p A^{-1/2}, \tag{5}
\]

which is labeled as LDM8 in later discussion.

The error between the LDM and the observed values is:

\[
e(A, Z) = BE(A, Z)_{\text{LDM}} - BE(A, Z)_{\text{Expt}}. \tag{6}
\]

The mean value and the standard deviation of the error is \( m \) and \( \sigma \), respectively. Table \[IV\] presents four sets of the parameters for LDM5, LDM6, LDM8, and LDM8'. In the fitting of the former three sets of the parameters, we consider 2350 nuclei with \( Z > 7 \) and \( N > 7 \), of which the observed value are from AME2012 \[12\]. The exclusion of the light nuclei is because they are too light to be considered as a liquid drop. In the fitting of the parameters of LDM8', 312 nuclei with \( Z > 81 \) and \( N > 125 \) are considered. It is seen that the original five parameters in LDM5 is stable when the model is modified. The two statistical quantities of the error between LDM and observed value are also listed in Table \[IV\]. The mean values \( m \) of four sets of error are close to zero because of the fitting. The stand deviation \( \sigma \) decreases obviously from LDM5 to LDM6, and to LDM8. The much smaller \( \sigma \) given by LDM8' indicate the well description of LDM in heavy nuclei. With the inclusion of the deformation and the other terms, it is expected that the Eq. \[5\] can be used to study the properties of superheavy nuclei.

The error normally comes from three parts, the model, the experiment, and the numerical method \[1\]. The experimental error of nuclear binding energy is generally much smaller comparing with the theoretical error \[12\].

The error from the numerical method is negligible here because the formulas used in this paper are analytical. Thus, we only consider the error from the model, which consists two parts, the statistical error from the parameters and the systematic error from the deficiency of the model. If the model is perfect, the error, \( e(A, Z) \), shows normality, \( N(m, \sigma) \), where the mean value \( m \) is close to zero and the standard deviation \( \sigma \) is small. The systematic error breaks the normality because of the missing important terms in the model. Table \[IV\] presents the distribution of the error of the LDM6 and LDM8, and the standard normal function, \( N(0,1) \), for 2350 elements. It is clearly that the normality of the error is better when LDM is improved from LDM6 to LDM8. Because in LDM8 the shell correction is not exactly included and the other physical terms, such as deformation, are also not included. The error of LDM8 still distributes deviated from the standard normal distribution.

**TABLE I.** Four sets of parameters including uncertainty of each parameters in parentheses, and the mean value \( m \) and the stand deviation \( \sigma \) of the error between LDM calculations and observed values. All data are in the unit of MeV except the dimensionless quantity \( a_v^2 \).

| Model   | \( a_v \)   | \( a_s \)   | \( a_e \)   | \( a_{av} \)  | \( a_{as} \)  | \( a_v \)   | \( V_{Z_0, N_0} \)  | \( a_0^2 \)  | \( m \) | \( \sigma \) |
|---------|-------------|-------------|-------------|--------------|--------------|-------------|------------------------|-------------|--------|--------|
| LDM5    | 15.634(24)  | 17.569(76)  | 0.709(17)   | 23.06(6)     | 12.12(88)    | -0.02       | 3.0                     |
| LDM6    | 15.673(21)  | 17.801(69)  | 0.7046(14)  | 28.83(16)    | 36.72(77)    | 0.05       | 2.5                     |
| LDM8    | 15.660(12)  | 17.865(38)  | 0.7007(8)   | 29.41(9)     | 39.24(43)    | -0.04      | 1.4                     |
| LDM8'   | 15.96(17)   | 19.81(74)   | 0.70(7)     | 33.2(1.3)    | 63.3(7.0)    | 0.0648(9)  | 40(1) -0.04 1.4        |

**TABLE II.** The distributions of the error of LDM6 and LDM8, and the standard normal function for 2350 element.

| Model   | \((-\infty, -2\sigma)\) | \((-2\sigma, -\sigma)\) | \((-\sigma, 0)\) | \(0, \sigma\) | \((\sigma, 2\sigma)\) | \((2\sigma, +\infty)\) |
|---------|--------------------------|--------------------------|------------------|---------------|------------------------|-------------------------|
| LDM6    | 122                      | 183                      | 587              | 1183          | 275                    | 0                       |
| LDM8    | 83                       | 316                      | 699              | 907           | 327                    | 18                      |
| N(0, 1) | 53.5                     | 319.4                    | 802.2            | 802.2         | 319.4                  | 53.5                    |
Because the number of data is large, the error can be written as the sum of two normal functions, one is statistical and another is systematic:

\[ e(A, Z) = aN(m_1, \sigma_1)_{\text{stat}} + bN(m_2, \sigma_2)_{\text{syst}}, \]

where \( a + b = 1 \). This function means that the statistical and systematic error may have different centroids which is the main reason that the error of binding energies distribute different from the standard normal function. Figure 1 presents the fitting of the function (1) to the error of LDM6 and LDM8. The error of LDM6 and LDM can be written as:

\[ e(A, Z)_{LDM6} = 0.72N(1.2,1.3)_{\text{stat}} + 0.28N(-2.1,2.0)_{\text{syst}}, \]
\[ e(A, Z)_{LDM8} = 0.74N(0.6,1.0)_{\text{stat}} + 0.26N(-1.6,1.0)_{\text{syst}}. \]

Purely from a statistical view, we can see the LDM8 is better than LDM6. Firstly, the standard dilation of the statistical error is a little smaller in LDM8 because of the two more parameters in LDM8. Secondly, both the standard deviation of the systematic error and the distance between two centroids in LDM8 (1.0 and 2.2 MeV) are smaller than those in LDM6 (2.0 and 3.3 MeV) because of the inclusion of shell correction. With a large number of data, the error can be considered as a statistical error distributes as a normal function with systematical error distributes also as a normal function of which the centroid has a certain distance. The mean values and the standard deviations of these two normal distributions can be used to verify the quality of the model.

Because the shell correction is included in LDM8, its error needs to be less dependent on the shell effect. We use the \( F \)-test for the single-factor analysis of variance (ANOVA) to see the dependence of the error on the shell effect. The error, \( e(A, Z) \), is grouped by the distance to the nearest closed shell, \( D^2 = (Z - Z_0)^2 + (N - N_0)^2 \), which can be used to scale the shell effect, the further distance the less contribution of the shell effect. Each error is grouped as the \( j \)th element in the \( j \)th group of distance \( D, e(i, j) \). The mean value in the \( i \)th group is \( \bar{e}_i \). Then the between-group variability \( S_A^2 \) and within-group variability \( S_R^2 \) can be defined:

\[ S_A^2 = \frac{1}{k-1} \sum_{i=1}^{k} n(i)(\bar{e}_i - m)^2, \]
\[ S_R^2 = \frac{1}{T-k} \sum_{i=1}^{k} \sum_{j=1}^{n(i)} (e(i, j) - \bar{e}_i)^2, \]

where \( k \) and \( T \) are the number of groups and the total number of errors in these \( k \) groups, respectively. \( F = S_A^2 / S_R^2 \) is used to scale the dependence on the factor \( D \) which is used to group. Table III presents the result of ANOVA. \( k \) is the number of group from group one, \( D = 0 \). From LDM6 to LDM8, both the \( S_A^2 \) and \( S_R^2 \) decrease obviously. From Table III we can see, without shell correction, the average binding energy grouped by \( D \) show large deviation between the groups comparing with the small deviation within the groups. The dependence on the shell effect is scaled by \( F \), the larger the more dependence. The error is much less dependent on shell effect in LDM8, especially when \( k \) become larger. The results of ANOVA shows that the Eq. (4) definitely add the shell correction to LDM. More exactly treatment of the shell correction is expected to further reduce the

![Graph](Image)

FIG. 1. The distributions of the error of LDM6 and LDM8, and the function (1) fitted to these two distributions (Color online).

| Model | \( k \) | \( S_R^2 \) | \( S_A^2 \) | \( F = S_R^2 / S_A^2 \) |
|-------|--------|--------|--------|------------------|
| LDM6  | 10     | 4.04   | 9.86   | 2.44             |
|       | 15     | 3.25   | 7.80   | 2.40             |
|       | 20     | 2.89   | 6.77   | 2.34             |
| LDM8  | 10     | 6.33   | 32.66  | 5.16             |
|       | 15     | 5.40   | 52.05  | 9.64             |
|       | 20     | 4.90   | 61.00  | 12.45            |

TABLE III. The ANOVA of error of LDM6 and LDM8. \( k \) is the number of the groups from group one, \( D = 0 \). \( S_A^2 \) and \( S_R^2 \) are the between-group variability and the within-group variability, respectively. \( F = S_R^2 / S_A^2 \) scales the dependence on \( D \).
dependence of error on shell effect.

Figure 2 shows the chart of nuclide scaled by the error of LDM8. Around 68.3% of total 2350 nuclei are “measured” within $\sigma = 1.4$ MeV by LDM8. The deviation between the model and the observed value demands more exactly treatment of the shell correction and the inclusion of other important terms, such as deformation. More exact models can give around 500 keV standard deviation, such as finite-range droplet model [3], the Hartree-Fock-Bogoliubov model [6], and the Weizsäcker-Skyrme mass model [13]. It is worth to mention that present model is in an analytical form and limited to totally eight parameters. It is interesting to see that the huge part of nuclear binding can be understood by a simple formula.

In conclusion, the statistical methods can be used to examine the improvement of the theory. As an example, we use the LDM to “measure” the 2350 binding energy in AME2012. The improvement of the LDM is the inclusion of the shell effect by adding a new simple and analytical function. Purely from a statistical view, we can conclude that the LDM is improved after shell correction. Because the error between LDM calculations and observed values shows smaller standard deviation, better normality, smaller standard deviation in both the systematic and statistical part, smaller centroid distance between systematic and statistical part, and less dependent on shell effect. It is expected that more theory works can be improved through the consideration of the statistical methods.

The shell correction introduced in this paper shows its validity in the description of the binding energy. The LDM with such shell correction term gives 1.4 MeV standard deviation for 2350 observed binding energies by eight parameters.

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