Article ID: 1007-4627(2017) 01-0110-06

Which Nuclei are Well Described by Liquid Drop Model: A Statistical Study Based on Uncertainty Decomposition Method

YUAN Cenxi

(*Sino-French Institute of Nuclear Engineering and Technology, Sun Yat-Sen University, Zhuhai 519082, Guangdong, China*)

Abstract: Which data are well described by a theoretical model? Such questions can be answered through the physical origin of the model. For example, the liquid drop model (LDM) well describes the heavy and far from shell nuclei. Because the liquid-drop assumption is more suitable for nuclei with more nucleons and LDM does not include the shell effect. Such answer is qualitative and needs a clear view on the physical origin of the model. Is it possible to give an semi-quantitatively answer only from the mathematical form of the model and the observed data. In the present work, the recently suggested uncertainty decomposition method (UDM) is used to answer which nuclei are well described by LDM. The residues between LDM and the observed data can be decomposed through UDM to systematic and statistical uncertainties, which represent the uncertainty of the deficiency of the model and the indeterminate parameters, respectively. Based on UDM, the chart of nuclides are semi-quantitatively divided into three parts, areas dominated by the systematic and statistical uncertainties, and the cross area. Contrary to the common sense, the well described nuclei by LDM are not the nuclei with small residues, but actually the nuclei of which the residues are dominated by the statistical uncertainty. These nuclei are indeed the heavy and far from shell nuclei, which agrees with the physical consideration of LDM. But only the mathematical form of the model and the experimental data are needed during the use of UDM. The nuclides dominated by the statistical uncertainty can be well described by LDM (standard deviation less than 0.7 MeV) with parameters fitting to these nuclei.

Key words: atomic nuclei; uncertainty decomposition method; liquid drop model; statistical uncertainty; systematic uncertainty

CLC number: O571.2 **Document code:** A **DOI:** 10.11804/NuclPhysRev.34.01.110

http://www.npr.ac.cn

1 Introduction

A theoretical model aims to describe observed data and predict unknown quantities. For a model, it is significant to investigate its uncertainty, which is essential for the evaluation of its predicted power[1]. The standard statistical methods are widely used to obtain the parameters of various models, taking nuclear mass model for example, the liquid drop model (LDM)[2], the finite-range droplet model[3], Lublin-Strasbourg Drop model[4], the Hartree-Fock-Bogoliubov model[5, 6], and the Weizsäcker-Skyrme mass model[7, 8]. The uncertainties of the modern nuclear mass models are around 0.5 MeV through the fitting procedure[3–8].

The detail of the total uncertainty is of great interesting, normally from three origins: the model, the experiment, and the numerical method[1]. The uncertainty from the model itself consists the statistical uncertainty and the systematic uncertainty, which come from the indeterminate parameters and the deficiency of the model, respectively. It is very difficult to evaluate the systematic uncertainty because its origin is the imperfection of the model itself[1]. How to derive the systematic uncertainty became a popular topic in recent years. For example, the systematic uncertainty

Received date: 18 Oct. 2016

Foundation item: National Natural Science Foundation of China(11305272); Specialized Research Fund for Doctoral Program of Higher Education(20130171120014); Guangdong Natural Science Foundation (2014A030313217); Pearl River S&T Nova Program of Guangzhou (201506010060)

Biography: YUAN Cenxi(1984–), male, Zhengzhou, Henan, Lecturer, working on nuclear physics;
E-mail: yuancx@mail.sysu.edu.cn.

of the energy density functional theory is obtained by comparing a variety of models[9], two illustrative cases are shown to estimate the systematic uncertainty by analysing the residues[1].

Very recently, we suggested a so-called uncertainty decomposition method (UDM) to decompose the statistical and systematic uncertainty from the residue of a simple model under simple statistical assumptions[10]. The uncertainties of LDM with and without shell correction term are investigated based on UDM, which shows that the systematic uncertainty is much reduced when the shell correction is included in LDM[10]. In addition, the statistical investigation provides a consistent view with physical consideration, such as, the residues of the light and closed shell nuclei distribute mostly inside the systematic uncertainty, which means the light and closed shell nuclei are not suitable to be described by LDM[10].

One may ask which observed data are well described by a theoretical model? There are many answers from the physical concern of the origin of the model. In the present work, such questions are tried to be answered by a statistical analysis based on UDM. In a statistical view, the observed data are well described when their uncertainties are dominated by the statistical uncertainty not by the systematic uncertainty. With the help of UDM, the simple nuclear mass model, LDM, is also used as an example. The present work aims to show that the well described mass data may be contrary to the common sense, those with the least total uncertainty, which extends the usefulness of UDM and provide a statistical insight on a theoretical model.

2 Uncertainty decomposition method and liquid drop model

A theoretical model described a quantity Y. After fitting procedure, the parameters of the model, $(X_1, X_2 ...)$, are obtained, including the values and the uncertainties, for the ith parameters, X_i and σ_i, respectively. The residues between the model and the observed data, $e = Y(X_1, X_2...) - Y(\text{Expt.})$, include three parts of the uncertainties, from the model, the experiment, and the numerical method[1]. Because the experimental uncertainty for nuclear mass is very small[11] and the numerical uncertainty of the linear and analytical model, LDM, can be neglected. Thus only the uncertainty from the model itself are considered in the present work, including statistical and systematic uncertainties.

The main consideration of UDM is that the distribution of the residues can be recognized as two distributions, the statistical and the systematic uncertainties. Furthermore, in the case of a large sample, it is reasonable to assume that the statistical and systematic uncertainties follow the normal distribution, although not exactly. A normal distribution is described as $N(m, \sigma)$, where m and σ are the mean value and the standard deviation, respectively. The distribution of the residues is:

$$\begin{aligned} f(e) &= f(\text{stat}) + f(\text{syst}) \\ &= \frac{1}{2} N(m_{\text{stat}}, \sigma_{\text{stat}}) + \frac{1}{2} N(m_{\text{syst}}, \sigma_{\text{syst}}) \ , \end{aligned} \tag{1}$$

where $\frac{1}{2}$ is the factor for normalization. The mean values m_{stat} and m_{syst} may be separated, which is rarely discussed before.

A distribution can be characterized by the moments, such as the mean value (first moment), variance (second moment), skewness (third moment), kurtosis (fourth moment). Applying the calculations of moments to Eq. (1):

$$\begin{aligned} m(e) &= \frac{1}{2}(m_{\text{stat}} + m_{\text{syst}}) \\ \sigma^2(e) &= \frac{1}{2}(m^2_{\text{stat}} + \sigma^2_{\text{stat}} + m^2_{\text{syst}} + \sigma^2_{\text{syst}}) \\ p_3(e) &= \frac{1}{2}(m^3_{\text{stat}} + 3m_{\text{stat}}\sigma^2_{\text{stat}} + m^3_{\text{syst}} + 3m_{\text{syst}}\sigma^2_{\text{syst}}) \\ p_4(e) &= \frac{1}{2}(m^4_{stat} + 6m^2_{\text{stat}}\sigma^2_{\text{stat}} + 3\sigma^4_{\text{stat}} + \\ &\quad m^4_{\text{syst}} + 6m^2_{\text{syst}}\sigma^2_{\text{syst}} + 3\sigma^4_{\text{syst}}) \ . \end{aligned} \tag{2}$$

The moments in the left hand side can be calculated through the residues, $Y(X_1, X_2...) - Y(\text{Expt.})$. The right hand side can be obtained through the properties of the normal distribution. In principal the four unknown quantities, the mean values and the variances of the statistical and systematic uncertainties, can be obtained through Eq. (2). But it normally has no physical solution because the assumption of normal distribution is not exactly.

Because the statistical uncertainty comes from the uncertainty of the parameters of the model. To obtain the mean values and the variances of the statistical and the systematic uncertainties, one can firstly simulate the variances of the statistical uncertainty through X_i and σ_i obtained in the fitting procedure:

$$\sigma^2_{\text{stat}} = \frac{\Sigma^M_{k=1}[Y(X'_i)_k - Y(X_i)_k]^2}{M} \ , \tag{3}$$

where X'_i is randomly generated through the normal distribution $N(X_i, \sigma_i)$. The kth Y_k and one parameter X_i is randomly selected from all possible candidates, while other parameters keep the same as the best fitted values. The number M is chosen to be large enough compared with the number of the observed data. Such simulation obtains the deviation comes from the uncertainty of the parameters, which is the estimation of the variance of the statistical uncertainty.

After obtaining the variance of the systematic uncertainty, one can express $m_{\rm syst}$ and $\sigma_{\rm syst}$ by $m(e)$, $\sigma(e)$, $\sigma_{\rm stat}$, and $m_{\rm stat}$ through the first two equations in Eq. (2). The remaining one unknown in the latter two sub-equations in Eq. (2) can be obtained by minimizing the p_3 and p_4 as the function of $m_{\rm stat}$,

$$\triangle p = |p_3^{1/3}(e) - p_3^{1/3}(m_{\rm stat})| + |p_4^{1/4}(e) - p_4^{1/4}(m_{\rm stat})|.$$

This is the criteria for UDM.

As the two distributions in Eq. (1) is obtained, more statistical understandings on the model can be presented, such as how to quantitatively define which data are well described by a theoretical model. A model normally gives very small residue on some observables after fitting procedure. One may considers that these observables are well described by the model. But it may not be true. In a statistical view, the systematic uncertainty represents the deficiency of the model and the statistical uncertainty comes from the indeterminacy of the parameters. If the centroids of the two uncertainty are separated, the small residue of certain observable is the balance of systematic and statistical uncertainty during fitting. The well described observable actually has the residue dominated by statistical uncertainty.

Here we use the functions $f({\rm stat})$ and $f({\rm syst})$ to divide the distribution of the residues to several areas. The areas defined by $f({\rm stat})/f({\rm syst}) < 0.5$, $0.5 \leqslant f({\rm stat})/f({\rm syst}) \leqslant 2$, and $f({\rm stat})/f({\rm syst}) > 2$ are dominated by systematic uncertainty, cross area, and dominated by statistical uncertainty, respectively. The residues distribute inside $f({\rm stat})/f({\rm syst}) > 2$ is well described by the model.

In the present work, we try to explain which nuclei are well described by LDM based on UDM. Because the physical origin of LDM is very clear, the usefulness of UDM can be examined compared with the physical consideration of LDM. LDM is an semi-classical formula describing the binding energies and other bulk properties of nuclei. Microscopic model can give nice descriptions on the binding energies of most nuclei, such as the energy density functional theory[9] and the Hartree-Fock-Bogoliubov method[5]. The nuclear shell model, another microscopic approach, concentrates on the light and medium mass nuclei in a truncated model space. The previous works show that the shell model can give very precise description on the light nuclei from the stability line to both the neutron and proton drip line[12].

The original LDM includes the volume energy, the surface energy, the Coulomb energy, the volume term of asymmetry energy, and the paring energy[13]. Many additional terms are introduced to include more physical effect, such as the surface term of asymmetry energy is introduced to LDM[2], given as:

$$BE(A,Z)_{\rm LDM} = a_v A - a_s A^{2/3} - a_c Z(Z-1)A^{-1/3} - a_a^v I(I+1)/A + a_a^s I(I+1)/A^{4/3} + \delta a_p A^{-1/2}, \quad (4)$$

where $I = |A-2Z|$ and $\delta = 1, 0, -1$ for even-even, odd-even, and odd-odd nuclei, respectively. These six parameters are considered to be the most important terms for nuclear binding in a macroscopic view and describe observed binding energies generally within the precision of 1%. The largest deviation comes from the lack of the shell effect. It should be noted that LDM can give well description on the binding energies[3] with the standard Strutinsky shell correction procedure[14].

3 Results and discussion

The application of UDM is performed on LDM based on the introduction in Section 2. The parameters of LDM are determined by fitting to the experimental data, AME2012[11]. In the fitting, 2 302 observed data are considered with experimental uncertainty less than 0.2 MeV. The light nuclei ($Z < 7$ and $N < 7$) are also excluded. Then UDM is used to decompose the statistical and the systematic uncertainties after the parameters and their uncertainties are obtained.

Fig. 1 presents the distribution of the residues and the obtained three uncertainties, total, systematic, and statistical. Around 5% of the data have residues smaller than −5 MeV (smallest one −11.515 MeV), but no residues larger than 5 MeV (largest one 4.388 MeV). The distribution of the residues shows the effect of the systematic uncertainty. Because LDM does not include the shell effect, the theoretical binding energies

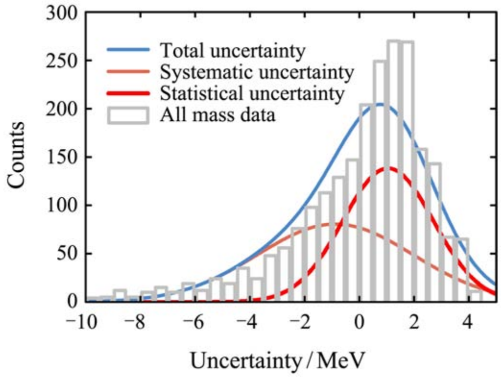

Fig. 1 (color online) Distributions of the residues and the obtained uncertainties.

http://www.npr.ac.cn

of the closed shell nuclei are underestimated compared with the observed data. Such deficiency of LDM is the most important origin of the systematic uncertainty. UDM can give an approximate systematic uncertainty for models with a large deficiency. More detailed discussions about the application of UDM to LDM can be found in Ref. [10].

The present work concentrates on the discussion on which nuclei are well described by LDM. After fitting procedure, many data are described by LDM with small residues. Fig. 2 presents the nuclei with residues around zero (-1.5 MeV$\leqslant e \leqslant 1.5$ MeV). It is clearly seen that many nuclei are not shown on the figure, which should be included. For example, the heavy nuclei around $Z=100$, $N=150$ should be well described by LDM, because liquid-drop assumption is suitable for the heavy nuclei. Some nuclei far from shell, around $Z=60$, $N=70$ and $Z=70$, $N=90$, should be well described by LDM, because the shell effect is not obvious in these nuclei. But these heavy and far from shell nuclei are not presented in Fig. 2. The nuclei with small residues seem not to be the well described nuclei by LDM from the physical consideration.

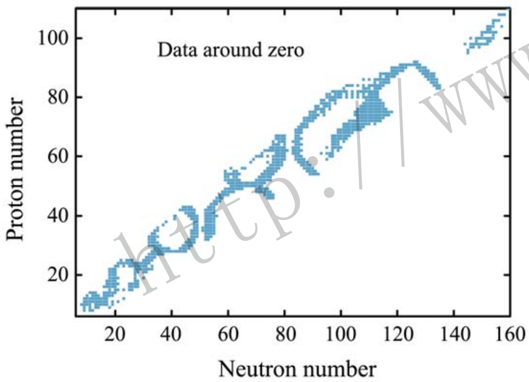

Fig. 2　(color online) Nuclei with residues around zero (-1.5 MeV$\leqslant e \leqslant 1.5$ MeV).

Then we start from the statistical view introduced in Section 2, that the well described data is dominated by f(stat), defined by $f(\text{stat})/f(\text{syst}) > 2$. Fig. 3 presents such nuclei. It is seen that many nuclei are included in the figure besides the nuclei around magic number $Z=28$, 50, 82 and $N=28$, 50, 82, 126. It should be noted that the number of nuclei in Fig. 2 and 3 are both around 1 000. The nuclei in Fig. 3 agrees more with the physical consideration of LDM compared with those in Fig. 2. It is interesting to see that the application of UDM on LDM provides a purely statistical investigation on which nuclei are well described by LDM. During the fitting procedure and applying UDM, only the mathematical form of LDM is needed, no physical meaning of LDM needs to be considered. After the use of UDM, the statistical results agree with the physical consideration of LDM, that the heavy and far from shell nuclei are suitable to be described by LDM. In addition, the residues dominated by statistical uncertainty show that the corresponding nuclei are suitable to be described by LDM, contrary to the common sense that small residue means well described.

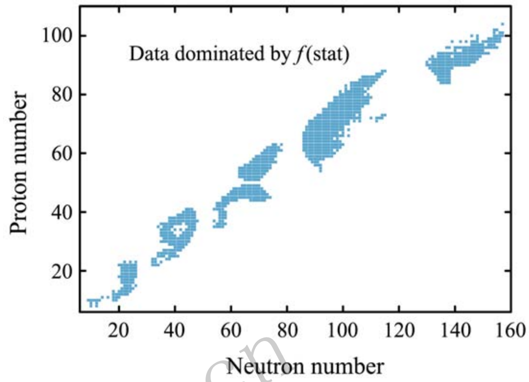

Fig. 3　(color online) Nuclei dominated by f(stat) ($f(\text{stat})/f(\text{syst})>2$).

Fig. 4 presents the chart of nuclides scaled by $f(\text{stat})/f(\text{syst})$, which gives a semi-quantitative result on the performance of LDM on all nuclei. The blue areas dominated by f(syst) are mainly the light nuclei and the nuclei around doubly magic number, especially around the doubly magic nuclei. The red areas dominated by f(stat) are mainly the heavy and far from shell nuclei. The cross areas are mainly between the blue and red areas, especially in the heavy region, which means the cross areas are closed to the doubly magic nuclei in the heavy region because the lack of the shell effect is the most important deficiency of LDM. It should be noted that two cross areas are found in super heavy region, around $Z=110$, $N=150$ and $Z=82$, $N=150$, which indicates the possible magic number located at $Z>110$ and $N>150$.

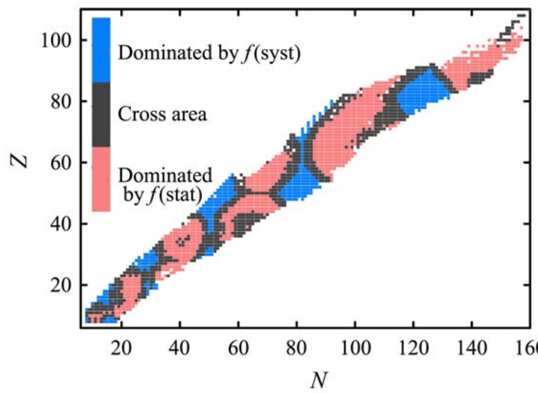

Fig. 4　(color online) Chart of nuclides scaled by $f(\text{stat})/f(\text{syst})$.

http://www.npr.ac.cn

It is interesting to see how well LDM works on the nuclides dominated by statistical uncertainty. The LDM parameters (parameter set 2) are refitted to 1011 nuclides dominated by statistical uncertainty and compared with the original parameters (parameter set 1) fitted to all 2 302 nuclides, as shown in Table 1. Certain differences are found between two sets of the parameters, especially between the surface energy term and the surface term of asymmetry energy in each set, respectively. As expected, the variance for the nuclides dominated by statistical uncertainty is much reduced in the second line. The standard deviation is less than 0.7 MeV, which is comparable with those from the modern models (around 0.5 MeV). The results clearly show that LDM works quite well on part of nuclides. Further investigation on the origin of the changes of the parameters would be helpful for further understanding LDM.

Table 1 The LDM parameters fitting to all 2 302 nuclides (first line) and to 1 011 nuclides dominated by statistical uncertainty (second line), and the corresponding variance for the data dominated by statistical uncertainty.

a_v	a_s	a_c	a_{av}	a_{as}	a_p	$\sigma^2(e)$
15.7	17.8	0.704	29.0	37.7	12.1	3.5
15.8	18.3	0.708	29.6	39.8	12.1	0.4

The global comparison is shown in Fig. 5 for the two sets of the parameters. Although the parameter set 2 gives a larger total variance, the distribution of the residues of it, with a peak around zero, has much more nuclides with small variance (less than 1 MeV).

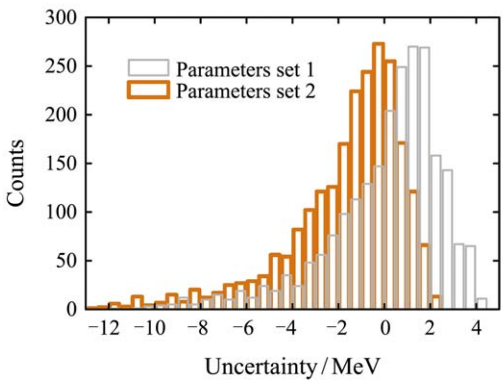

Fig. 5 (color online) Distribution of the residues from two sets of LDM parameters, fitting to all 2302 nuclides (parameter set 1) and to 1011 nuclides dominated by statistical uncertainty (parameter set 2).

If a model is fitted to all data, a better global description can be obtained. But one problem remains. The fitting results are the balance of the good and bad data, which means data well or poorly described by the model. The parameters from the fitting may include information which should not be included in the model. The present method provides a possible way to find more suitable parameters for the model.

4 Conclusions

In summary, the recently suggested UDM is applied to LDM to give an statistical study on which nuclei are well described by LDM. Contrary to the common sense, the well described nuclei by LDM are not those with small residues, but dominated by the statistical uncertainty, which is decomposed from the distribution of the residues through UDM. The definition, $f(\text{stat})/f(\text{syst})$, well scales the chart of nuclides and provides a semi-quantitative study on the performance of LDM on all nuclei, which is an example of the application of UDM. LDM works very well on the nuclides dominated by the statistical uncertainty with the refitted parameters.

http://www.npr.ac.cn

References:

[1] DOBACZEWSKI J, NAZAREWICZ W, REINHARD P G. J Phys G: Nucl Part Phys, 2014, **41**: 074001.
[2] MYERS W D, SWIATECKI W J. Nucl Phys, 1966, **81**: 1.
[3] MÖLLER P, NIX J R. At Data Nucl Data Tabl, 1995, **59**: 185.
[4] POMORSKI K, DUDEK J. Phys Rev C, 2003, **67**: 044316.
[5] GORIELY S, CHAMEL N, PEARSON J M. Phys Rev Lett, 2009, **102**: 152503.
[6] GORIELY S, CHAMEL N, PEARSON J M. Phys Rev C, 2013, **88**: 061302(R).
[7] LIU M, WANG N, DENG Y, WU X. Phys Rev C, 2011, **84**: 014333.
[8] WANG N, LIU M, WU X Z. MENG J. Phys Lett B, 2014 **734**: 215.
[9] ERLER J, BIRGE N, KORTELAINEN M, *et al.* Nature, 2012, **486**: 510.
[10] YUAN C X. Phys Rev C, 2016, **93**: 034310.
[11] WANG M, AUDI G, WAPSTRA A H, *et al.* Chin Phys C, 2012, **36**(12): 1603.
[12] YUAN C X, SUZIKI T, OTSUKA T, *et al.* Phys Rev C, 2012, **85**: 064324 (2012); YUAN C X, QI C, XU F R, *et al.* ibid, 2014, **89**: 044327.
[13] HEYDE K. Basic Ideas and Concepts in Nuclear Physics, 2nd ed, 1999, IOP, Bristol.
[14] STRUTINSKY V M. Nucl Phys A, 1967, **95**: 420.

哪些核适合被液滴模型描述：基于不确定度分解方法的统计研究

袁岑溪[1)]

（中山大学中法核工程与技术学院，广东 珠海 519082）

摘要： 一个模型适合描述哪些物理量？这个问题可以通过模型的物理来源来回答。比如，液滴模型适合描述重核和远离满壳核。这是因为液滴近似更适用于核子数多的核以及液滴模型不包含壳效应。这样的回答是定性的并需要清楚模型的物理来源。是否可能仅通过模型的数学形式和实验数据就能给出半定量的解答？利用最近提出的不确定度分解方法尝试对液滴模型适合描述哪些核这一问题进行半定量的回答。并且不需已知液滴模型的物理来源，仅需其数学形式以及实验数据。通过不确定度分解方法，液滴模型与实验数据间的残差可以分解为系统不确定度和统计不确定度。两者分别代表了模型的缺陷和模型不精确的参数带来的不确定度。基于这一分解，核素图上的原子核可以按其对应的残差被半定量地划分为系统不确定度主导、统计不确定度主导、以及中间区域。液滴模型适合描述的核就是统计不确定度主导残差的核而不是像通常认为的是残差最小的核。从核素图上看，统计不确定度主导残差的核正是重核以及远离满壳核，与液滴模型物理来源一致，但得到这一结果的过程是半定量的且仅需液滴模型的数学形式以及实验数据。如果对由统计不确定度主导残差的核重新拟合液滴模型的参数，模型可以很好地描述这些核(标准差小于0.7 MeV)。

关键词： 原子核；不确定度分解方法；液滴模型；统计不确定度；系统不确定度

http://www.npr.ac.cn

收稿日期： 2016-10-18

基金项目： 国家自然科学基金资助项目(11305272)；高等学校博士学科点专项科研基金项目(20130171120014)；广东省自然科学基金项目(2014A030313-217)；广州市科技计划珠江科技新星项目(201506010060)

1) E-mail: yuancx@mail.sysu.edu.cn。