Refining the nuclear mass model via the α decay energy

Weihu Ye and Yibin Qian*
Department of Applied Physics, Nanjing University of Science and Technology, Nanjing 210094, China

Zhongzhou Ren
School of Physics Science and Engineering, Tongji University, Shanghai 200092, China

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Besides the direct comparison with the experimental mass values, the α decay energy (Q_α), as one type of the mass difference, can be considered as another factor to judge the accuracy and validity of modern nuclear mass models. In the present study, the Duflo-Zuker (DZ) mass model is employed to match the measured Q_α value besides the mass data. This procedure can not only provide us a new way to evaluate and predict the α decay energy, but also raise one more constraint on the theoretical mass scheme. It is found that all the experimental α decay energies, from the ground state (g.s.) to g.s. transition of even-even nuclei above $A = 100$, can be well reproduced in a quite improved accuracy. Moreover, the symmetry term, involved in the macroscopic part of the DZ model, is refined further to regulate the behavior of the ambiguous symmetry energy coefficient in the nuclear equation of state. Through the relationship between the slope parameter of the symmetry energy and the neutron skin thickness, the neutron thickness ΔR_{np} of ^{208}Pb is determined in the vicinity of 0.201 fm, which is compatible to the very recent measurement.

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I. INTRODUCTION

The accurate calculation of nuclear masses (or binding energies) is one of the most central issues not only in nuclear physics but also in nuclear astrophysics [1], due to its fundamental role acted in the nuclear theory. In very recent years, although the measurement of nuclear masses is constantly improved by the development of experimental facilities like CERN and HIRFL-CSR [1–5], it is rather difficult for directly or indirectly measuring masses of unstable nuclei towards the dripline. For example, those nuclear masses are still experimentally unknown for many nuclei participating in the rapid proton (rp) and the rapid neutron (r) capture processes [1]. Therefore, the theoretical mass models are urgently requested to provide very reliable and precise extrapolations when it comes to these unknown but attractive regions. At present, the available experimental mass data have been well reproduced by various global mass models, such as the Weizsäcker-Skyrme (WS*4) [6], Duflo-Zuker (DZ) [7,8], Hartree-Fock-Bogoliubov (HFB) [9,10], finite range droplet model (FRDM) [11,12], and so on, with the root mean square deviation (RMSD) from 300 keV to 600 keV.

Especially, the RMSD, between the calculated nuclear masses and measured ones, has been reduced by 10–40% for some of the above models by taking into account the radial basis function approach or the mirror nuclei constraint [13–15]. In addition, the increasingly popular neural networks or machine learning strategies have lead the precision of mass predictions into a higher level [16–19]. However, one question would naturally arise: Is the ability of extrapolation proportional to the decreasingly RMSD for these mass models? Whatever the answer is, there indeed exists serious problems. On one hand, despite the quite good agreement between theory and experiment in known mass regions, the difference of extrapolated values, from current mass formulas, can be up to tens of MeV for those nuclei far way from the β stability line or in the superheavy mass regime [10,19–21]. On the other hand, there are still obvious gaps between the evaluated and measured "byproducts" of masses, like the separation energy or the decay energy, which may be caused by the overfitting of algorithms or missing physics in mass models.

To conquer the above dilemmas, one possible solution may be taking the decay energies into the fitting process of mass models, aiming at one more constraint to make the prediction reliable and avoid the overfitting problem from a new perspective. In the meantime, α decay spectra have been exploited as a unique tool in recognizing the very neutron-deficient nuclei plus the superheavy nuclei [22–26]. With these in mind, the α decay energy is considered as another target in the present study, when determining the coefficients of the mass model. This can give a more accurate prediction on α decay energy, which will be very valuable for the proposal on the future synthesis of short-lived α emitters. Of course, one can imagine that the corresponding masses should be worse matched against the experimental values at that time. In other words, the mass model has to meet the multi-objective design problem, which will be somewhat figured out as shown in the following. As for the mass model, the DZ10 method is chosen

*qyibin@njust.edu.cn

here due to its relative simplicity and accuracy. Besides the microscopic term based on the shell model picture, the DZ model also incorporates the macroscopic part mapped from the liquid drop model. The symmetry energy term of finite nuclei in the latter has been subtly connected with the symmetry energy of nuclear matter. Additionally, the very recent measurement on the neutron skin thickness of ^{208}Pb, from the PREX collaboration, is expected to stringently restrict the nuclear equation of state, i.e., the slope of the symmetry energy coefficient [27]. Based on the dipole polarizability, the Coulomb energies or the displacement energies of mirror nuclei and so on, extensive efforts have been actually devoted to the extraction of the significant neutron skin thickness [28–31] before that. It is of physical interest to see what will happen to these crucial quantities, namely the slope parameter and the neutron skin thickness, after the present reexamination of the symmetry term derived from the systematics of α decay energy plus the binding energy. Specifically, a brief introduction of the DZ10 framework is given in Sec. II, and the refining procedure via the measured α decay energies is then described along with the detailed results. In Sec. III, one can see the consequent influence on the symmetry energy and the thickness of neutron skin. A summary is given in the last section.

II. DZ10 FRAMEWORK AND ITS ADJUSTMENT TO THE α DECAY ENERGY

The DZ10 formula, as mentioned above, consists of four macroscopic terms and six microscopic monopole ones, namely [8,20],

$$B_{\rm DZ} = B_{\rm LD} + a_5(M+S) - a_6\frac{M}{\rho} + a_7 s_3 - a_8\frac{s_3}{\rho} + a_9 s_4 + a_{10} d_4 \quad (1)$$

with

$$\begin{aligned} B_{\rm LD} &= a_1 V_C - a_2 V_T + a_3 V_{TS} + a_4 V_P \\ &= a_1 \frac{-Z(Z-1) + 0.76[Z(Z-1)]^{2/3}}{A^{1/3}\left(1 - 0.25\frac{T^2}{A^2}\right)} \\ &\quad - a_2\frac{T(T+2)}{A^{2/3}\rho} + a_3\frac{T(T+2)}{A^{2/3}\rho^2} + a_4\frac{2-T/A}{\rho}, \end{aligned} \quad (2)$$

where $\rho = A^{1/3}[1 - 0.25\frac{T^2}{A^2}]^2$ is the scaling factor, and the isospin term is taken as the form $T = |N - Z|$ [8]. Given that the macroscopic part is kind of rooted from the traditional liquid droplet (LD) model, these terms are labeled together as $B_{\rm LD}$, which contains the Coulomb, symmetry, surface symmetry, and pairing energies. Note that the pairing term V_P has been restricted to even-even nuclei, due to the present requirement about the α emitters. Different from the conventional LD or macro-micro mass models, the volume and surface energies are actually included in the so-called mater term $M + S$ as well as $\frac{M}{\rho}$. As for the remaining terms, the s_3, $\frac{s_3}{\rho}$, and s_4 present the spherical term, while the last term d_4 comes from the nuclear deformation. The details and physics about the DZ10 model can be found in Refs. [7,8,21]. Those parameters a_i are mainly determined by fitting the experimental α decay energy Q_α, while the previous target, namely the measured mass, will be partially satisfied. Based on the DZ10 mass formula, the Q_α can be calculated as the mass difference between the parent nucleus and the decay products,

$$Q_\alpha = B_{DZ}(Z-2, N-2) - B_{DZ}(Z, N) + B_\alpha, \quad (3)$$

where B_α is taken as the experimental binding energy of ^{4}He. Regardless of whether this equation is trivial, one can combine it with the DZ10 formula, namely Eq. (1), to restrain the parameter set a_i, by adjusting the available experimental α decay energies. Considering that the DZ10 model is well analytically expressed, the above Q_α formula can be expected to be reduced via the total differential approximation to the first order,

$$Q_\alpha \approx \frac{\partial B_{\rm DZ}}{\partial Z}\Delta Z + \frac{\partial B_{\rm DZ}}{\partial A}\Delta A + B_\alpha, \quad (4)$$

where $\Delta Z = -2$, $\Delta A = -4$. It is very easy to perform the differentiation for the $B_{\rm LD}$ part. However, it seems to be impossible to take the derivative of the rest monopole terms, which is caused by the fact there are summed terms plus the cross-shell situations. Hence a slightly modified version of Eqs. (3) and (4) can be

$$\begin{aligned} Q_\alpha \approx &\left(\frac{\partial B_{\rm LD}}{\partial Z}\Delta Z + \frac{\partial B_{\rm LD}}{\partial A}\Delta A\right) + B_\alpha \\ &+ B_{\rm mic}(Z-2, N-2) - B_{\rm mic}(Z, N), \end{aligned} \quad (5)$$

where the binding energy $B_{\rm mic}$ is from the microscopic monopole part. For convenience, the adjustments of the DZ10 to the α decay energy via Eqs. (3) and (5) are, respectively, denoted as "Case I" and "Case II". The experimental Q_α values are selected from the g.s. to g.s. transitions of 275 even-even nuclei in the latest AME2020 [32]. With the help of the differential evolution algorithm [33], the set of parameters a_i for the two cases are separately obtained and listed in Table I. Note that although the fitting target is settled as the α decay energy at present, one additional and necessary requirement is that the final parameters should correspond to the minimum σ_B in the last series of iterations towards the convergence. In the meantime, the iteration was performed for more than 10^4 times plus the various initializations to get the optimized parameter set in the DZ10 mass formula as possible as we can. This is implemented in the "Case I", which is beneficial for the refinement of mass formulas and the subsequential analysis on the equation of state (EOS) as discussed in the following section. The original parameter set, determined from the mass data [8], is also shown in the second column of the same table for comparison. The last two lines of the table separately present the RMSD of Q_α and binding energies for the chosen mass region beyond $A = 100$ with the form

$$\sigma = \sqrt{\frac{\sum_{i=1}^{N}(A^{\rm exp} - A^{\rm theo})^2}{N}}, \quad (6)$$

where the quantity A means the α decay energy or the binding energy B. As one can see from Table I, the RMSD of Q_α is as expected to decrease (more than 30%) after the refinement in the present two cases. The agreement between theoretical

TABLE I. The parameters of the DZ10 mass model. For comparison, the original parameters from Ref. [8], by fitting the AME03 mass, are listed in the second column. The last two columns are, respectively, the new parameters determined by fitting the α decay energies with Eqs. (3) and (5). The experimental values of Q_α are taken from the latest AME2020 [32]. The RMSD values of the Q_α and the binding energy are also given in the last two lines for the presently focused region above $A = 100$.

Parameters	Original	Case I	Case II
a_1	0.707	0.703	0.692
a_2	37.515	37.776	38.561
a_3	53.351	54.992	61.814
a_4	6.199	4.023	3.611
a_5	17.766	17.734	17.742
a_6	16.314	16.207	16.647
a_7	0.478	0.342	0.359
a_8	2.183	1.525	1.580
a_9	0.022	0.022	0.024
a_{10}	41.388	39.189	35.104
σ_{Q_α}	0.511	0.358	0.365
σ_B	0.762	0.725	3.803

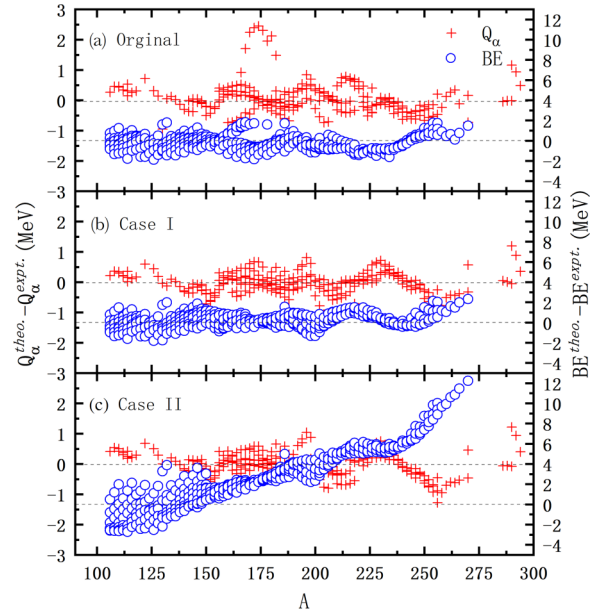

FIG. 1. Difference between experimental values and theoretical evaluations obtained from the DZ10 model for three different kinds of parameters. The blue circle and the red cross, respectively, correspond to the α decay energy and the binding energy for heavy nuclei beyond $A = 100$.

B values and experimental ones becomes worse for "Case II", while the σ_B is slightly lower in "Case I" than that from the original parameter set. The latter unexpected situation may come from the efficiency of the adopted fitting algorithm. Another important factor is that the original parameter set, as mentioned in Ref. [8], is determined from the AME03, while the present fitting is adjusted to the recent AME20 [32] with the concentration on the α emitters. For a better insight, the discrepancies between calculation and measurement are also displayed in Fig. 1 for the selected α emitters. An interesting point is that the DZ10 mass formula seems to produce a relatively large deviation from the experimental baseline in the superheavy mass region, no matter which version of parameters is employed. This may be caused by the fact the shell structure are different from the traditional scenario employed in the DZ model, which cannot be fully covered by the present spherical monopole Hamiltonian [20]. With the above in mind, let us pay special attention to the obtained parameters. When the α decay energy is taken as another matching target, some new parameters, corresponding to the pairing, spherical, surface symmetry, and deformation energies, are quite different in contrast with the original ones. As additional information, we have performed the fitting process aimed at the single α decay energy, in which the parameters would change more drastically. In this sense, when separately fitting two objective quantities, the involved coefficients in the same model (DZ10) behave in a different manner. One may conclude that these coefficients in the inaccurate mass model are overfitted to pursue the single accuracy, leading the introduction of the missing physics into the fitted parameters rather than in the complete physical picture. The ability of extrapolation in mass models (at least in DZ10) appears to be ambiguous particularly for those nuclei near the dripline of the nuclide chart. Hence the balance between multi-objectives, i.e., the binding energy and the α decay energy, may be instrumental to avoid the overfitting and improve the predictive power of current mass formulas. As mentioned before, we have made an attempt in this direction. The more rigid multiconstraints on the mass model is in progress. Before proceeding to the next section, it is noted that the parameters in "Case II" bring us the large RMSD and the unreasonable trend of binding energy. However, one should notice that the one-order approximation has been employed in the Q_α fitting, while these parameters are directly put back into the binding energy evaluations. This may be the main reason why the σ_B is so much higher in "Case II". Yet, it is hoped that this case can be an initial step towards an analytical tool for the quick and accurate Q_α calculator serving the experimental design.

III. SYMMETRY ENERGY

In previous studies, α decay has been treated as a probe into the symmetry energy or the incompressibility of nuclear matter (NM). This is actually a natural story as shown in the following logic. The symmetry energy term of the nuclear mass is found to contribute greatly to the α decay energy [26,34,35]. On the other hand, the coefficient of the symmetry term in finite nuclei has been revealed to be in a sophisticated relationship with the symmetry energy of NM [36,37]. In this sense, it is interesting to see the new results on the symmetry energy of NM when the DZ mass formula is directly adjusted to the α decay energy plus the harmony with the binding energy.

The EOS of the asymmetric nuclear matter, defined as the energy per nucleon, is $e(\rho, \delta) = e(\rho, 0) + S(\rho)\delta^2 + O(\delta^4)$ with the nucleon density $\rho = \rho_n + \rho_p$ plus the isospin asymmetry $\delta = (\rho_n - \rho_p)/\rho$. As compared to the well-known

energy per nucleon of the symmetric nuclear matter $e(\rho, 0)$, the ambiguousness or say challenge comes from the isospin asymmetry term [38–40]. If ignoring the higher term in the EOS, the key point is the symmetry energy coefficient $S(\rho)$, which can be expanded to the second order by

$$S(\rho) = S(\rho_0) + L\left(\frac{\rho-\rho_0}{3\rho_0}\right) + \frac{K_{\rm sym}}{2}\left(\frac{\rho-\rho_0}{3\rho_0}\right)^2, \quad (7)$$

where $S(\rho_0)$ is the symmetry energy coefficient at the NM saturation density. The slope parameter $L = 3\rho\frac{\partial S(\rho)}{\partial\rho}|_{\rho_0}$ and the curvature parameter $K_{\rm sym} = 9\rho^2\frac{\partial^2 S}{\partial\rho^2}|_{\rho_0}$ are the fundamental factors to govern the behavior of symmetry energy coefficient as well as the EOS. Extensive efforts have been devoted to elucidating the $S(\rho)$ code or these vital parameters L and $K_{\rm sym}$ [38–44]. Starting from the extraction of transport model or the systematics of energy density functional [38–40,45], several specific formulas of $S(\rho)$ are proposed to explore the its density dependence around the saturation density ρ_0. Three of them, employed here, are listed as follows:

$$S(\rho) = S(\rho_0)\left(\frac{\rho}{\rho_0}\right)^{\gamma}, \quad (8)$$

$$S(\rho) = 12.5\left(\frac{\rho}{\rho_0}\right)^{2/3} + C_1\left(\frac{\rho}{\rho_0}\right)^{\gamma}, \quad (9)$$

$$S(\rho) = 17.47\left(\frac{\rho}{\rho_0}\right)^{2/3} + C_1\left(\frac{\rho}{\rho_0}\right) + C_2\left(\frac{\rho}{\rho_0}\right)^{1.52}. \quad (10)$$

When it comes to the determination of the two constants of each above formula, one requires two conditions. As mentioned in Ref. [35] and references therein, the $S(\rho_0)$ is relatively well known, which can be a reliable condition. Considering that the symmetry energy coefficient in the EOS equals to that in the mass of finite nuclei [36], namely $S(\rho_A) = a_{\rm sym}(A)$, the $a_{\rm sym}$ value of the typical nucleus ^{208}Pb can offer another factor to confirm the $S(\rho)$ expression. The $a_{\rm sym}$ in the nuclear mass, as suggested in the traditional droplet model, is usually written as $a_{\rm sym}(A) = S(\rho_0)/(1+\kappa A^{-1/3})$ or approximately $a_{\rm sym}(A) = S(\rho_0)(1-\kappa A^{-1/3})$ (used here). The symmetry energy coefficient $S(\rho_0)$ of NM is identically adopted here, which can be readily put forward from the asymptotic situation $a_{\rm sym}(A\to\infty) = S(\rho_0)$. In the present study, the symmetry energy coefficient in the DZ10 formula is actually expressed as $a_{\rm sym}(A) = a_2 - a_3A^{-1/3}$. After inserting the detailed values of a_2 and a_3 from the original and the "Case I" sets, as listed in Table I, we can obtain easily the remaining parameters in Eqs. (8), (9), and (10). To proceed this, one necessary quantity is the density of ^{208}Pb. Given a series of calculations based on the energy density functionals [36], this input ρ_{208} is fixed in the range of 0.093 fm^{-3}–0.105 fm^{-3}. The slope L and curvature $K_{\rm sym}$ parameters are accordingly determined by the derivative of the NM symmetry energy coefficient, which are shown in Table II. In the meantime, the neutron skin thickness, as a subtle bridge between the finite nuclei and the asymmetric nuclear matter, is receiving special attention due to its unique role played in the studies of nuclear structure and astrophysics [46–49]. Based on the systematics of microscopic many-body calculations, the neutron skin thickness of atomic nuclei is found to be in a linear relation with the slope parameter L in $S(\rho)$, i.e., $\Delta R_{np} = 0.101 + 0.00147L$ [46]. In this way, the resultant values of ΔR_{np} are also presented in the table for ^{208}Pb. The neutron skin thickness of ^{208}Pb is very recently reported as $\Delta R_{np} = 0.283 \pm 0.071$ fm from the PREX II [27] and $\Delta R_{np} = 0.278 \pm 0.035$ fm from the proton scattering [50], which is slightly more compatible with those extracted from the "Case I" as compared to the original situation aimed at the mass. On the other hand, as stated in Refs. [44,51], the S_{ρ_0} is fixed as 38.1 ± 4.7 MeV if the neutron skin thickness of ^{208}Pb is adopted from the PREX II, which is consistent with the present extraction, namely the a_2 value. On the whole, the obtained values of one certain quantity in Table II are close but different with each other for the two former referred cases. Again, it may be more reasonable to extract the information on the symmetry energy from the systematics of binding energies when proceeding the multi-objective optimization on the mass formulas. Can the latter be another kind of "more is different"?

TABLE II. Three resulting quantities L, $K_{\rm sym}$, and ΔR_{np} of ^{208}Pb, based on the symmetry energy coefficient in the DZ10 mass formula. Note that three $S(\rho)$ expressions, namely Eqs. (8), (9), (10), are employed for the proceeding extraction.

Quantity	$S(\rho)$	Original	Present
L (MeV)	Eq. (8)	64.5 ± 8.5	67.5 ± 8.5
	Eq. (9)	65 ± 8	67.5 ± 8.5
	Eq. (10)	55.5 ± 12.5	59.5 ± 12.5
$K_{\rm sym}$ (MeV)	Eq. (8)	−80 ± 4	−80 ± 5
	Eq. (9)	−78 ± 2	−78 ± 3
	Eq. (10)	−211 ± 57	−202 ± 58
ΔR_{np} (fm)	Eq. (8)	0.196 ± 0.012	0.201 ± 0.013
	Eq. (9)	0.197 ± 0.011	0.201 ± 0.013
	Eq. (10)	0.183 ± 0.018	0.189 ± 0.018

IV. SUMMARY

In conclusion, the α decay energy is considered as an alternative optimized objective of the modern model of nuclear masses, in which the DZ10 mass formula is employed to implement this kind of theoretical experiment. During this procedure, besides the subtraction of the DZ10 binding energy of daughter nuclei from that of parent nuclei, the macroscopic part are approximated under the first order to pursue a more quick calculator of α decay energies. Whichever case of these two options is switched, the accuracy of evaluating the α decay energy is largely improved plus the partial concord with the nuclear masses. The clear discrepancies between the present DZ10 parameter sets from both the mass and the Q_α and the original ones based on the B value hint the existence of overfitting problem in current nuclear mass formulas. This study, as an initial step towards the multi-objective optimization for masses, is expected to further refine modern mass models and make their extrapolations compatible and reliable serving the astrophysical demand. On the other hand, the reex-

amined symmetry energy coefficients of finite nuclei provide another constraint on the density dependence of symmetry energy coefficient in the EOS of nuclear matter, leading to new results on the involved slope and curvature parameters. The consequent ΔR_{np} (around 0.201 fm) of ^{208}Pb is comparable with the new experimental result $\Delta R_{np} = 0.283 \pm 0.071$ fm, which may in turn be supportive for the present treatment on the determination of coefficients in mass formulas via the α decay energy besides the binding energy.

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