Kinetic Energy Distribution of Fragments for Thermal Neutron-Induced $^{235}\text{U}$ and $^{239}\text{Pu}$ Fission Reactions

Xiaojun Sun$^1$, Haiyuan Peng$^1$, Liying Xie$^1$, Kai Zhang$^1$, Yan Liang$^1$, Yinhu Han$^{1,2}$, Nengchuan Su$^2$, Jie Yan$^3$, Jun Xiao$^3$, and Junjie Sun$^3$

$^1$College of Physics, Guangxi Normal University, Guilin 541004, People’s Republic of China
$^2$China Institute of Atomic Energy, P. O. Box 275(41), Beijing 102413, People’s Republic of China
$^3$Institute of Nuclear Physics and Chemistry, China Academy of Engineering Physics, Mianyang 621990, People’s Republic of China

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Focused on the generation and evolution of vast complementary pairs of the primary fission fragments at scission moment, Dinuclear and Statistical Model (DSM) is proposed. (1) It is assumed that the fissile nucleus elongates along a symmetric coaxis until it breaks into two primary fission fragments. (2) Every complementary pair of the primary fission fragments is approximatively described as two ellipsoids with large deformation at scission moment. (3) The kinetic energy in every complementary pair of the primary fragments is mainly provided by Coulomb repulsion, which is explicitly expressed through strict six-dimensional integrals. (4) Only three phenomenological coefficients are obtained to globally describe the quadrupole deformation parameters of arbitrary primary fragments both for $^{235}\text{U}(n_{th}, f)$ and $^{239}\text{Pu}(n_{th}, f)$ reactions, on the basis of the common characteristics of the measured data, such as mass and charge distributions, kinetic energy distributions. In the framework of DSM, the explicit average total kinetic energy distribution $\overline{\text{KE}}(A)$ and the average kinetic energy distribution $\overline{\text{KE}}(A)$ are consistently represented. The theoretical results in this paper agree well with the experimental data. Furthermore, this model is expected as the reliable approach to generally evaluate the corresponding observables for thermal neutron-induced fission of actinides.

I. INTRODUCTION

The description of nuclear fission has presented exceptional challenges to the theoretical research since its discovery in the late 1930s [1]. The evolution of a nucleus from a compact configuration into two separated fragments is an intricate puzzle [2], and it has not only the collective movement of large-scale nucleons, but also the influence of various structural effects. The current theoretical descriptions of fission reflect the complexity and richness revealed in experimental studies, emphasizing the multidimensional, dynamic, and microscopic aspects [3]. Despite the many theoretical advances, there is not yet a quantitative theory of fission [3]. This is unfortunate because nuclear fission remains important to society at large due to its many practical applications, including safeguards, accelerator technology, homeland security, medicine, energy production, and waste transmutation at nuclear reactors [4–6], and r-process in the merging of neutron stars [7, 8].

The majority of energy released in neutron-induced fission of actinides is in the form of kinetic energy in the fission fragments [9]. The kinetic energy in the fission fragments measured by experiments is generally expressed in the relationship with the mass number $A$ of the light and heavy fragments, including the average total kinetic energy $\overline{\text{KE}}(A)$ and average kinetic energy $\overline{\text{KE}}(A)$. The kinetic energy is an important part of observables, which has a close relationship with other observables (such as mass distribution, charge distribution, neutron multiplicity, and so on). Moreover, kinetic energy is closely related to shell effect [10], which is helpful for the research of nuclear structure.

It is universally acknowledged that the transformation of fissile nucleus from a single system to two systems is one of the critical problems. Therefore, a comprehensive description of the deformation of these large primary fragments is indispensable to quantitatively predict the fission products. Some macroscopic models, macroscopic and microscopic models, microscopic models, and time-dependent microscopic theories [11–17] have been used to calculate deformation parameters from fissile nucleus to fission fragments. The physics of these models are well, but the calculated results of fission products vary greatly, and there are still a lot of obscure problems concerning the microfission theory. For example, the dissipation coefficient in the fission process is difficult to be calculated by microscopic method. The evolution relationship between temperature and entropy in the fission process, the competitive relationship between quantum tunneling effect and dissipation effect, and the coupling of different dimensional degrees of freedom in multi-dimensional fission are necessary to be further considered. It is widely shared that the results of these micromodels have not yet been adopted by the latest evaluation nuclear data libraries, such as ENDF/B-VIII.0 [18], JEFF-3.3.1 [19], JENDL-4.0u2 [20], CENDL-3.1 [21], and so on.
The machine learning method developed in recent years plays a very important role in the evaluation of nuclear data [22, 23]. This method optimizes the theoretical data and greatly improves the accuracy, but it ignores some physical evolution processes. The semi-empirical GEF model [2] summarizes the fundamental laws of physics and general properties of microscopic systems and mathematical objects. Many fission observables can be calculated with higher accuracy, and without having to make specific adjustments to the measurement and empirical data of a single system. This unique feature is of great valuable in evaluating nuclear data, but it is difficult to account for the fission process. The pre-scission configuration (PSC) approach represents that the part of the neck will be incorporated into the nascent light tail. In section II, the deformation parameters of the nuclei are employed to describe the kinetic energy. This approach can provide with trust enough $\langle TKE \rangle$ distributions and extend the fissioning systems for which experimental $\langle TKE \rangle$ data do not exist [24].

In this paper, a new Dinuclear and Statistical Model (DSM) is proposed to concurrently calculate the average total kinetic energy $\langle TKE \rangle(A)$ and average kinetic energy $\langle KE \rangle(A)$ of fragments for thermal neutron-induced $^{235}$U and $^{239}$Pu fission reactions. In section II, The derivation process of Coulomb interaction is introduced in detail. In section III, the deformation parameters of the primary fragments at scission moment are generally described. The calculated results and analyses are shown in section IV. And simple conclusions are given in section V.

II. COULOMB REPULSION

It is widely shared that the fissile nucleus $\{Z_f, A_f\}$ elongates along the coaxial of symmetry because of the deformation energy. While increasing its elongation enough large, the fissile nucleus will attain the scission point and split into a multitude of complementary fission fragment pairs $\{Z_{L0}, A_{L0}; Z_{H0}, A_{H0}\}$ [25]. These complementary primary fragments are unstable neutron-rich nuclei and possess large kinetic energy under Coulomb repulsion. Furthermore, they de-excite through emitting fast neutrons and $\gamma$ photons, and evolve to initial fission products $\{Z_{L0}, A_{L}; Z_{H0}, A_{H}\}$. These initial fission products will further de-excite through emitting slow neutrons and $\beta$ ray to form relatively stable secondary fission products $\{Z_L, A_L; Z_H, A_H\}$.

Complementary primary fragments have complex shapes at scission moment. Although the expression for the Coulomb interaction of two deformed, arbitrarily oriented, axially symmetric nuclei is obtained [26], it is difficult to derive the analytical formula. To vividly describe the fissile system at the scission point, the dinuclear concept is used in this paper. It is assumed that the fissile nucleus is stretched along the axis of symmetry until it breaks into two primary fission fragments. Every complementary pair of the primary fission fragments is approximately described by two ellipsoids with large deformation at scission moment. The schematic of dinuclear and coordinate system at the scission point are shown in Fig. 1. The kinetic energy in every complementary pair of the primary fragments is mainly provided by Coulomb repulsion. The representation of the Coulomb interaction is as follows [26]:

$$V_C = e^2 \int \frac{\rho_{L0} (\vec{R}_{L0}) \rho_{H0} (\vec{R}_{H0})}{|\vec{R}_{12}|} d\vec{R}_{L0} d\vec{R}_{H0}, \quad (1)$$

the amount of $e^2$ in Eq. (1) is a charge constant with a value of 1.44 MeV-fm. The distance $\vec{R}_{12}$ between $d\vec{R}_{L0}$ and $d\vec{R}_{H0}$ for the primary fission fragment pairs can be obtained from Fig. 1 as

$$\vec{R}_{12} = \vec{R} + \vec{R}_{H0} - \vec{R}_{L0}. \quad (2)$$

The denominator [26, 27] in Eq. (1) is

$$\frac{1}{|\vec{R}_{12}|} = \sum_{l_{L0}, l_{H0}=0}^{\infty} \frac{R_{l_{L0}l_{H0}} R_{l_{L0}l_{H0}+1}}{R_{l_{L0}l_{H0}+1} R_{l_{L0}l_{H0}}}. \quad (3)$$

Here, $Y_{lm}(\theta, \varphi)$ is a spherical harmonic function, and $R_{l_{L0}}, \vec{R}_{H0}, \theta_{L0}, \varphi_{L0}, \theta_{H0}, \varphi_{H0}$ are the spherical coordinates in the laboratory coordinate system $O_1$ and $O_2$, respectively.
The numerator $\rho_{L0}(<R_{L0})$ and $\rho_{H0}(<R_{H0})$ in Eq. (1) is the proton density in the light and heavy primary fragments, respectively. Because of the high excited energy of the primary fragments, it is assumed that the proton distribution is uniform in their ranges $R_i(\theta_i)$ ($i = L0$ or $H0$) denotes the light and heavy primary fragments, as the same in the next text if not specifically marked). So in this paper, a homogeneous charged drop with a sharp surface is adopted, and its proton density is expressed as

\[ \rho_i(\vec{r}) = \begin{cases} \rho_i & 0 \leq r \leq R_i(\theta_i) \\ 0 & r \geq R_i(\theta_i) \end{cases}. \]  

(4)

$R_i(\theta_i)$ defines the distance from the origin of the coordinate system to the point on the nuclear surface. For an axially deformed system, $R_i(\theta_i)$ is expressed as

\[ R_i(\theta_i) = R_i[1 + \beta_i Y_{lm}(\theta_i)]. \]  

(5)

Here, $R_i = r_0 A_i^{1/3}$, $r_0 = 1.226$ fm [28]. $\beta_i$ is a quadrupole deformation parameter, which is very important to describe the tensile strength of the primary fragments [17]. So the distance between the centers of mass of light and heavy primary fragments is rewritten as

\[ R = R_{L0}[1 + \beta_{L0} Y_{20}(0)] + R_{H0}[1 + \beta_{H0} Y_{20}(\pi)]. \]  

(6)

In order to obtain the explicit form of Coulomb repulsion $V_C$ as expressed in Eq. (1) for different complementary fragment pairs, the charge densities should be firstly calculated through the definition of proton number, i.e. $Z_i = \int \rho_i(\vec{r})d\vec{r}$. Thus the expression of the light and heavy kernel densities is expressed as

\[ \rho_i = \frac{3 Z_i}{4 \pi R_i^3 (1 + \frac{\rho_i}{16} B_i^2 + \frac{3 \rho_i}{180} B_i^2)}, \]  

(7)

\[ B_i = \sqrt{5} \sqrt{\beta_i} / \sqrt{16\pi}. \]

Eq. (1) requires six-dimensional integral. Firstly, Eq. (1) can be rewritten as

\[ V_C = e^2 \int \rho_{L0}(\vec{R}_{L0})d\vec{R}_{L0}Q_1. \]  

(8)

Where, $Q_1$ is represented as

\[ Q_1 = \int_0^{2\pi} \int_0^\pi \sin \theta_{H0} d\theta_{H0} d\varphi_{H0} \times \int_{R_{H0}(\theta_{H0})} R_{H0}^2 dR_{H0}. \]  

(9)

The spherical harmonic function $Y_{lm}(\theta, \varphi)$ can be expanded as

\[ Y_{lm}(\theta, \varphi) = \sqrt{\frac{(2l + 1)(l - m)!}{4\pi(l + m)!}} P_{lm}(\cos \theta)e^{im\varphi}. \]  

(10)

If $m \neq 0$, $\int_0^{2\pi} e^{im\varphi} d\varphi = 0$, thus Eq. (10) is meaningless. Conversely, if $m = 0$, $\int_0^{2\pi} e^{im\varphi} d\varphi = 2\pi$. So $Q_1$ can be expressed as

\[ Q_1 = \sqrt{\pi} \rho_{H0} \sum_{l=0}^{\infty} 4\pi(-1)^l l_{L0}^4 R_{L0}^4 Y_{l0,0}(\theta_{L0}, \varphi_{L0}) \]  

\[ \times \int_0^1 \sum_{l=0}^{\infty} \frac{(l_{L0} + l_{H0})!R_{H0}^{l_{H0}+3}}{l_{H0}!R_{H0}^l(l_{H0} + 3)} \]  

\[ \times (1 - B_{H0} + 3B_{H0}^2)^{l_{H0}+3} P_{l_{H0}}(x_1)dx_1. \]  

(11)

Here, $x_1 = \cos \theta_{H0}$ and $x_1 \in [-1, 1]$.

Obviously, the integral and summation can be exchanged. Thus, $Q_1$ can be rewritten as

\[ Q_1 = \sqrt{\pi} \rho_{H0} \sum_{l=0}^{\infty} 4\pi(-1)^l l_{L0}^4 R_{L0}^4 Y_{l0,0}(\theta_{L0}, \varphi_{L0}) \]  

\[ \times \int_0^{l_{L0}} \int_0^{l_{L0}} \int_0^{l_{L0}} \frac{(l_{L0} + l_{H0})!R_{H0}^{l_{H0}+3}}{l_{H0}!R_{H0}^l(l_{H0} + 3)} \]  

\[ \times (1 - B_{H0} + 3B_{H0}^2)^{l_{H0}+3} P_{l_{H0}}(x_1)dx_1. \]  

(12)

While $l_{H0} = 0$, 2, 4, 6, and $l_0$, $p_0$, $p_2$, $p_4$, $p_6$ are expressed as follows

\[ p_0 = \frac{R_{H0}^3}{3} (2 + \frac{24}{5} B_{H0}^2 - \frac{32}{35} B_{H0}^3), \]  

\[ p_2 = \frac{R_{H0}^3}{10R^2} (4B_{H0}^2 + \frac{32}{7} B_{H0}^4 + \frac{96}{7} B_{H0}^3), \]  

\[ + \frac{640}{77} B_{H0}^4 + 3392 B_{H0}^5), \]  

\[ p_4 = \frac{R_{H0}^3}{168R^4} (\frac{48}{5} B_{H0}^2 + \frac{192}{11} B_{H0}^4 + \frac{658}{143} B_{H0}^3, \]  

\[ + \frac{6144}{143} B_{H0}^5 + \frac{5376}{187} B_{H0}^6 + 334848 B_{H0}^6), \]  

(13)

\[ p_6 = \frac{R_{H0}^3}{6480R^6} (\frac{3456}{143} B_{H0}^3 + \frac{4145}{715} B_{H0}^1, \]  

\[ + \frac{373248}{2431} B_{H0}^5 + \frac{8736708}{46189} B_{H0}^7, \]  

\[ + \frac{7796736}{46189} B_{H0}^5 + \frac{8559208}{1062347} B_{H0}^8, \]  

\[ + \frac{467361792}{26558675} B_{H0}^9). \]  

(14)

By substituting Eqs. (12) and (13) into Eq. (8), $V_C$ can be rewritten as

\[ V_C = e^2 \rho_{L0} \rho_{H0} \sqrt{\pi} Q_2. \]  

Where, $Q_2$ is expressed as

\[ Q_2 = \sqrt{\pi} \int_{-1}^{1} \sum_{l_{L0}=0}^{\infty} (l_{L0} + 3) R_{L0}^{l_{L0}+1} \]  

\[ \times ([l_{L0}]p_0 + (l_{L0} + 2)p_2 + (l_{L0} + 4)p_4) \]  

\[ + (l_{L0} + 6)p_6 + \ldots ) (1 - B_{L0} + 3B_{L0}^2)^{l_{L0}+3} \]  

\[ \times P_{l_{L0}}(x_2)dx_2. \]  

(15)

Here, $x_2 = \cos \theta_{H0}$ and $x_2 \in [-1, 1]$. 
As same as \( Q_1 \), \( Q_2 \) can be rewritten as

\[
Q_2 = \sqrt{\pi}(s_0 + s_2 + s_4 + s_6 + \ldots). \tag{16}
\]

While \( l_{LO} = 0, 2, 4, 6 \), and \( s_0, s_2, s_4, s_6 \) are expressed as follows

\[
s_0 = \frac{4\pi R_0^3}{3R} \left( p_0 + 2!p_2 + 4!p_4 + 6!p_6 + \ldots \right)
\times \left( 2 + \frac{24}{5} B^2_{LO} + \frac{32}{35} B^3_{LO} \right).
\]

\[
s_2 = \frac{4\pi R_0^3}{3R} \frac{3R_0^4}{10R^2} \left( 2p_0 + 4!p_2 + 6!p_4 + 8!p_6 + \ldots \right)
\times \left( 4B_{LO} + \frac{32}{7} B^2_{LO} + \frac{96}{7} B^3_{LO} + \frac{640}{77} B^4_{LO} + \frac{3392}{1001} B^5_{LO} \right).
\]

\[
s_4 = \frac{4\pi R_0^3}{3R} \frac{3R_0^4}{168R^4} \left( 4!p_0 + 6!p_2 + 8!p_4 + 10!p_6 + \ldots \right)
\times \left( \frac{48}{5} B^2_{LO} + \frac{92}{11} B^3_{LO} + \frac{6528}{143} B^4_{LO} + 6144 \right)
\times \frac{B^5_{LO} + \frac{5376}{187} B^6_{LO} + \frac{334848}{46189} B^7_{LO}}{B^5_{LO}},
\]

\[
s_6 = \frac{4\pi R_0^3}{3R} \frac{3R_0^4}{6480R^6} \left( 6!p_0 + 8!p_2 + 10!p_4 + 12!p_6 + \ldots \right)
\times \left( \frac{3456}{143} B^3_{LO} + \frac{41472}{715} B^4_{LO} + 373248 \right)
\times \frac{B^5_{LO} + \frac{8736768}{46189} B^6_{LO} + \frac{7796736}{46189} B^7_{LO}}{B^5_{LO}},
\]

\[
+ \frac{85598208}{1062347} \frac{B^8_{LO}}{B^9_{LO}}.
\]

After sorting out and omitting the higher order terms, one can obtain the explicit Coulomb repulsion as

\[
V_C = \frac{\epsilon^2 Z_{LO} Z_{HO}}{R_{LO}(B_{LO})/f_{LO}(B_{HO})} \left\{ [f_0(B_{HO})
+ 2!f_2(B_{HO}, R_{HO}) + 4!f_4(B_{HO}, R_{HO})]f_0(B_{LO})
+ [2!f_0(B_{HO}) + 4!f_2(B_{HO}, R_{HO})]
+ 6!f_4(B_{HO}, R_{HO})]f_2(B_{LO}, R_{LO})
+ 4!f_0(B_{HO}) + 6!f_2(B_{HO}, R_{HO})
+ 8!f_4(B_{HO}, R_{HO})]f_4(B_{LO}, R_{LO}) \right\}. \tag{18}
\]

Where the compact forms of \( f \) function are listed as follows

\[
f_0(x) = 1 + \frac{12}{5} x^2 + \frac{16}{35} x^3,
\]

\[
f_2(x, y) = \frac{3y^2}{10R^2} \left( 2x + \frac{16}{7} x^2 + \frac{48}{11} x^3 + \frac{320}{1001} x^4 \right),
\]

\[
f_4(x, y) = \frac{3y^4}{168R^4} \left( \frac{24}{5} x^2 + \frac{96}{11} x^3 + \frac{3264}{143} x^4 + \frac{3072}{143} x^5 + \frac{2688}{187} x^6 + \frac{167424}{46189} x^7 \right).
\]

Thus, the total kinetic energy of every complementary primary fragment pair is rewritten as

\[
TKE = V_C(A_{LO}, Z_{LO}, \beta_{LO}; A_{HO}, Z_{HO}, \beta_{HO}). \tag{20}
\]

And the average total kinetic energy of the complementary primary fragment pairs is expressed as

\[
\bar{TKE}(A) = \frac{1}{\sum_k} \sum_k TKE(A_{LO}(j), Z_{LO}(j, k), \beta_{LO}(j, k); A_{HO}(j), Z_{HO}(j, k), \beta_{HO}(j, k)), \tag{21}
\]

where \( j \) denotes the number of the primary fragment pairs, and \( k \) denotes the isobar numbers of the \( j \)-th primary fragment pair.

From the Eqs. (18) - (21), one can see that the deformation parameters \( \beta_{LO,H0} \) are indispensable. Unfortunately, it is impossible that the deformation parameters \( \beta_{LO,H0} \) of the primary fragments at scission moment are accurately derived from both experimental and theoretical approaches. So in this paper, these quantities are obtained by the following methods in the next sections.

### III. DEFORMATION PARAMETER

#### A. Most Probable Primary Fragment Pair

It is widely shared that the primary fragments at scission moment must keep the laws, i.e.,

\[
Z_f = Z_{LO} + Z_{HO},
A_f = A_{LO} + A_{HO}. \tag{22}
\]

In addition, the neutron separation energy of every primary fragment must hold the positive value, i.e., \( S_n(Z_i, A_i) > 0 \). Furthermore, the neutron-proton ratio of every possible primary fragment is larger than that of the fissile nucleus. Thus, one can predict all of the possible primary fragment pairs, as shown in Figs. 2 and 3 for \( ^{235}U(n_{th}, f) \) and \( ^{239}Pu(n_{th}, f) \) reactions, respectively. In these two figures, the gray points denote the measured mass nuclei compiled in AME2016 [29], and the black points denote the stable nuclei located in the vicinity of the beta stable line. The blue hollow points denote the possible primary fragments predicted in this paper. It is obvious that there are hundreds of possible primary fragment pairs \( \{A_{LO}(j), Z_{LO}(j, k); A_{HO}(j), Z_{HO}(j, k)\} \). Here, \( j \) denotes the sequence number of the primary fragment pairs, and \( k \) labels the sequence number of the isobar pairs for the \( j \)-th primary fragment pair. From Figs. 2 and 3, one can see that there is slightly discrepancies at the positions of the symmetrical fission points \( \{A_f/2, Z_f/2\} \) for \( ^{235}U(n_{th}, f) \) and \( ^{239}Pu(n_{th}, f) \) reactions, respectively. And the amount of the total primary fragments of \( ^{235}U(n_{th}, f) \) reaction is a bit fewer than that.
Most Probable Primary Fragment Pair, dominates the kinetic energy, named after the isobar holding the largest kinetic energy, can be selected on the basis of the characteristics of the ground state (such as half-life) of the primary fragment pairs. In this paper, it is assumed that only a pair of isobar holding the largest kinetic energies can be selected on the basis of the characteristics of the ground state (such as half-life) of the primary fragment pairs.

Tables I and II list the partial possible primary fragment pairs and their half-lifes in the ground states for \(^{235}\text{U}(n_{th}, f)\) and \(^{239}\text{Pu}(n_{th}, f)\) reactions, respectively. The experimental data are taken from IAEA - Nuclear Data Section [30]. The first column denotes the \(j\)-th primary fragment pair, and the second column labels the \(k\)-th isobar pair of the \(j\)-th primary fragment pair. And the last two columns denote the half-lifes of the light and heavy primary fragments, respectively. Here, units such as \(s\), ms, min, h, d and y, denote second, millisecond, minute, hour, day and year, respectively. From tables I and II, one can see that the half-lifes of the light and heavy primary fragments exhibit large discrepancies. In this paper, it is assumed that the isobar pairs with the smallest values \(\tau_{L0} + \tau_{H0}\) are the candidates of the Most Probable Primary Fragment Pairs holding the largest kinetic energies. All of the Most Probable Primary Fragment Pairs is listed in Tables III and IV for \(^{235}\text{U}(n_{th}, f)\) and \(^{239}\text{Pu}(n_{th}, f)\) reactions, respectively. It is worth mentioning that there are several isobar pairs, of which the values \(\tau_{L0} + \tau_{H0}\) are roughly equal, for some primary fragment pairs. Therefore, the isobar pairs with the smallest values of \(|\tau_{L0} - \tau_{H0}|\) are selected as the candidates of the Most Probable Primary Fragment Pairs.

### B. Deformation Parameter

It is widely acknowledged that the shapes of the primary fragments at scission moment are hardly obtained not only by the measurements but also by the theories. In order to obtain the general descriptions of the deformation parameters of the primary fragment pairs, it is assumed that the average total kinetic energies are only provided by the Most Probable Primary Fragment Pairs. And the effects of the excited energies on the deformation parameters are ignored at scission moment because of the large deformation energies. Therefore, it is presumed that the deformation parameters of the primary fragments are dependent on the isospin asymmetry degree \(I\), and can be expressed as

\[
\beta_i = \alpha_i I_i, \tag{23}
\]

where \(\alpha_i\) is the phenomenological parameter, and \(I_i = (N_i - Z_i)/A_i\) \((i = L0 \text{ or } H0\) denotes the light and heavy primary fragment, respectively).

Substituting Eq. (23) into Eq. (21), one can get the relationship between the mass number \(A\) and the phenomenological parameter \(\alpha\), as shown in Figs. 4 and 5. From Figs. 4 and 5, one can see that there are same slopes of the isotopes shown as the blue lines in the range of \(^{235}\text{U}(n_{th}, f)\) reaction. It is the slightly unexpected results because one generally believe that larger mass nucleus perhaps produce more primary fragments.

Theoretically, each primary fragment pair has different contribution to the kinetic energy. However, the measured average total kinetic energy \(TKE(A)\) and average kinetic energy \(KE(A)\) for fission reactions are only the functions of the mass number. It is one of the critical problems that how describe the partial contributions of each isobar pairs for the same mass number \(A\). In order to solve this problem, the common characteristics of the deformation for the vast primary fragments must be revealed. In this paper, it is assumed that only a pair of isobar holding the largest kinetic energy, named after Most Probable Primary Fragment Pair, dominates the contributions of each primary fragment pair. And the excited energies of the primary fragments are not high because of the large deformation energies at scission moment. Thus, the Most Probable Primary Fragment Pairs holding the largest kinetic energies can be selected on the basis of the characteristics of the ground state (such as half-life) of the primary fragment pairs.
TABLE I. Partial possible primary fragment pairs and their half-lives in the ground states for $^{235}$U($n_{th}, f$) fission reaction. The experimental data are taken from IAEA - Nuclear Data Section [30]. Here, units such as s, ms, min, h, d and y denote second, millisecond, minute, hour, day and year, respectively.

| $j$ | $k$ | $A_{lo}(j)$ | $Z_{lo}(j,k)$ | $A_{ho}(j)$ | $Z_{ho}(j,k)$ | $\tau_{lo}$ | $\tau_{ho}$ |
|-----|-----|-------------|--------------|-------------|--------------|-----------|-----------|
| 1   | 1   | 118        | 46           | 118         | 46           | 1.9s      | 1.9s      |
| 1   | 2   | 118        | 45           | 118         | 47           | 26ms      | 3.76s     |
| 1   | 3   | 118        | 44           | 118         | 48           | 99ms      | 2.69min   |
| 1   | 4   | 118        | 43           | 118         | 49           | 30ms      | 5s        |
| 2   | 1   | 117        | 46           | 119         | 46           | 4.3s      | 0.92s     |
| 2   | 2   | 117        | 45           | 119         | 47           | 0.44s     | 2.1s      |
| 2   | 3   | 117        | 44           | 119         | 48           | 151ms     | 2.69min   |
| 2   | 4   | 117        | 43           | 119         | 49           | 45.5ms    | 27.03h    |
| 3   | 1   | 116        | 46           | 120         | 46           | 11.8s     | 0.492s    |
| 3   | 2   | 116        | 45           | 120         | 45           | 0.68s     | 1.23s     |
| 3   | 3   | 116        | 44           | 120         | 48           | 204ms     | 50.8s     |
| 3   | 4   | 116        | 43           | 120         | 49           | 57ms      | 3.08s     |
| 4   | 1   | 115        | 46           | 121         | 46           | 25s       | 0.285s    |
| 4   | 2   | 115        | 45           | 121         | 47           | 0.99s     | 0.78s     |
| 4   | 3   | 115        | 44           | 121         | 48           | 0.318s    | 13.5s     |
| 4   | 4   | 115        | 43           | 121         | 49           | 78ms      | 23.1s     |
| 5   | 1   | 114        | 46           | 122         | 46           | 2.42min   | 0.108s    |
| 5   | 2   | 114        | 45           | 122         | 47           | 1.58s     | 0.529s    |
| 5   | 3   | 114        | 44           | 122         | 48           | 0.54s     | 5.24s     |
| 5   | 4   | 114        | 43           | 122         | 49           | 0.1s      | 6.17s     |
| 5   | 5   | 114        | 42           | 122         | 50           | 58ms      | Stable    |
| 6   | 1   | 113        | 46           | 123         | 46           | 93s       | 0.108s    |
| 6   | 2   | 113        | 45           | 123         | 47           | 2.8s      | 0.298s    |
| 6   | 3   | 113        | 44           | 123         | 48           | 0.8s      | 2.1s      |
| 6   | 4   | 113        | 43           | 123         | 49           | 0.152s    | 6.17s     |
| 6   | 5   | 113        | 42           | 123         | 50           | 80ms      | 129.2d    |
| 6   | 6   | 113        | 41           | 123         | 51           | 32ms      | Stable    |
| 7   | 1   | 112        | 46           | 124         | 46           | 21.04h    | 38ms      |
| 7   | 2   | 112        | 45           | 124         | 47           | 3.6s      | 0.191s    |
| 7   | 3   | 112        | 44           | 124         | 48           | 1.75s     | 3.4s      |
| 7   | 4   | 112        | 43           | 124         | 49           | 0.271s    | 3.12s     |
| 7   | 5   | 112        | 42           | 124         | 50           | 0.12s     | Stable    |
| 7   | 6   | 112        | 41           | 124         | 51           | 33ms      | 60.2d     |
| 8   | 1   | 111        | 46           | 125         | 46           | 23.4min   | 57ms      |
| 8   | 2   | 111        | 45           | 125         | 47           | 11s       | 0.150s    |
| 8   | 3   | 111        | 44           | 125         | 48           | 2.12s     | 0.68s     |
| 8   | 4   | 111        | 43           | 125         | 49           | 0.29s     | 2.36s     |
| 8   | 5   | 111        | 42           | 125         | 50           | 0.186s    | 9.64d     |
| 8   | 6   | 111        | 41           | 125         | 51           | 5.4ms     | 2.76y     |
| 9   | 1   | 110        | 46           | 126         | 46           | Stable    | 48.6ms    |
| 9   | 2   | 110        | 45           | 126         | 47           | 3.35s     | 0.052s    |
| 9   | 3   | 110        | 44           | 126         | 48           | 12.04s    | 0.515s    |
| 9   | 4   | 110        | 43           | 126         | 49           | 0.9s      | 1.53s     |
| 9   | 5   | 110        | 42           | 126         | 50           | 0.296s    | 2.3×107y |
| 9   | 6   | 110        | 41           | 126         | 51           | 0.082s    | 12.35d    |
| 9   | 7   | 110        | 40           | 126         | 52           | 37.5ms    | Stable    |
| 10  | 1   | 109        | 45           | 127         | 47           | 80.8s     | 0.109s    |
| 10  | 2   | 109        | 44           | 127         | 48           | 34.4s     | 0.37s     |
| 10  | 3   | 109        | 43           | 127         | 49           | 0.91s     | 1.09s     |
| 10  | 4   | 109        | 42           | 127         | 50           | 0.61s     | 2.1h      |
| 10  | 5   | 109        | 41           | 127         | 51           | 0.108s    | 3.85d     |
| 10  | 6   | 109        | 40           | 127         | 52           | 0.056s    | 9.35h     |
A large amount of the measured average total kinetic energy distributions, such as $^{231}\text{Pu}$, $^{232}\text{U}$, $^{235}\text{U}$, $^{237}\text{Np}$, $^{239}\text{Pu}$, $^{241}\text{Pu}$, $^{241}\text{Am}$ and $^{243}\text{Am}$ induced by thermal neutrons, shows that their peaks are located at $A \approx 132$ [31–33, 37–41]. And many measured charge distributions show that their peaks are located at $Z \approx 54$ [42–44]. It is widely acknowledged that $A \approx 132$ and $Z \approx 54$ are closely related to the shell structure. It is inspired that $A \approx 132, 140, A_f/2$ and $Z \approx 54, Z_f/2$ are some crucial values for the average total kinetic energy distributions for the actinide fission reactions induced by thermal neutron. Therefore, the expression of the phenomenological parameter $\alpha$ is presumed as

$$\alpha = a_L, H + a_k(A - A^p_f)^2,$$

$$\delta \leq \delta_f, f \leq Z \leq Z_f/2 \quad \text{or} \quad Z_f/2 \leq Z \leq 54,$$

$$\alpha = \delta_L, HbZ + c_L, H + \delta_k, HkA,$$

$$Z \leq (Z_f - 54) \quad \text{or} \quad Z \geq 54.$$  

Where $A^p_{H_0} = 132$, $A^p_{I_0} = A_f - A^p_{H_0}$ and $\delta_L = -1$, $\delta_H = 1$. It is assumed that the deformation parameter $\beta$ is a smooth function of $A$ and $Z$ for a large amount of the primary fragments, so the coefficients in Eqs. (24a) and (24b) can
be derived as

\[
\begin{aligned}
  a_k &= k/16 \\
  a_L &= -(Z_f - 54)b + c_L - (A_f - 136)k \\
  a_H &= 54b + c_H + 136k \\
  c_H &= -Z_f b - A_f k + c_L.
\end{aligned}
\]

(25)

Thus, there are only three adjustable free coefficients \(\{k, b, c_L\}\) for describing the general rule of the deformation parameter \(\beta\). Furthermore, this rule is extended to describe the deformation parameters of arbitrary primary fragments for \(^{235}\text{U}(n_{th}, f)\) and \(^{239}\text{Pu}(n_{th}, f)\) reactions.

IV. RESULT AND ANALYSIS

A. Average total kinetic energy

On the basis of the Dinuclear and Statistic Model (DSM) introduced in the last sections II and III, the explicit average total kinetic energy distribution \(TKE(A)\) is expressed as Eq. (21), and the quadrupole deformation parameters of the arbitrary primary fragments are also expressed as Eqs. (23)-(25). Thus, root-mean-square deviation \(\sigma\), expressed as

\[
\sigma = \sqrt{\frac{1}{\sum_j \sum_j} [TKE_{th}(A_j) - TKE_{exp}(A_j)]^2},
\]

(26)
is adopted to determine the agreement between the theoretical calculations and the experimental data. Where the $\overline{TKE}_{th}$ and $\overline{TKE}_{exp}$ denote the theoretical values and experimental data, respectively. The recently published experimental data with a small relative errors [32, 39] are selected to obtain a set of the optimal parameters $\{k, b, c_L\}$ listed in Table V both for $^{235}\text{U}(n_{th}, f)$ and $^{239}\text{Pu}(n_{th}, f)$ reactions.

Figs. 6 and 7 show the comparisons of the calculated average total kinetic energies $\overline{TKE}(A)$ with the measurements for $^{235}\text{U}(n_{th}, f)$ and $^{239}\text{Pu}(n_{th}, f)$ reactions, respectively. The experimental data are derived from Refs. [31, 39, 45–49]. Red line and green lines denote the theoretical results of this work and PSC approach [24], respectively.

mean-square deviations $\sigma_{\text{TKE}}$ are listed in Table VI. It is obvious that the results of this work is slightly superior to those of the PSC approach.

From Eq. (18), one can see that the distance $R$ between the mass centers of the complementary light and heavy primary fragments is critical. In terms of Eq. (6), the average distance $\overline{R}$ between the mass centers of complementary primary fragments can also be rewritten as a
Fig. 8. (Color online) The average distance $\bar{R}$ versus mass number $A$ for $^{235}$U$(n_{th}, f)$ reaction (a) and $^{239}$Pu$(n_{th}, f)$ reaction (b).

Fig. 9 shows the deformation at scission moment and half-life in the ground state of the possible isobar pairs of $A_{L0} = 96$ and $A_{H0} = 140$ for $^{235}$U$(n_{th}, f)$ reaction. And Fig. 10 shows the deformation at scission moment and half-life in the ground state of the possible isobar pairs of $A_{L0} = 100$ and $A_{H0} = 140$ for $^{239}$Pu$(n_{th}, f)$ reaction. It is obvious that the isobar pair with the smallest half-life in the ground state holds the smallest deformation at scission moment. This implies that the largest kinetic energy of the primary fragments can be manifested by some properties of their ground state. And this isobar pair is corresponding the Most Probable Primary Fragment Pair with highest kinetic energy introduced in the last section. Several properties of the Most Probable

TABLE V. The optimal coefficients of the deformation parameter (no units).

| $k$  | $b$   | $c_L$  |
|------|-------|--------|
| 0.1943 | -0.4151 | 7.7924 |

TABLE VI. Root-mean-square deviations $\sigma$ of the different models.

| Fission system | $\sigma_{TKE}$ (MeV) | $\sigma_{KE}$ (MeV) | Models |
|----------------|------------------------|----------------------|--------|
| $^{235}$U$(n_{th}, f)$ | 1.32 | 1.26 | DSM |
| $^{239}$Pu$(n_{th}, f)$ | 2.11 | 1.09 | DSM |
| / | 2.01 | / | PSC [24] |
| / | 1.73 | / | GEF [53] |
| $^{239}$Pu$(n_{th}, f)$ | 2.95 | 2.22 | GEF [53] |
Primary Fragment Pairs, such as the quadrupole deformation parameter $\beta$, phenomenological parameter $\alpha$ and the isospin asymmetry degree $I$, are listed in Tables III and IV for $^{235}\text{U}(n_{th}, f)$ and $^{239}\text{Pu}(n_{th}, f)$ reactions, respectively.

B. Average kinetic energy

The subjects of total kinetic energy $TKE$ are the complementary primary fragment pairs. However, the energy allocation of light and heavy primary fragments is different. In terms of the conservations of momentum and kinetic energy, i.e.,

$$\begin{align*}
    m_{L0}v_{L0} + m_{H0}v_{H0} &= TKE, \\
    \frac{1}{2}m_{L0}v_{L0}^2 + \frac{1}{2}m_{H0}v_{H0}^2 &= TKE,
\end{align*}$$

the kinetic energy distribution of the heavy primary fragment $KE_{H0}$ is defined as

$$KE_{H0} = \frac{1}{2}m_{H0}v_{H0}^2 = \frac{m_{L0}}{m_{L0} + m_{H0}} TKE, \quad (29)$$

And the kinetic energy distribution of the light primary fragment $KE_{L0}$ can be easily written as

$$KE_{L0} = TKE - KE_{H0} = \frac{A_{H0}}{A_f} TKE. \quad (30)$$
Thus, the average kinetic energy distribution $\overline{KE}(A)$ is expressed as
\begin{equation}
\overline{KE}(A) = \frac{1}{\sum_k} \sum_k K\varepsilon(A_{L0}(j), Z_{L0}(j, k); A_{H0}(j), Z_{H0}(j, k)),
\end{equation}
and
\begin{equation}
\overline{KE}(A) = \frac{A_f - A}{A_f} \overline{KE}(A).
\end{equation}

Further, one can find that the results of Eqs. (31) and (32) are roughly equal. Evidently, Eq. (32) is simple and convenient, and is used in this paper.

Figs. 11 and 12 show the comparisons of the calculated and measured $\overline{KE}(A)$ for $^{235}$U(n$_{th}$, f) and $^{239}$Pu(n$_{th}$, f), respectively. Red and blue lines denote the results of this work and GEF model [53], respectively. And the root-mean-square deviations $\sigma_{KE}$ of this work and GEF are listed in Table VI. From Figs. 11 and 12 and Table VI, one can see that all of the calculated results of this paper is reasonable and slightly superior to those of GEF model.

V. CONCLUSION

Based on the dinuclear concept, it is assumed that the fissile nucleus elongates along an coaxis and attains the scission point. Thus the kinetic energy of the complementary primary fragment pairs is mainly provided by the Coulomb repulsion. After performing strictly the six-dimensional integral and omitting the higher order terms, the compact expression of Coulomb repulsion is explicitly obtained. In terms of the statistical properties of the abundant experimental total kinetic energy distributions, mass and charge distributions, and our previous theoretical results, some special quantities (such as mass numbers $A = 132$ and 140, charge number $Z = 54$, and symmetrical fission point $\{A_f/2, Z_f/2\}$) are used to derive the phenomenological expression of the deformation parameters of the different primary fragments at scission moment. And a set of optimal coefficients $\{k, b, c_L\}$ of the deformation parameters of arbitrary complementary fragments is obtained both for $^{235}$Pu(n$_{th}$, f) and $^{239}$Pu(n$_{th}$, f) reactions. The calculated results concurrently agree well with the measured total kinetic energy distributions $\overline{KE}(A)$ and experimental kinetic energy distributions $\overline{KE}(A)$, and also slightly better than the previous theoretical results.

However, Dinuclear Statistical Model (DSM) omits the rotational energy, which contributes larger portion for heavy-ion induced reactions due to the big angular momenta of the incident particle. In addition, nuclear charge densities have exponential tails rather than a sharp surface, so DSM ignores the attractive nuclear force at scission moment because of the super coaxial deformation. Due to the fact that DSM model can provide with enough trust for the average total kinetic energy distributions $\overline{KE}(A)$ and the average kinetic energy distributions $\overline{KE}(A)$, the feasibility is expected to extend the arbitrary incident energies and/or other fissile systems.

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