

Calculation of prompt fission neutron spectra for $^{235}\text{U}(\text{n},\text{f})^*$

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Abstract: The prompt fission neutron spectra for the neutron-induced fission of ^{235}U at $E_n < 5$ MeV are calculated using nuclear evaporation theory with a semi-empirical model, in which the nonconstant and constant temperatures related to the Fermi gas model are taken into account. The calculated prompt fission neutron spectra reproduce the experimental data well. For the $\text{n}(\text{thermal})+^{235}\text{U}$ reaction, the average nuclear temperature of the fission fragment, and the probability distribution of the nuclear temperature, are discussed and compared with the Los Alamos model. The energy carried away by γ rays emitted from each fragment is also obtained and the results are in good agreement with the existing experimental data.

Key words: fission fragment, prompt fission neutron spectra, nuclear temperature, neutron multiplicity

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1 Introduction

Prompt fission neutron spectra (PFNS) from neutron-induced fissions play an important role in various types of nuclear engineering and technologies, both in energy and non-energy applications. From a more fundamental point of view, studying the prompt fission neutron spectrum in detail can reveal some interesting properties of the nuclear fission process itself. The early representations of the prompt fission neutron spectrum, in which many of the physical effects were covered up, are the Maxwellian and Watt spectrum representations with one or two parameters adjusted to reproduce the experimental spectrum. The Los Alamos (LA) model [1] is one of the most successful models for predicting PFNS with an assumption of the same triangular-shaped initial nuclear temperature distribution for both light and heavy fragments. However, the LA model cannot describe the more specific physical quantities of a given fission fragment.

In recent years, the concepts of the multi-modal

random neck-rupture model [2, 3] and the multi-modal Los Alamos model (MMLA) have been used to quantitatively predict the fission fragment properties, and have been applied to some calculations of the prompt neutron spectrum and the multiplicity of actinide nuclei isotopes [4–8]. However, the nuclear temperature adopted in these two models is still the triangular distribution.

In the present work, the prompt fission neutron spectrum for the neutron induced fission of ^{235}U with a semi-empirical model was calculated, which is very different from the LA model. More physical quantities are taken into account, such as the initial excitation energy of every fission fragment, the nuclear temperature of each fragment and the prompt fission neutron multiplicity distribution. We are only concerned with low-energy (0–5.0 MeV) fission in this paper, for which only the first-chance fission compound is formed. The present work is the continuation of Refs. [9, 10], where only the prompt fission neutron multiplicity of $\text{n}+^{235}\text{U}$ was studied.

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2 Formulation

The total excitation energy $E_{\text{TXE}}(A_{\text{L}} + A_{\text{H}})$ of the fission fragment pair is given as follows:

$$E_{\text{TXE}}(A_{\text{L}} + A_{\text{H}}) = E_{\text{r}}^*(A_{\text{L}} + A_{\text{H}}) + B_{\text{n}}(A_{\text{c}}) + E_{\text{n}} - E_{\text{TKE}}(A_{\text{L}} + A_{\text{H}}), \quad (1)$$

where $B_{\text{n}}(A_{\text{c}})$ is the neutron binding energy of the fission compound nucleus, and the subscript c refers to the compound nucleus. E_{n} is the kinetic energy of the incident neutron. $E_{\text{TKE}}(A_{\text{L}} + A_{\text{H}})$ is the total kinetic energy of both light and heavy fragments, and is taken from experimental data. $E_{\text{r}}^*(A_{\text{L}} + A_{\text{H}})$ is the energy released in the fission process, which can be calculated with the following:

$$E_{\text{r}}^*(A_{\text{L}} + A_{\text{H}}) = M(Z_{\text{c}}, A_{\text{c}}) - M(Z_{\text{L}}, A_{\text{L}}) - M(Z_{\text{H}}, A_{\text{H}}), \quad (2)$$

where $M(Z_{\text{c}}, A_{\text{c}})$, $M(Z_{\text{L}}, A_{\text{L}})$ and $M(Z_{\text{H}}, A_{\text{H}})$ are the mass of the compound nucleus, the light fragment and the heavy fragment, respectively.

For a given fragment pair, the $E_{\text{TXE}}(A_{\text{L}} + A_{\text{H}})$ is distributed among the light and heavy fragments by means of the energy partition $R_{E_{\text{n}}}$, as in Ref. [10]. Then, $E^*(A)$, the excitation energy for a given fission fragment, can be obtained:

$$E^*(A) = R_{E_{\text{n}}}(A) \times E_{\text{TXE}}(A_{\text{L}} + A_{\text{H}}). \quad (3)$$

Within the Fermi gas model, the initial fission fragment energy $E^*(A)$ is simply related to the nuclear temperature T . The probability for the fission fragment to emit a neutron at a given kinetic energy is obtained by the Weisskopf spectrum at this particular temperature [11]. Assuming a constant value of the cross section of the inverse process of compound nucleus formation, the normalized prompt fission neutron spectrum $\phi(\varepsilon)$ in the center-of-mass system is

$$\phi(A, T, \varepsilon) = \frac{\varepsilon}{T^2} \exp(-\varepsilon/T), \quad (4)$$

where ε is the center-of-mass neutron energy, and T is the residual nuclear temperature of the fission fragment. There is a matching energy ($E_{\text{match}}(A)$) for every nucleus in the Fermi gas model. At higher nuclear excitation energies ($E^*(A) > E_{\text{match}}(A)$), the nuclear temperature T is simply written as:

$$T = \sqrt{\frac{E^*(A) - B_{\text{n}}(A)}{a_{A-1}}}, \quad (5)$$

with a_{A-1} being the level density parameter of the $(A-1)$ nucleus, and $B_{\text{n}}(A)$ being the neutron separation energy of the given fragment.

When the excitation energy is lower than the matching energy, a constant temperature is taken for neutron evaporation.

For a fragment with excitation energy $E^*(A)$, it could de-excite by emitting neutrons and γ rays. Here we assumed that the neutrons are emitted first, and only in the case that the excitation energy is lower than the neutron binding energy, i.e. the neutron could not be emitted again, and then the γ rays are emitted. The excitation energy of the fragment will decrease after a neutron is emitted from a fragment, which will decrease the nuclear temperature T as well. The prompt fission neutron spectra at different temperature, T , are calculated using Eq. (4) for each fragment. The total prompt fission neutron spectrum of every fragment is obtained by summing all of them up. The following shows how these spectra are weighted.

Usually the $\bar{\nu}$ is the average total prompt neutron number, but actually there are distributions for neutron emission, i.e. the prompt neutron multiplicity distribution $P(\nu)$. The average value of this distribution is $\bar{\nu}$. Considering the neutron emission of every fission fragment as a Poisson process [12], the neutron multiplicity distribution $P(N)$ of fragment A can be obtained:

$$P(N) = \frac{\bar{\nu}^N(A)}{N!} e^{-\bar{\nu}(A)}, \quad (6)$$

where $P(N)$ is the probability of the N neutron emitting by fragment A , and $\bar{\nu}(A)$ is the mean prompt fission neutron number emitted by fragment A [9]. Then, the number of emitting the i -th neutron for emitting the total N neutrons can be written as:

$$P_N''(i) = NP(N) \times \frac{P'(i)}{\sum_i P'(i)}, \quad (7)$$

where,

$$P'(i) = \frac{P(i)}{P(i-1)}, \quad P'(0) = P(0). \quad (8)$$

For a given fragment A , the sum of $P_N''(i)(i=1, N)$ is equal to $\bar{\nu}(A)$.

According to the statistical theory, a fragment can emit N neutrons. Only the probability of each neutron is different. In this work, 11 neutron emissions are considered for every fragment, regardless of its average prompt neutron number $\bar{\nu}(A)$. Therefore, there are 11 excitation energies and 11 nuclear temperatures for every fragment. This means that 11 neutron spectra should be considered for every fragment. The total prompt fission neutron spectra of each fragment

in the center-of-mass system is written as $\phi(A, \varepsilon)$, and calculated as a superposition of the 11 neutron spectra by weighting with the $P_N''(i)$,

$$\phi(A, \varepsilon) = \sum_{i=1}^{11} \frac{\varepsilon}{T_i^2} \exp(-\varepsilon/T_i) \times P_N''(i), \quad (9)$$

where T_i is the nuclear temperature corresponding to the i -th neutron emitted by a fragment.

Given the center-of-mass neutron energy spectra of every fragment, the corresponding neutron energy spectra $\Phi(A, E)$ in the laboratory system can be obtained by assuming that neutrons are emitted isotropically in the center-of-mass frame of a fission fragment. The total prompt fission neutron spectra of all fragments in the laboratory system can be expressed as:

$$N(E) = \sum_j Y(A_j) \bar{\nu}(A_j) \Phi(A_j, E), \quad (10)$$

where j stands for all fission fragments, $Y(A)$ is the chain yield and $\bar{\nu}(A)$ is the average prompt fission neutron number.

3 Results and discussions

For every fission fragment, 11 center-of-mass neutron energy spectra are calculated using Eq. (4), then the normalized center-of-mass neutron energy spectra are calculated from Eq. (9). Fig. 1 shows the neutron energy spectra for the thermal neutron induced fission of ^{235}U , and the fragment mass number A is 88. The dashed curves indicate the 11 center-of-mass neutron energy spectra with their weight $P_N''(i)$, and the thin solid curve indicates the total normalized center-of-mass neutron energy spectrum. Transformation to the laboratory system yields the thick solid curve shown in Fig. 1.

In Fig. 1, the dashed spectra correspond to T_1, T_2, \dots and T_{11} from top to bottom. It is clear that the neutron energy spectra (dashed curves) become softer overall with neutron emission. This is because neutron emissions lead to a decrease in the excitation energy as well as the nuclear temperature. In addition, it can be seen in Fig. 1 that the normalized neutron spectra in the center-of-mass system is dominantly contributed by the first few neutron emissions by the fragment, and this is due to the very fast decrease in neutron emission probability with the number of emitted neutrons.

The total prompt fission neutron spectra in the laboratory system are calculated with Eq. (10), and the mass number range of the fragment is $78 \leq A \leq 158$. Fig. 2 gives the total prompt fission

neutron spectra in the laboratory system for the $n(\text{thermal})+^{235}\text{U}$ fission. The solid curve indicates the calculated neutron energy spectrum, and the other symbols are the experimental data. The present calculation agrees well with the experimental data. At the spectrum tail, the calculation spectrum is a little harder relative to the experiment, but remains within the experimental error limit.

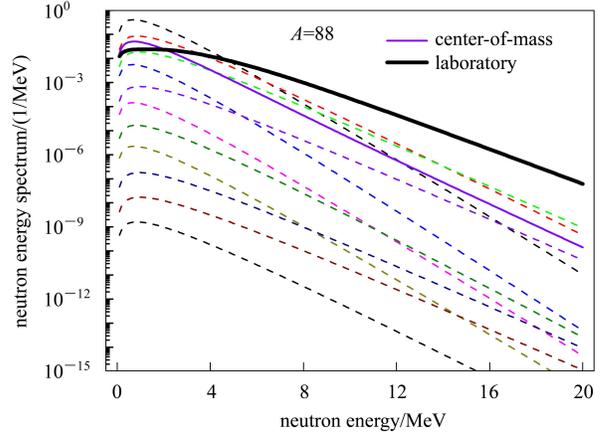


Fig. 1. The prompt fission neutron spectra for a given fragment ($A=88$) in the fission of ^{235}U induced by thermal neutrons.

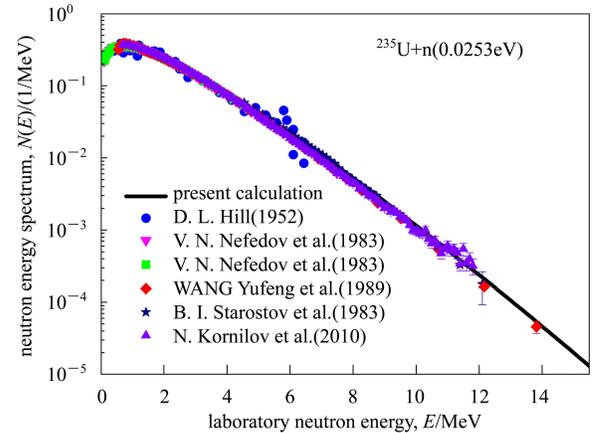


Fig. 2. The total prompt fission neutron spectra for the $n(\text{thermal})+^{235}\text{U}$ reaction. The solid curve is the calculated results, and the other symbols are the experimental data from EXFOR [14].

In Fig. 3, the comparisons of the calculated spectrum of this work with recent calculations of the Los Alamos model [13] and the multi-modal Los Alamos model [8] are shown. In general, the agreement is good. The small difference between 4–10 MeV and above 13 MeV may be due to the different nuclear temperature distributions.

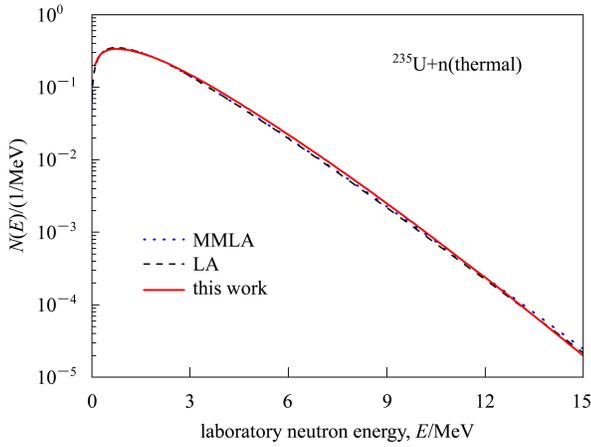


Fig. 3. The calculated prompt fission neutron spectra at $E_n=0.0253$ eV in comparison with the the recent calculations of the Los Alamos model and the multi-modal Los Alamos model.

Figure 4 shows the calculated results for the $n+^{235}\text{U}$ reaction with the incident neutron energy being 0.4, 0.53, 1.5 and 2.9 MeV, respectively, where experimental data exist. It can be seen that the calculated spectra are in good agreement with the experiment data when the incident neutron energy is 0.4, 0.53 and 1.5 MeV. For the case of $E_n=0.53$ MeV, the calculated spectrum is shown to be a little bit harder than the experiment in the region from 5.5 MeV to

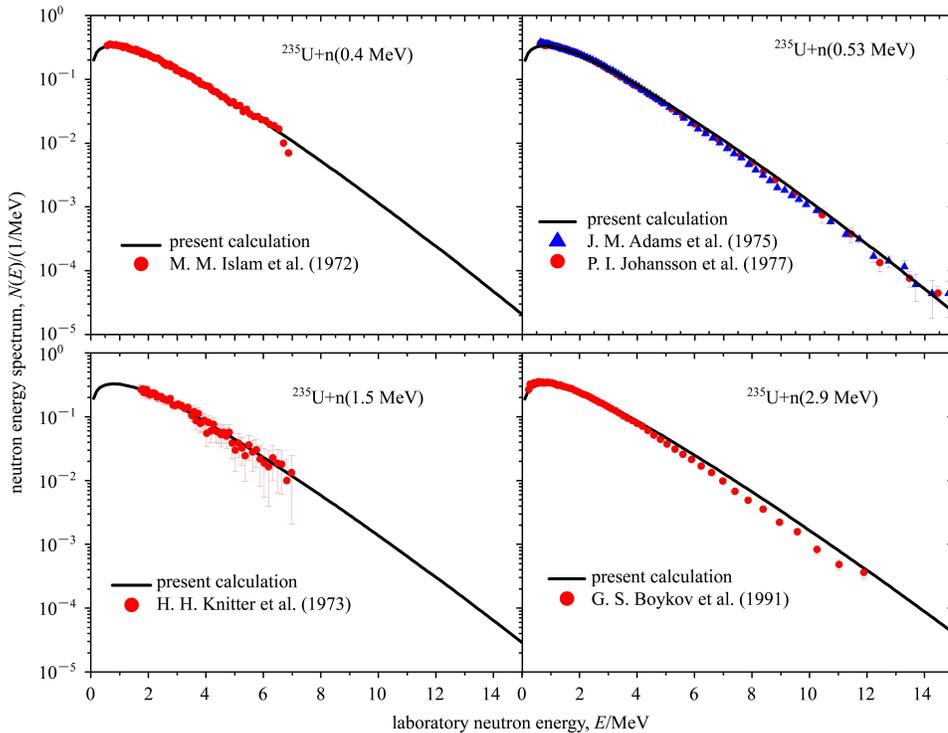


Fig. 4. The calculated total prompt fission neutron spectra for the $n+^{235}\text{U}$ reaction. The incident neutron energy is 0.4, 0.53, 1.5 and 2.9 MeV, respectively. The solid curve is the calculated results, and the other symbols are the experimental data from EXFOR [14].

10 MeV, but agrees with the experiment well above 10 MeV and below 5.5 MeV. While for $E_n=2.9$ MeV, the calculated data disagree with the experimental data above ~ 5.0 MeV, where the calculated spectrum appears to be too hard. We compare the experimental spectra at 0.53 MeV and 2.9 MeV, and show this in Fig. 5. It can be seen that the two spectra have the same shape below 6.5 MeV. While at the region above 6.5 MeV, the spectrum with a 2.9 MeV incident neutron energy is even softer than that of 0.53 MeV. This is not reasonable, because in physics the prompt fission neutron spectrum should become harder with increasing incident neutron energy. Therefore, the experimental data at 2.9 MeV may not be acceptable.

In the case of the $n(\text{thermal})+^{235}\text{U}$ reaction, the following quantities are calculated and discussed for cross checking and gaining an insight into some of the properties of the fragment.

1) The nuclear temperature

In this work, 11 excitation energies and 11 nuclear temperatures are considered for every fragment. For a given fragment A , the average nuclear temperature can be obtained by weighting with the $P_N''(i)$, and this is shown in Fig. 6 as a function of fragment mass A . It is shown that the average nuclear temperature of the light and heavy fission fragments is different, especially in the symmetric fission region, where a considerable symmetric variation appears.

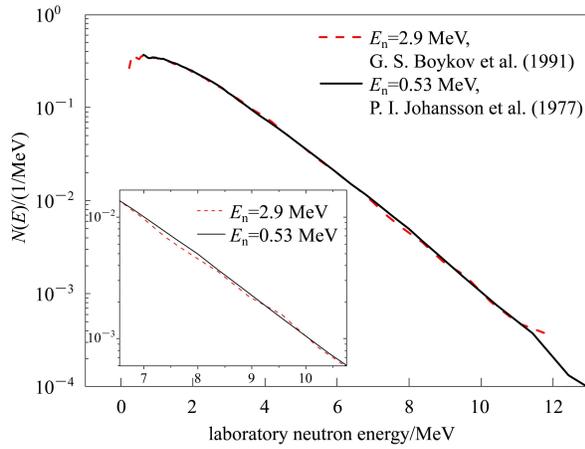


Fig. 5. The experimental data at $E_n=2.9$ MeV in comparison with the experimental data at 0.53 MeV.

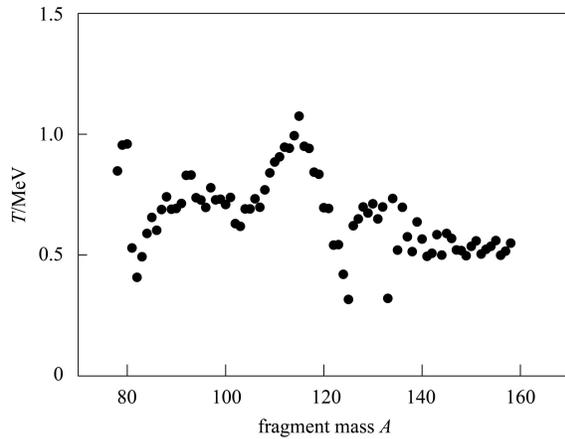


Fig. 6. The average nuclear temperature of the fission fragment for the $n(\text{thermal})+^{235}\text{U}$ reaction.

Using the Fermi gas model, Terrell transformed the distributions of residual fragment energies to the distributions of nuclear temperature ($P(T)$), as shown in the upper part of Fig. 6 [15]. The calculated distributions of the nuclear temperature in this work are also shown in the lower part of Fig. 7. It can be seen that both have the same trend, i.e. an approximately Gaussian distribution, but with different FWHM. The FWHM is 0.385 in this work, and 0.772 in Ref. [15]. The probability of a nuclear temperature of 0.6 to 0.8 MeV in this work is larger than that in Ref. [15]. This is because some constant temperatures are used for some of the fragments in this work, and the nuclear temperatures in Ref. [15] are transformed according to the estimated distributions of the residual fragment energies. The distribution of the nuclear temperature in this work is calculated one fragment by one fragment exactly, with excitation energy partitioning, so it is more reasonable.

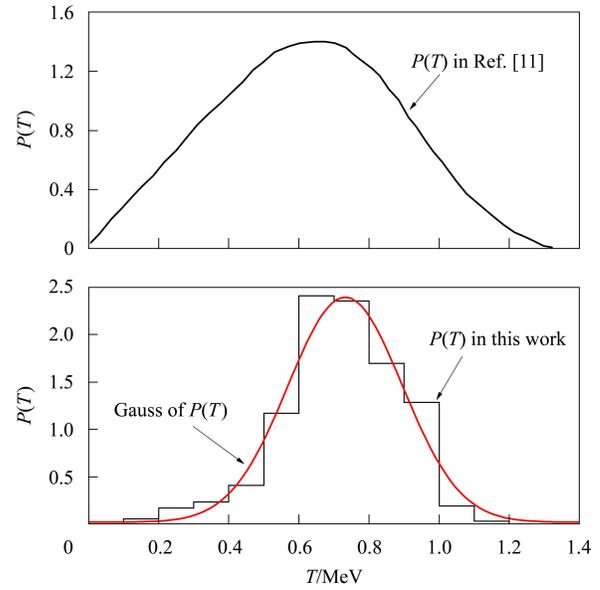


Fig. 7. The distributions of the nuclear temperature of the fission fragments. The upper part of the figure shows the temperature distributions given in Ref. [15].

The average nuclear temperature \bar{T} of all fission fragments is also calculated and compared. In this work, the \bar{T} is given as a superposition of each fragment temperature, taking the chain yield $Y(A)$ and the average prompt fission neutron number $\bar{\nu}(A)$ as weight. In the LA model, the average nuclear temperature \bar{T} of all fragments is $\frac{2}{3}T_m$, and T_m is the maximum temperature. For the $n(\text{thermal})+^{235}\text{U}$ reaction, \bar{T} is 0.663 MeV for the LA model, and is 0.652 MeV for this work. The average nuclear temperature given in Ref. [15] is 0.6 to 0.7 MeV. They are in good agreement. But in this work, the average nuclear temperature for light fragments is 0.72 MeV, while for the heavy fragments it is 0.56 MeV. They are very different, and the ratio is 1.28, while they are assumed the same in the LA model and Ref. [15].

2) The average neutron kinetic energy $\langle \varepsilon \rangle$

The average kinetic energy $\langle \varepsilon \rangle$ of the neutron emitted from a given initial fission fragment used in Ref. [9] is the experimental data. While in this work, the $2T$ is the mean energy of the neutron emitted with an evaporation spectrum distribution corresponding to the average temperature T of the fission fragment. Fig. 8 shows comparisons of the $\langle \varepsilon \rangle$ values for the $n+^{235}\text{U}$ reaction. The solid circles are the experimental data, the open circles are the calculated values in this work, and the triangular symbols are the calculated results in Ref. [16]. The values obtained for the light fragments are in good agreement with the experimental data. For the heavy fragments, the calculated $\langle \varepsilon \rangle$ values are lower than the experimental data.

There are no experimental data between $113 \leq A \leq 125$, and we give the same trend as Ref. [16] in this mass region.

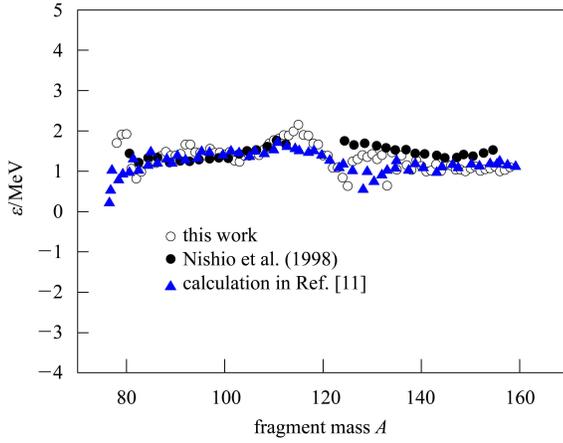


Fig. 8. Average neutron kinetic energy $\langle \varepsilon \rangle$ for the $n(\text{thermal})+^{235}\text{U}$ reaction.

3) The energy carried away by γ rays

Another quantity of interest is $E_\gamma(A)$, the energy carried away by γ rays emitted from a fragment. $E_\gamma(A)$ used in Ref. [9] is the experimental data. While in this work, the average total energy carried away by γ rays ($E_\gamma(A)$) is considered as the average excitation energy left when no further neutron emission occurs. Fig. 9 gives the experimental $E_\gamma(A)$ values used in Ref. [9] and the calculated results for the $n(\text{thermal})+^{235}\text{U}$ reaction in this work. The closed circles show the experimental data and the open circles are the calculated values. One can see that the experimental E_γ trend as a function of fragment mass A is well reproduced, although this is somewhat different for heavy fragments. This indicates that the calculation of this work is reasonable in physics and programming.

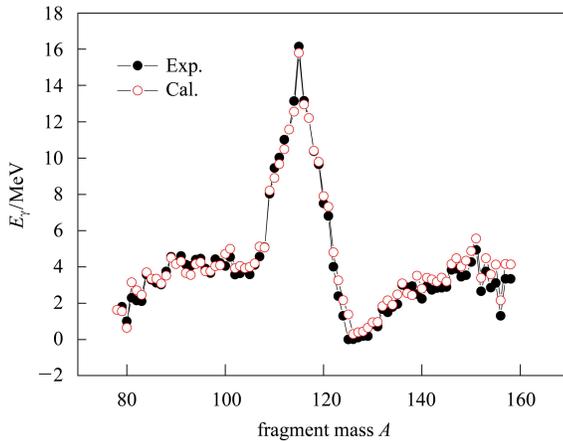


Fig. 9. $\bar{E}_\gamma(A)$ for the $n+^{235}\text{U}$ reaction.

4) The average fission fragment neutron separation energy

In Ref. [9], the average fission fragment neutron separation energy $B_n(A)$ is determined by weighting with the independent fission-fragment yields of the same mass chain. While in this work, it is obtained by weighting with $P_N''(i)$. In general, the agreement is good (Fig. 10).

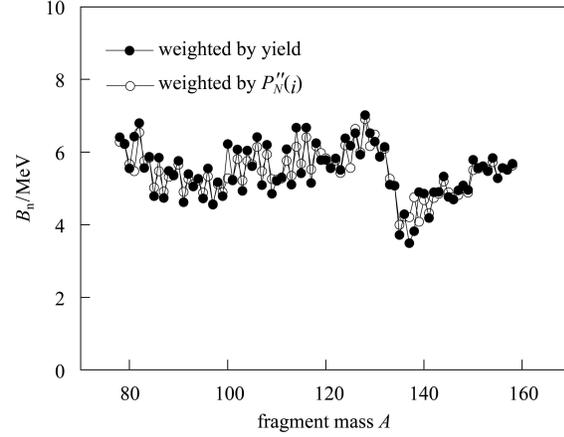


Fig. 10. B_n as a function of fission fragment mass for the $n+^{235}\text{U}$ reaction.

5) Energy conservation

For the $n(\text{thermal})+^{235}\text{U}$ fission reaction, E_{fission} , the total energy of the fission system is given by

$$E_{\text{fission}} = E_r^*(A_L + A_H) + B_n(A_c) + E_n, \quad (11)$$

which is distributed between the total excitation energy E_{TXE} and the total kinetic energy E_{TKE} . Then E_{TXE} is divided into a pair of fission fragments, i.e. the excitation energy of each initial fission fragment, $E^*(A_L)$ and $E^*(A_H)$, and they could de-excite by emitting neutrons and γ rays. So, the E_{fission} can also be expressed using the following formula:

$$\begin{aligned} E_{\text{fission}} &= E_{\text{TKE}}(A_L + A_H) + E_{\text{TXE}}(A_L + A_H) \\ &= E_{\text{TKE}}(A_L) + E_{\text{TKE}}(A_H) + E^*(A_L) + E^*(A_H) \\ &= E_{\text{TKE}}(A_L) + E_\gamma(A_L) + \bar{\nu}(A_L) \times [\langle \varepsilon \rangle(A_L) \\ &\quad + \langle B_n \rangle(A_L)] + E_{\text{TKE}}(A_H) + E_\gamma(A_H) \\ &\quad + \bar{\nu}(A_H) \times [\langle \varepsilon \rangle(A_H) + \langle B_n \rangle(A_H)]. \end{aligned} \quad (12)$$

In this work, $\langle \varepsilon \rangle(A)$, $E_\gamma(A)$ and $B_n(A)$ are the calculated results shown in Figs. (8)–(10), E_{TKE} is the experimental data and $\bar{\nu}(A)$ is the calculated result with Ref. [9]. In the physics, the E_{fission} from Eq. (11) and Eq. (12) should be equal, i.e. the energy should be conserved in the calculation. Fig. 11 gives both of the two calculated results. It can be seen that the energy is conserved very well in the present work.

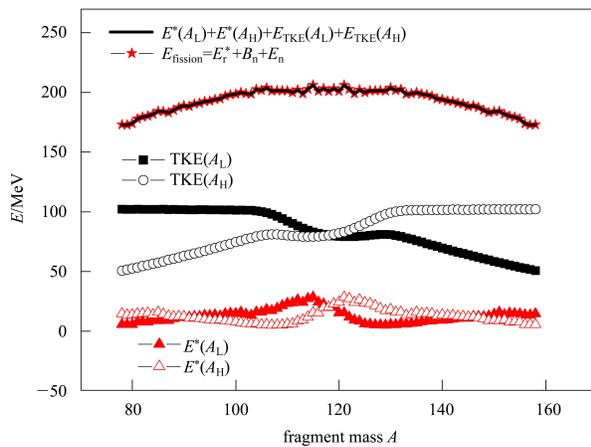


Fig. 11. The energy conservation for the $n(\text{thermal})+^{235}\text{U}$ reaction.

4 Conclusion

In conclusion, we have calculated the prompt fission neutron spectra for the neutron-induced fission of ^{235}U at $E_n=0.0253$ eV, 0.4, 0.53, 1.5 and the results are different. Therefore, the hypothesis of two fission fragments which have the same nuclear temperature is not reasonable. The ratio of the average nuclear temperature for light fragments and heavy fragments is 1.28 in this work, and this is very close to the $R_T=1.2$ or 1.4 used in Ref. [17]. In addition, the nuclear temperature in the symmetric fission region varies considerably, from 1.07 MeV to 0.31 MeV.

2.9 MeV with a semi-empirical method. The prompt fission neutron multiplicity distribution and nonconstant and constant temperatures were taken into account. The calculated neutron spectra display good agreement with the experimental spectra, except for the case of the $n(2.9\text{ MeV})+^{235}\text{U}$ reaction, for which the experimental data may be not reasonable. The average nuclear temperature of the fission fragment and the probability distribution of the nuclear temperature were calculated and compared with the LA model. The energy carried away by γ rays for the case of the $n(\text{thermal})+^{235}\text{U}$ reaction was also calculated and compared with the experimental data.

As the prompt fission neutron spectrum is calculated according to the excitation energy of each fragment, and there is no parameter in the present work, the results reported could shed some light on the properties of fission fragments.

- 1) The evaporation mechanism is the main mechanism for neutron emission from fission fragments.
- 2) The nuclear temperature of the two fission fragments is different.
- 3) The calculated energy carried away by the γ rays is in good agreement with the experimental data, which proves that the two-step model of fragment de-excitation is reasonable: first the emittance of neutrons, and then, only in the case where the excitation energy is not enough to emit neutrons, the emittance of γ rays. During the emittance of neutrons, there is some competition from the emittance of γ rays.

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