Approximate Relationships to Reproduce the Values of Shell Correction Energy for Fission Fragments

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Although the shell correction has been studied for years, calculating shell correction values is still complicated. Strutinsky suggested a simple method for calculating shell correction energy. However, this method still require numerical calculations. Since shell correction values are widely used, here linear relationships are presented to reproduce the shell correction energy values of fission fragments.

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The first model to describe the properties of the nucleus was the liquid drop model. When Haxel [1] and Mayer [2] introduced the spin-orbit force that could predict the increase in the binding energy of the magic nuclei, the shell model became the basis of discussion on the properties of the excited nucleus states. The slow development of the calculation of shell correction energy was at first due to the limited power of computers and recently due to the complexity of the theoretical models. This complexity, together with the large volume of computations required, demonstrates the importance of a simple relationship.

Of course, the simplification expression for nuclear parameters is presented from the beginning of the discovery of fission. The first approximate relationship is the semi-empire formula of mass in the Liquid drop model (LDM). Although this approximate relation does not have good results for magic nuclei, it can be used for most nuclei. Also, the mass distribution of fission fragments can be presented as a Gaussian form despite minor differences with the experimental results [3–5]. Viola [6] declared the systematic relationship for fission fragment total kinetic energy release ($<\overline{TKE}>= 0.1189\frac{Z_{cn}^2}{A_{cn}^{1/3}} + 7.3$ MeV). Terrel [7] presented the deformability parameter as the mass and atomic numbers ($\alpha = 4.86 - 0.063\,\frac{{Z_i}^2}{A_i}$). The average total prompt gamma emission energy and total prompt fission energy release for neutron-induced of isotopes uranium is presented by Madland [8] (eg. $T_f^{total} = 170.93 - 0.1544E_n$ for neutron fission of ^{235}U). Recently the amounts of energy released in the reaction ($< Q >= 90.2398 + 1.0127TKE - 0.0017TKE^2$) and the average neutron separation energy ($< B_n >= 16.2275 - 0.1221TKE + 0.0003TKE^2$ for ^{252}Cf(SF)) are expressed in terms of the average total kinetic energy [9]. Also, the ratio of the neutron multiplicity of heavy fragment on the total neutron multiplicity (ν_H/ν) is presented by Ref. [10]. For example, it is formulated for ^{252}Cf(SF) as

$$\nu_H/\nu = \begin{cases} -0.1A_H + 13.1\, for\ 126 \le A_H < 130 \\ 0.0286A_H - 3.6143\ \ for\ \ 130 \le A_H \le 144 \\ 0.5 \qquad for \quad 144 \le A_H \le 145 \\ 0.0163A_H - 1.8563 for\ 145 \le A_H \le 176. \end{cases} \tag{1}$$

The first shell correction energy approximation was performed with the Strutinsky method. With the introduction of the Strutinsky method, the methods of calculation for the shell correction made a major leap [11, 12]. Although the Strutinsky model simplifies calculations of shell correction, this method still requires intricate and usually numerical calculations. In the Strutinsky method, the shell correction is a difference between the sum of single-particle energies of occupied states and the averaged of those energies. The occupied states are always calculated numerically and the averaged energy is obtained with the single-particle levels. Despite these complex calculations, the Strutinsky method has been widely used [13–19]. On the other hand, the shell correction energy can be calculated in the semi-classical methods by the WignerKirkwood expansion [20–25]. They has claimed that Strutinsky shell correction method is essentially a semi-classical approximation [26, 27]. This is clear that the semi-classical method and Hartree-Fock-Bogoliubov method are inherently complex calculations.

On the other hand, the shell correction energy is simply defined as the difference between the experimental mass and the calculated mass with Liquid drop model (LDM) [28]. According to this definition, Myers [29] presented the different between the calculated values of the Finite-Range liquid drop model (FRLDM) [30] and experimental data. The shell correction values for all nuclei are presented in Ref. [29], from which the shell correction energy values are taken in the present study.

On the other hand, shell correction values are widely used in nuclear calculations and calculating these values is complex. This prompted us to systematically present the easiest way to obtain these values for the fission fragment. The initial idea comes from an phenomenological method in which the values of shell correction energy of fission fragments at zero excitation energy are plotted

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over the fission fragments. It can be seen from these plots that these values do not change much except for magic fragments. Therefore, the shell correction energy values of fission fragments can be approximated with a simple linear relationship for each reaction. Also, using the values of shell correction for each model (eg FRDL or HFB models), a linear relationship can be provided for the same model, which have a minimum error.

Simple relationships for shell correction not only reduce the volume of nuclear calculations but can also lead to the formation of systematic methods for calculating mass and energy distributions. For example, the mass yield of cold and spontaneous fission of ^{252}Cf and ^{238}U are calculated using the systematic scission point [31–33] by these approximated relationships. Also, the total kinetic energy of actinides is evaluated by this approximated [34].

I. METHOD

Ruben plotted phenomenologically the shell correction energy values of some reactions over the mass numbers of fission fragments (figure 2 of Ref.[35]). Manailescu [10] also plotted the same plotting. The shell correction energy does not depend on the mass number of fragments and the atomic number of fission fragments, but this plotting can present the approximation relationship to obtain shell correction energy values of fragments for some reactions.

Also, the atomic numbers of the fission fragments are calculated by the most probable charge based on the unchanged charge-density distribution as [10, 36]

$$Z_{UCD} = \frac{Z_{cn}\,(A+\nu)}{A_{cn}}, \tag{2}$$

where ν is the post-scission neutrons [37, 38]. Comparing the fission fragments for photofission of ^{238}U (Table 1 from [39]) and neutron fission of ^{238}U (Tables 1-4 from [40]), it can be seen that the fission fragments of these reactions are generally the same. For example, the fragments ^{84}Br, ^{85,87,88}Kr, and ^{92,93}Sr are found in the neutron fission and photofission of ^{238}U. However, fragments such as ^{101}Mo and ^{104}Tc are only found in photofission experimental data, which may depend on the experiment process. Of course, the method of measuring these references is the same, but similar results have been obtained with another measurement method [41].

On the other hand, the damping of the shell corrections with increasing the excitation energy is presented by Ignatyuk [42] as

$$E_{shell}(T) = E_{shell}(0)\left(\frac{(e^{-E_1/E_0}-1)}{(e^{(E-E_1)/E_0}-1)} + \frac{TS_0\,(\tau\cosh(\tau)-1)}{\sinh(\tau)}\right), \tag{3}$$

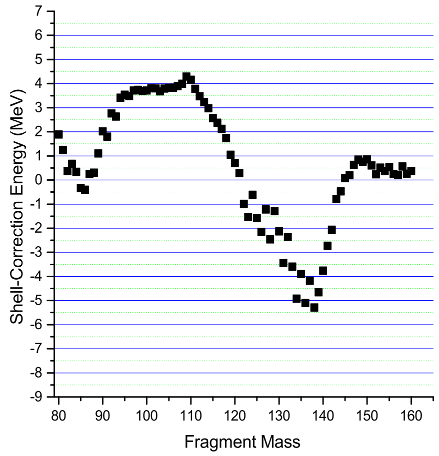

FIG. 1: Mass-dependent shell correction energy for ^{232}Th fission.

where $E_{shell}(0)$ is the shell correction energy at zero excitation energy, $S_0 = 2.5MeV^{-1}$, $\tau = 2\pi^2 A^{1/3}T/41$, E_1 =-18.54 MeV, E_0=42.28 MeV.

II. LINEAR RELATIONSHIPS

The values of shell correction energy are plotted over mass number of fragments in Figs. 1-5. From these Figures, the linear approximate relationships are presented for several reactions.

The shell correction energy of fission fragments is plotted over mass number of fragments for ^{232}Th fission in FIG. 1. According to FIG. 1, the shell correction energy of fission fragments could be approximated as a linear relationship for fission of ^{232}Th as

$$E_{shell}(MeV) = \begin{cases} 1.89 + 0.65(A-80) \quad for\ A < 83 \\ 0.1 \quad for\ 83 \le A \le 88 \\ 0.3 + 3.1(A-88)/6 \\ \quad for\ 88 \le A \le 96 \\ 3.5 \quad for\ 96 \le A \le 110 \\ 4.16 - 7.86(A-110)/30 \\ \quad for\ 110 < A < 140 \\ 0.86 + 0.45(A-150) \\ \quad for\ 140 < A < 150 \\ 0.5 \quad for\ A > 150, \end{cases}$$

where A is mass number of fission fragments.

The shell correction energy of fission fragments is plotted over mass number of fragments for ^{235}U fission in FIG. 2. According to FIG. 2, the shell correction energy of fission fragments could be approximated as a linear relationship for fission of ^{235}U as

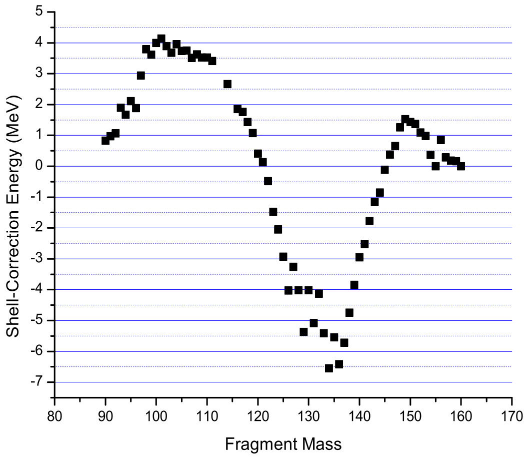

FIG. 2: Mass-dependent shell correction energy for ^{235}U fission.

$$E_{shell}(MeV) = \begin{cases} 0 \quad for \;\; A < 100 \\ 0.2(A-100) \;\; for \;\; 100 \leq A \leq 110 \\ 4 - 11(A-110)/20 \quad for \;\; 110 < A < 130 \\ 3 + 10(A-165)/35 \;\; for \;\; A > 130. \end{cases} \tag{4}$$

This multifunction relation is similar to the ratio of ν_H/ν formalisms in appendix A of Ref. [10] (Eq. 1).

The shell correction energy of fission fragments is plotted over mass number of fragments for ^{238}U fission in FIG. 3. According to FIG. 3, the shell correction energy of fission fragments could be approximated as a linear relationship for fission of ^{238}U as

$$E_{shell}(MeV) = \begin{cases} 2 - 0.35(A-80) \quad for \;\; A < 90 \\ A - 91.5 \;\; for \;\; 90 \leq A \leq 95 \\ 3.5 \;\; for \;\; 95 \leq A \leq 110 \\ 3.5 - 3.5(A-110)/15 \; for \, 110 < A < 125 \\ -4.5(A-125)/15 \quad for \;\; 125 < A < 140 \\ -4.5 + 5.5(A-140)/8 \, for \; 140 < A < 148 \\ 1 \;\; for \;\; A > 148. \end{cases} \tag{5}$$

These relations are also used in [31] to evaluate mass yield of spontaneous fission of ^{238}U.

The shell correction energy of fission fragments is plotted over mass number of fragments for $^{239-240}Pu$ fission in FIG. 4. According to FIG. 4, the shell correction energy of fission fragments could be approximated as a linear relationship for fission of $^{239-240}Pu$ as

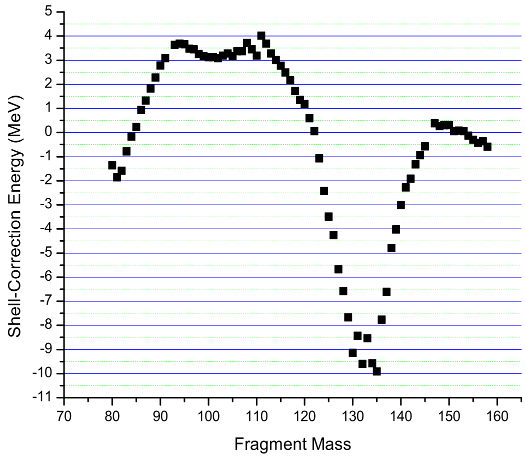

FIG. 3: Mass-dependent shell correction energy for ^{238}U fission.

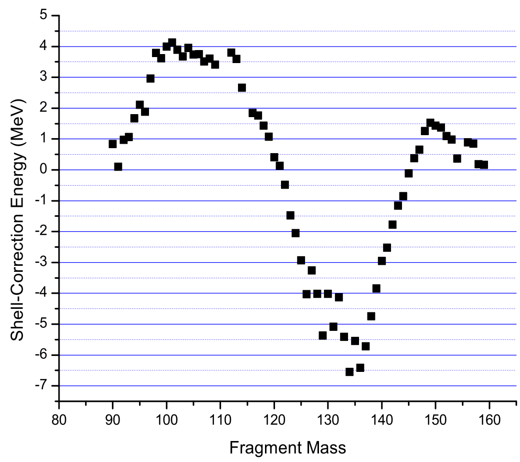

FIG. 4: Mass-dependent shell correction energy for ^{239}Pu fission.

$$E_{shell}(MeV) = \begin{cases} 1 - (A-100)/15 \quad for \;\; A < 100 \\ 1 + 0.3(A-100) \;\; for \;\; 97 \leq A \leq 111 \\ -4(A-125)/15 \quad for \;\; 110 < A < 125 \\ -4(A-125)/5 \quad for \;\; 125 < A < 130 \\ 4 + 8(A-155)/25 \;\; for \;\; A > 147. \end{cases} \tag{6}$$

The shell correction energy of fission fragments is plotted over fragments for fission of ^{252}Cf in FIG. 5. According to FIG. 5, the shell correction energy of fission fragments could be approximated as a linear relationship for fission of ^{252}Cf as

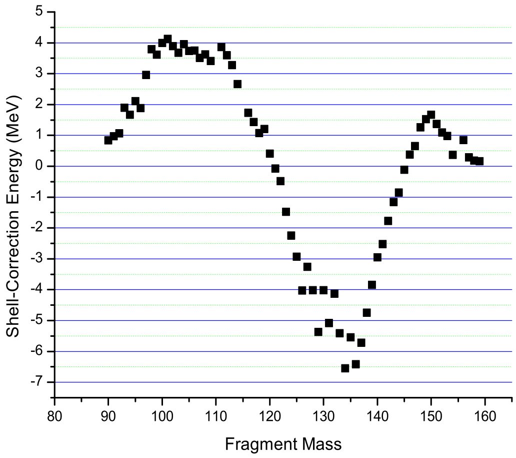

FIG. 5: Mass-dependent shell correction energy for ^{252}Cf fission.

$$E_{shell}(MeV) = \begin{cases} -1.86 + 2(A-81)/12 \quad for \;\; A < 97 \\ 3.3 \quad for \;\; 97 \leq A \leq 111 \\ 4.02 - 10.16(A-111)/19 \\ \qquad\qquad for\, 111 < A < 130 \\ 0.38 + 8.52(A-147)/17 \\ \qquad\qquad for\, 130 < A < 147 \\ 0.36 - 0.025(A-148) \;\; for \;\; A > 147. \end{cases}$$

Also, for cold and Spontaneous fission of ^{252}Cf, mass yield are investigated by the same relations using statistical scission point model [33].

Of course, for more accuracy, all relationships can be divided into more sections.

III. SUMMARY

The shell correction values of fission fragments is plotted for different reactions of actinides at zero excitation energy. Approximate linear relationships are presented for fission of ^{232}Th, ^{235}U, ^{238}U, $^{239-240}$Pu, and ^{252}Cf.

The shell correction values of fission fragments could be systematically obtained without complication calculation at zero excitation energy, so the damping of the shell corrections must be used to estimate its values for excitation energy E.

The results of these relationships are not accurate for a few fission fragments with magic numbers, but they can be estimated well for a large numbers of fission fragments. Also, the presented relationships may be the first order of approximation, so in the future they can be developed for more accuracy and other models.

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