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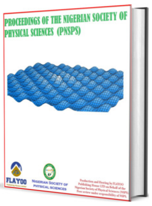

Effect of deformation on alpha decay of super-heavy nuclei within a Woods-Saxon model

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ABSTRACT

In this research, alpha decay study of super-heavy nuclei has been carried out by employing the Woods-Saxon model potential. The spherical and deformed Woods-Saxon model have been employed to investigate the effect of deformation on the super-heavy nuclei via alpha decay. When compared with experimental data, the two models are found to perform very well in describing the experimental half-life data. Moreover, results obtained by considering deformation is found to give better agreement with the experimental data than the results using spherical configuration. This is mainly because the super-heavy nuclei have non-zero deformation parameters. The study concludes that deformation should be considered when studying super-heavy nuclei, and that the deformed Woods-Saxon model is more complete in describing the interaction between the alpha decay and the daughter nuclei as it has a low standard deviation value of 0.5012 compared to 0.6260 when only sphericity is considered.

Keywords: Alpha decay, Woods-Saxon model, Deformation, Super-heavy nuclei.

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1. INTRODUCTION

Alpha (α) decay, discovered by Ernest Rutherford and his collaborators in 1899 is a fundamental radioactive decay mode that plays a crucial role in understanding nuclear structure, stability, and interactions [1–3]. The theoretical foundation of alpha decay was established in 1928 by Gamow, along with Condon and Gurney [4–6], who successfully explained the process using quantum mechanical tunneling. Their work provided a theoretical interpretation of the Geiger–Nuttall law, the first empirical formula for predicting alpha decay half-lives. This law establishes a relationship between the decay half-life and the energy of the emitted alpha particle, showing that higher-energy emissions correspond to shorter half-lives.

Over the years, numerous theoretical models and empirical formulas have been developed to refine the calculation of alpha decay half-lives. Theoretical models include the fission-like model [7], cluster formation model [8, 9], preformed cluster model (PCM) [10], effective liquid drop model (ELDM) [11], generalized liquid drop model (GLDM) [12],modified generalized liquid drop model (MGLM) [13], two-potential approach [14, 15] and so on. These models utilize both phenomenological and microscopic potentials to describe the alpha decay process more accurately. Some of the empirical and semi-empirical formulas that have also been successful in the study of alpha decay half-lives are the Viola–Seaborg formula (VSS) [16], Royer formula [17, 18], Ren and modified Ren formulas [19, 20], universal decay law (UDL) [21], scaling laws of Brown and Horoi

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[22], Akrawy formula [23], and Denisov and Khudenko formula [24]. These formulas offer practical approaches to estimating decay half-lives across a wide range of nuclei. However, in this study, Woods-saxon model was considered over other theoretical models for nuclear potential because it assumes a finite nuclear surface which is more realistic and also, give better agreement with experimental data.

The consideration of deformation in the calculation of alpha-decay half-life is essential as many alpha emitters are deformed in their ground state configuration. Consequently, the alpha-daughter system potential is influenced by the emission angle (θ) of the alpha particle relative to the symmetry axis of the deformed nucleus [25]. This deformation significantly affects both the alpha decay half-life and the tunneling probability, as they depend on the angular dependence of the deformed potential [28]. Given the critical role of deformation, it is essential to account for it when calculating alpha decay half-lives, as this leads to more accurate predictions. Several studies have incorporated and demonstrated the importance of deformation in the study of alpha decay half-lives [26, 27, 29–32].

The study of alpha decay half-lives of super-heavy nuclei has been carried out both experimentally and theoretically. Super-heavy nuclei have been selected for this study because they have non-zero quadrupole and hexadecapole deformation parameters. This aids the effect of using deformed model on alpha decay have-lives. The paper is arranged as follows: In Section 2, the models employed for the description of the alpha-decay half-lives via a deformed Woods-Saxon (WSD) potential model and the Spherical Woods-Saxon (WSS) potential model were presented. The results of the description are presented and discussed in Section 3 while the conclusion is given in Section 4.

2. THEORETICAL FORMALISM

2.1. DEFORMED WOODS-SAXON POTENTIAL

Here, the effective interaction potential between the alpha particle and the deformed daughter nucleus is given by the sum of the deformed repulsive Coulomb potential $V_C(r,\theta)$, the deformed attractive nuclear potential $V_N(r,\theta)$ and the centrifugal term $V_\ell(r,\theta)$ [33]:

$$V_{eff}(r,\theta) = \eta V_N(r,\theta) + V_C(r,\theta) + V_{ell}(r,\theta), \tag{1}$$

where η is a quantization factor of the nuclear potential that is obtained by applying the requirement of the Bohr-Sommerfeld quantization condition, ℓ is the angular momentum carried by the α-particle and θ is its angle of orientation with respect to the symmetry axis of the daughter nucleus. The deformed Woods-Saxon potential is defined as [31]:

$$V_N(r,\theta) = \frac{V_0}{1 + \exp\left[\frac{r+R(\theta)}{a}\right]}, \tag{2}$$

where the potential depth is obtained via [34]:

$$V_0 = -44.16[1 - 0.40I_2]\frac{A_2^{2/3}A_1^{2/3}}{A_2^{2/3} + A_1^{2/3}}. \tag{3}$$

Here, the diffuseness parameter is obtained using the formula [35]:

$$a = 0.5 + 0.33I_2, \tag{4}$$

where I_2 is the relative neutron excess of the daughter nucleus, given as:

$$I_2 = \frac{(N_2 - Z_2)}{A_2}. \tag{5}$$

The daughter nucleus effective radius $R(\theta)$ is given by:

$$R(\theta) = 1.17 + R_2[1 + \beta_2 Y_{20}(\theta) + \beta_4 Y_{40}(\theta)], \tag{6}$$

where β_2 and β_4 are the quadrupole and hexadecapole deformation parameters of the daughter nucleus respectively. These deformation parameters describe the shape of the nucleus. $Y_\ell, m(\theta)$ is the spherical harmonics and

$$R_2 = (1 + 0.39I_2)A_2^{1/3}, \tag{7}$$

is the radius of the daughter nucleus. It is known that the inclusion of the quadrupole deformation parameter causes a decrease in the half-life calculated value by 2-7 orders of magnitude [36]. Due to reflection symmetry, the calculations have been carried out by considering the relative orientations $\theta = 0^o - 180^o$ with respect to the symmetry axis of the deformed nucleus. The deformed Coulomb potential and the centrifugal term have been computed using:

$$V_C(r,\theta) = \frac{Z_1 Z_2 e^2}{r}\left[1 + \frac{3R^2(\theta)}{5r^2}\beta_2 Y_{20}(\theta) + \frac{3R^4(\theta)}{9r^2}\beta_4 Y_{40}(\theta)\right], \tag{8}$$

and

$$V_\ell(r) = \frac{(\ell + 1/2)\hbar^2}{2\mu r^2}, \tag{9}$$

respectively. Here, $\mu = \frac{A_\alpha A_d}{A_\alpha + A_d}$ is the reduced mass of the alpha particle and the deformed daughter nucleus. The WKB barrier penetration probability P is calculated via:

$$P = \frac{1}{2}\int_0^\pi T_\ell \sin\theta d\theta. \tag{10}$$

The transmission coefficient is calculated using

$$T_\ell(\theta) = \frac{1}{1 + \exp[\frac{2}{\hbar}\int_{r_1(\theta)}^{r_2(\theta)} \sqrt{2\mu|[V(r,\theta) - Q]|dr}]}, \tag{11}$$

where the turning points $r_1(\theta)$ and $r_2(\theta)$ are determined using the condition $V(r,\theta) = Q$. The alpha-decay half-life is then computed via [37]:

$$T_{\frac{1}{2}} = \frac{\ln 2}{\upsilon P}. \tag{12}$$

Here, the assault frequency υ is determined using:

$$\upsilon = \frac{2E_\upsilon}{\hbar} = \frac{Q\left[0.056 + 0.039\exp\left(\frac{4-A_2}{2.5}\right)\right]}{\hbar}. \tag{13}$$

2.2. SPHERICAL WOODS-SAXON POTENTIAL

For the spherical Woods-Saxon case (WSS), the daughter nucleus is assumed to be spherical. The effective potential between the alpha and the daughter nuclei is also given by the sum of the repulsive Coulomb potential $V_C(r)$, the attractive nuclear potential $V_N(r)$ and the centrifugal term $V_\ell(r)$:

$$V_{eff}\left(r\right) = \eta V_N\left(r\right) + V_C\left(r\right) + V_\ell(r), \tag{14}$$

where η is a quantization factor.

For Coulomb potential (V_C):

$$V_C\left(r\right) = \frac{Z_1 Z_2 e^2}{r}, \tag{15}$$

and the centrifugal potential (V_ℓ) is computed using:

$$V_\ell\left(r\right) = \frac{\left(\ell + \frac{1}{2}\right)\hbar^2}{2\mu r^2}. \tag{16}$$

For attractive nuclear potential [35]:

$$V_N\left(r\right) = \frac{V_0}{1 + exp\left[\frac{r+R_s}{a}\right]}, \tag{17}$$

where

$$R_s = 1.17 + (1 + 0.39I_2)A_2^{\frac{1}{3}}. \tag{18}$$

The penetration probability is given as [32]:

$$P = exp\left[-\frac{2}{\hbar}\int_{r_1}^{r_2}\sqrt{2\mu\left(V\left(r\right) - Q\right)}dr\right]. \tag{19}$$

3. RESULTS AND DISCUSSION

Here, we present the results of the calculations on effects of deformation on alpha-decay half-lives of super-heavy nuclei. The codes used for all calculations were written in Python programming language. Libraries such as NumPy, SciPy, Matplotlib, Pandas and SymPy were utilised during the process of computation as they aid quick and efficient results. The data used in this study viz: the mass number (A), atomic number (Z), experimental Q_α values, orbital angular momentum (ℓ) carried by the emitted α-particle are all extracted from the NUBASE2020 database. The data for 52 alpha emitters were derived from the database. The data include the mass number, atomic number, spin and parity, mass excess, and half-lives. But it was observed that some nuclides do not have spin and parity values, and some do not have defined decay modes; this leaves the space blank (or inclusion of NaN). So a simple line of code was written to remove the "Not a Number" (NaN). This is necessary because some machine learning models do not work with missing features. After data cleaning, a total of 45 nuclei were obtained. The decay energy Q_α was computed using:

$$Q_\alpha = \Delta M_P - \Delta M_D + \Delta M_\alpha, \tag{20}$$

where ΔM_P, ΔM_α, and ΔM_D denote the mass excesses of the parent nucleus, the alpha particle and the daughter nucleus respectively.

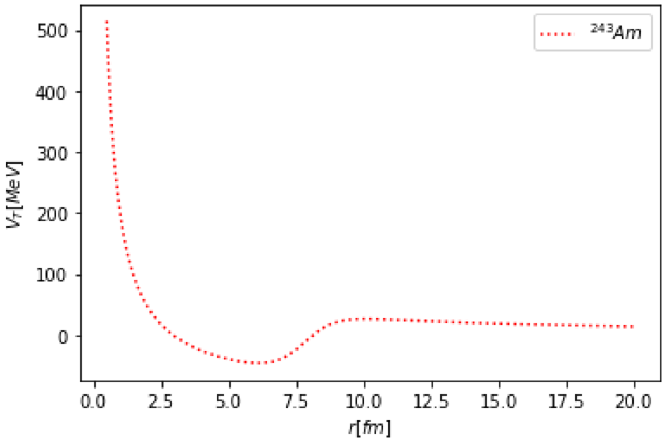

Figure 1. Calculated total (effective) potential, V_T (MeV) between alpha particle and daughter nucleus of Americium-243 (^{243}Am) against radial distance r (fm).

Alpha-particle emission obeys the spin-parity selection rule. When the spin and parity values are different, the alpha-emitter carries a non-zero angular momentum ℓ [38]. The minimum value of angular momentum ℓ_{min} at the α-transition between states with j_p, π_p, j_d and π_d is given as [20]:

$$\ell = \begin{cases} \Delta_j & \text{for even } \Delta_j \text{ and } \pi_d = \pi_p \\ \Delta_j + 1 & \text{for odd } \Delta_j \text{ and } \pi_d = \pi_p \\ \Delta_j & \text{for odd } \Delta_j \text{ and } \pi_d \neq \pi_p \\ \Delta + 1 & \text{for even } \Delta_j \text{ and } \pi_d \neq \pi_p \end{cases}, \tag{21}$$

where $\Delta_j = |jp{-}jd|$, and j_d, π_d, j_p, π_p are the spin and parity values of the daughter and parent nuclei, respectively. The extracted spin and parity values obtained from the NUBASE 2020 database were utilized to compute the angular momentum [35].

The potential which were measured in mega electron volts (MeV) are plotted against radial distance r in femtometer (fm) are shown in figure below for Americium-243 nucleus. Total (effective) potential V_T (MeV) was plotted against radial distance r(fm)]. When the mass number of the nucleus is 243, the nucleus is named Americium (^{243}Am) having proton number of 95 and neutron number to be 148. In the research, we also calculated the deformation effect on other nuclei which are Berkelium -247 (^{247}Bk) and Uranium-290 (^{290}U).

From Figure 1, one can observe that there is a drastic decrease to a point just below zero and rises to remain constant at a point slightly above zero. This shows that at small radial distances, the strong nuclear force between the alpha and daughter nucleus creates a deep potential well. At larger radial distances, the potential remains relatively constant due to the tunneling effect, which allows the alpha particle to penetrate the Coulomb barrier. Moreover, the input parameters such as the atomic number, mass number, orbital angular momentum, and Q_α values have been derived from the NUBASE2020 database [39]. The calculations was carried out using the deformed Woods-Saxon potential model. The calculations using the spherical Woods-Saxon nuclear potential has been included in order to see the effect of using deformed nuclear potential on the alpha-decay half-lives.

Table 1. Calculated α-decay half-lives of super-heavy nuclei ($Z = 100 \geq 118$) using the spherical Woods-Saxon, deformed Woods-Saxon models and experimental data.

Z	A	N	ℓ	Q_α	Expt	Z_d	A_d	β_2	β_4	WSS	WSD
100	243	143	1	8.689	-0.595	98	239	0.237	0.085	-0.4236	-0.33694
100	246	146	0	8.379	0.218	98	242	0.237	0.073	0.394327	0.515744
100	247	147	4	8.258	1.685	98	243	0.237	0.073	1.529912	1.595985
100	248	148	0	7.995	1.538	98	244	0.249	0.063	1.650364	1.743271
100	249	149	4	7.709	2.464	98	245	0.249	0.063	3.440644	3.464003
100	250	150	0	7.557	3.27	98	246	0.249	0.051	3.220886	3.329462
100	252	152	0	7.154	4.961	98	248	0.25	0.039	4.79693	4.91727
100	253	153	5	7.198	6.334	98	249	0.25	0.039	5.731352	5.804319
100	254	154	0	7.307	4.067	98	250	0.25	0.027	4.08242	4.260562
100	255	155	4	7.241	4.859	98	251	0.25	0.027	5.091663	5.234902
100	256	156	0	7.025	5.066	98	252	0.251	0.014	5.211799	5.406612
100	257	157	2	6.864	6.94	98	253	0.24	0.012	6.128801	6.347683
102	251	149	0	8.752	-0.016	100	247	0.249	0.051	-0.11378	0.082395
102	252	150	0	8.549	0.562	100	248	0.25	0.039	0.508163	0.73388
102	253	151	1	8.415	2.234	100	249	0.25	0.039	0.99562	1.206962
102	254	152	1	8.226	1.755	100	250	0.25	0.027	1.610986	1.852901
102	255	153	5	8.428	2.848	100	251	0.25	0.027	1.927247	2.142602
102	256	154	0	8.582	0.466	100	252	0.251	0.014	0.255466	0.562081
102	257	155	2	8.477	1.46	100	253	0.24	0.012	0.792841	1.125659
102	259	157	2	7.854	3.667	100	255	0.24	-0.001	2.936222	3.260715
103	254	151	3	8.822	1.224	101	250	0.25	0.027	0.441077	0.708842
103	255	152	4	8.556	1.494	101	251	0.25	0.027	1.570743	1.807667
103	256	153	1	8.855	1.516	101	252	0.251	0.014	-0.10907	0.211894
104	255	151	1	9.055	0.49	102	251	0.25	0.027	-0.26364	0.031195
104	256	152	0	8.926	0.328	102	252	0.251	0.014	0.027841	0.354474
104	257	153	5	9.083	0.748	102	253	0.24	0.012	0.607174	0.953568
104	258	154	0	9.196	-0.593	102	254	0.24	0.012	-0.87541	-0.49419
105	256	151	2	9.336	0.385	103	252	0.251	0.014	-0.5761	-0.23188
105	259	154	5	9.619	-0.292	103	255	0.24	-0.001	-0.63807	-0.2251
106	259	153	2	9.765	-0.396	104	255	0.24	-0.001	-1.50627	-1.06772
106	260	154	0	9.901	-1.768	104	256	0.24	-0.001	-2.13587	-1.68634
106	261	155	2	9.714	-0.729	104	257	0.229	-0.016	-1.43547	-0.94327
107	261	154	3	10.5	-1.893	105	257	0.229	-0.016	-2.91565	-2.38757
108	263	155	5	10.733	-3.046	106	259	0.23	-0.028	-2.54947	-2.00489
108	265	157	0	10.47	-2.708	106	261	0.219	-0.043	-3.01816	-2.44871
108	266	158	0	10.346	-2.404	106	262	0.219	-0.043	-2.73415	-2.17039
108	270	162	0	9.07	0.954	106	266	0.173	-0.013	0.804074	1.406413
110	267	157	0	11.777	-5	108	263	0.196	-0.034	-5.40027	-4.73151
110	270	160	0	11.117	-3.688	108	266	0.173	-0.013	-4.01516	-3.32955
114	286	172	0	10.355	-0.657	112	282	0	0	-1.07737	-0.18603
114	288	174	0	10.076	-0.185	112	284	0.023	0.002	-0.36084	0.51983
114	290	176	0	9.856	1.903	112	286	0.047	0.016	0.214783	1.067769
116	290	174	0	10.997	-2.046	114	286	0.047	0.016	-2.13489	-1.24603
116	292	176	0	10.791	-1.796	114	288	0.249	0.061	-1.66926	-1.47399
118	294	176	0	11.867	-3.155	116	290	0.249	0.061	-3.63105	-3.37401

The calculated description of alpha-decay half-lives are shown in Table 1. The first five columns show the atomic number (Z), mass number (A), neutron number (N), the angular momentum carried by he alpha particle (ℓ), the experimental Q_α values. The experimental alpha-decay half-lives (Expt. [$\log_{10}T_{\frac{1}{2}}(s)$]) are shown in the sixth column. Seventh and eight columns are for the daughter atomic number (Z_d) and the daughter mass number (A_d). The ninth column and tenth column is for the quadrupole (β_2) deformation parameters, the hexadecapole (β_4) deformation parameters. The Spherical Woods-Saxon potential (WSS) and the deformed Woods-Saxon potential (WSD) are shown in the eleventh and twelve columns, respectively.

However, in order to quantitatively compare the agreement between the experimental and theoretically calculated half-lives, the root mean square also known as standard deviation (σ) has

Table 2. Calculated standard deviation (σ) using the different models.

Model	σ
WSD	0.5012
WSS	0.6260

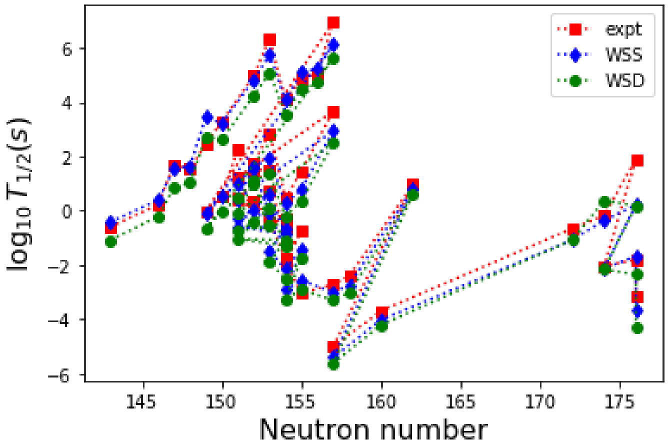

Figure 2. Plot of the calculated α-decay half-lives using the spherical Woods-Saxon, deformed Woods-Saxon models and experimental values.

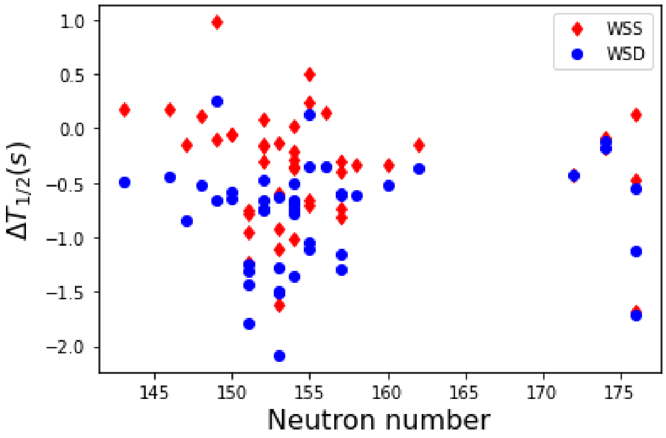

Figure 3. Plots of the $\Delta T_{1/2}$ against neutron number (N) for the super-heavy nuclei using the different models.

been computed using:

$$\sigma = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left[\left(\log_{10} T_{\frac{1}{2}}^{Theory}(s) - \log_{10} T_{\frac{1}{2}}^{Expt}(s)\right)\right]^{2}}, \tag{22}$$

where $\log_{10} T_{\frac{1}{2}}^{Theory}(s)$ is the theoretical α-decay half-lives calculated using the theoretical model and $\log_{10} T_{\frac{1}{2}}^{Expt}(s)$ is the experimental half-lives from the NUBASE2020 database [40, 41]. The standard deviation values for the WSD and WSS are 0.5012 and 0.6260 respectively. From these values, one observes that the WSD model gives the lowest standard deviation when compared to the WSS model and as such produces values of half-lives that are closer to the experimental values. This shows the importance of using a deformed nuclear potential over the spherical one for these super-heavy nuclei. This model has been proved to give excellent descriptions of α-decay half-lives [35].

Figure 2 shows the plots of the computed α-decay half-lives, $\log_{10} T_{\frac{1}{2}}(s)$, using the two theoretical models against the neutron number (N). The experimental values are shown in red squares, the Woods-Saxon Spherical are shown in blue diamond while Woods-Saxon Deformed are shown in black circle. The half-life can be seen to increase with increase in neutron number for the series of nuclei considered in the study. It can be observed from the graph that the half-lives are well concentrated within +5 to -4 region. One observes from the figure that all the models give very good descriptions of the alpha-decay half-lives, since only a slight difference between the calculated results and experimental can be seen. In figure 3, the difference between experimental and theoretical α-decay half-lives have been obtained using:

$$\Delta T_{1/2} = \log_{10} T_{1/2}^{Theory} - \log_{10} T_{1/2}^{Expt}. \tag{23}$$

$\Delta T_{1/2}$ has been plotted against neutron number in Figure 3 for the two models used in the study. It can be observed that, barring few exceptions, most of the points are near zero and within +0.5 to -1.5. Moreover, it can be observed that the WSD model gives lower $\Delta T_{1/2}$ values than the WSS model. This shows the advantage of using deformed model for the study of super-heavy nuclei.

4. CONCLUSION

The theoretical description of α-decay half-lives of super-heavy nuclei has been carried out via a deformed Woods-Saxon (WSD) potential model. Calculations using spherical Woods-Saxon (WSS) potential model was included to see the effect of using deformed nuclear potential on the α-decay half-lives of super-heavy nuclei. Both the models give very good descriptions of the α-decay half-lives when compared with experimental data, although the WSD reduces the deviation by approximately 19.9 %. The difference between theoretically calculated and experimental α-decay half-lives is also found to be within the range of +0.5 to -1.5 for most of the super-heavy nuclei. This gives a good representation and also showed the importance of using deformed nuclear potentials over spherical ones for super-heavy nuclei. The computed standard deviation indicates that the calculated half-lives using WSD model gives lower root mean square value when compare with the WSS model. Therefore, when studying super-heavy nuclei, deformation effect should be included in order to obtain a more accurate results. Exploring different models involving deformation and the inclusion of other higher correction of deformation such as hexacontatetrapole parameter can also be explored in the study of the half-lives of superheavy nuclei.

DATA AVAILABILITY

The data used in the study were obtained from the NUBASE2020 database [40, 41].

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