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Update to the Geiger-Nuttall Relationship for Determining the Half-Life of Heavy Nuclei Using a Least Square Method

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ABSTRACT

In this study, a set of empirical formulae such as the Royer formula, Modified Universal Decay Law (MUDL) formula, and Modified Viola-Seaborg (MVS) formula are used to calculate the half-lives of the heavy and super-heavy nuclei whose numbers of protons Z are in the range $67 \leq Z \leq 118$. New fitting parameters for these formulas are proposed and perfectly described, corresponding to the Royer, MUDL, and MVS formulas, respectively. The parameters are fitted using the least square fitting method using Python software. The calculated alpha decay half-lives are next compared to the experimental data with a minimal difference. Statistical processes, including standard deviation and comparison of theoretically estimated and experimentally observed half-lives, are used for this purpose. Also, the fitting curve intends to get the accuracy of the experimental and theoretical values of the half-lives.

Keywords: alpha decay, half-live, Geiger- Nuttall rule.

INTRODUCTION

Alpha decay is a valuable method for investigating nuclear structure (Delion *et al*., 2006). It can reveal important details about the lifetime of the nucleus in its lowest energy state, as well as provide insights into nuclear matter incompressibility, nuclear force, and parity and spin of nuclei (Basu, 2004; Chowdhury *et al.*, 2006; Delion *et al*., 2006; Seif, 2006). In 1896, Becquerel first observed alpha decay as an unknown radioactive phenomenon. More than a decade later, it was further described as a process in which the parent nucleus emits an alpha particle by Rutherford in 1899 (Santhosh *et al*., 2015). These radioactive elements undergo successive transformations and transition into other radioactive elements with lower atomic numbers. Throughout this process, these elements continue to emit alpha particles that undergo mass reduction and transition from one element to another. This sequence persists until the final stage is reached, forming lead, stable elements. The first empirical formula for alpha decay half-live was done by Geiger-Nuttall (Geiger and Nuttall, 1911). Subsequently, different authors have presented and developed many empirical and semi-empirical formulas (Poenaru *et al*., 2007; Poenaru *et al.*, 2012; Royer, 2000). Independently, Gamow (Gamow, 1928) and Gurney and Condon examined the one-body issue for alpha decay and derived the well-known Geiger-Nuttall correlation based on the fundamental principles of quantum mechanics. These fundamental relationships assist the experimentalists in accurately determining the half-live values of alpha decay during the experiment design process. From these relations, some use one set of parameters for all nuclei (Oganessian, 2007; Poenaru *et al*., 2006; Sobiczewski *et al*., 1989), and others use more sets of parameters by dividing it into four sets as Even–Even (E-E), Even–Odd (E-O), Odd–Even (O-E), and Odd–Odd (O-O) nuclei (Dasgupta-Schubert and Reyes, 2007) as an example Royer (Royer, 2000) uses 12 parameters four for each set of (E-E), (E-O), (O-E), and (O-O) nuclei. Subsequently other semi-empirical and analytical formulae were suggested to accurately predicted the half-lives of alpha decay, including the Viola-Seaborg-Sobiczewski (VSS) formula, the Sobiczewski-Parkhomenko (SP) formula, Royer formula (Royer, 2010; Royer and Zhang, 2008), (Akrawy) Universal Decay Law (UDL) formula (Akrawy and Poenaru, 2017), each of these formulae dependent on different elements that calculate the α-decay half-lives and compared with the experimental half-lives and the result in a good agreement. These formulae have undergone successive modifications and refinement (Ni *et al*., 2008; Ren *et al*., 2004; Sobiczewski *et al*., 1989; Viola and Seaborg, 1966) to establish a universal framework for all detected decay events. In 2009, a linear Universal Decay Law (UDL) was introduced for all known cluster decay events, relying on Q-values of the emitted particles and charges and the masses of nuclei contained in the decay process (Qi *et al*., 2009). This Universal Decay Law (UDL) has proven to be effective in various cluster decays (Ismail and Adel, 2020; Maroufi *et al*., 2019; Santhosh and Priyanka, 2014) and α-decays (Deng *et al.*, 2020; Yang *et al.*, 2021). Consequently, it has become the most widely utilized formula, recognized for its accuracy and extensive applicability.

The UDL has also undergone adjustments tailored for both α-decay and cluster decay (Akrawy *et al*., a2019; Soylu and Qi, 2021) by incorporating a few essential terms. While the negative and positive beta decay energy has been determined for the heavy and medium nuclei through the liquid drop model, by finding relationships that express these two energies regardless of the mass of the nuclei once the atomic number and the number of neutrons are known, even though it has been noticed that there is no effective effect on the half-life of the nuclei as opposed to the impact of the alpha decay energy on the nuclei that are dissolve by this type of decay (Abdullateef and Al-jomaily, 2021; Qasim and Al-jomaily, 2020).

This paper aims to calculate the alpha decay half-lives of heavy and super-heavy nuclei in the range $67 \leq Z \leq 118$. Using different formulas with new parameters obtained by the least square method using Python software and compares its theoretical values with experimental values.

THEORETICAL FREMWORK

A. Royer formula

In the year 2000, Royer (Royer, 2000) introduced a mathematical formula for alpha decay, explicitly addressing the logarithm of the half- lives $log_{10}T_{1/2}$ for alpha emitters. The effect of the mass number of the parent nuclei acquired into account by this formula, the proton numbers of the parent nuclei, and the energy discharged during the reaction on the logarithm of the alpha decay half-lives $log_{10}T_{1/2}$ and is expressed as follows:

$$log_{10}T_{1/2} = a + bA^{1/6} + \sqrt{Z} + \frac{cZ}{\sqrt{Q_\alpha}} \quad \ldots\ldots\ldots (1)$$

where Z and A represent the proton and the mass number of parent nuclei, respectively, Q_α represents the total energy of the alpha decay process expressed in MeV, and the parameters a, b, and c are fitting parameters in equation (1), and it given in the (Table 1). A new set of parameters (a, b, c) are obtained through a fitting procedure for equation (1) applied to the investigated nuclei. A total of 493 sets of nuclei were subjected to this fitting process utilizing the method of least squares implemented Python programming the new parameters are also listed in (Table 1), which contains the values of coefficients a, b, and c in both cases.

Table 1: The parameters of the Royer formula according to (Akrawy *et al.*, b2019) which are denoted as (a, b, and c) sub Royer, and the new parameters of the Royer formula obtained using Python software are denoted as (a, b, and c) sub Python.

Type	a_{Royer}	a_{Python}	b_{Royer}	b_{Python}	c_{Royer}	c_{Python}	*No. nuclei*
E-E	-25.31901	-24.262506	-1.15847	-1.233881	1.58439	1.606957	152
E-O	-31.98969	-29.680151	-1.03520	-1.197367	1.72656	1.765118	120
O-E	-31.39063	-28.377173	-1.09816	-1.048555	1.74562	1.617160	118
O-O	-29.78787	-26.968969	-1.10322	-1.045913	1.70604	1.578311	103

B. Modified universal decay law (MUDL)

Qi *et al.*, in 2009 introduced a linearly Universal Decay Law formula establish a relationship between the half-lives of monopole radioactive decays with a Q-value of outgoing particles, the masses, and charges of the involved nuclei (Ni *et al*., 2008) which is given as:

$$Log_{10}T_{1/2} = aZ_\alpha Z_\alpha\sqrt{\frac{A}{Q_\alpha}} + b\sqrt{A\,Z_\alpha Z_d(A_\alpha^{\frac{1}{3}} + A_d^{\frac{1}{3}})} + c \quad \ldots\ldots\ldots (2)$$

Akrawy *et al.* (Akrawy *et al*., b2019) introduced modifications to the Universal Decay Law formula by incorporating two asymmetry–dependent terms (I and I^2), linearly correlated with the logarithm of alpha decay half-lives. The MUDL formula expressed as follows:

$$\log_{10}T_{1/2} = aZ_\alpha Z_d\sqrt{\frac{A}{Q_\alpha}} + b\sqrt{A\,Z_\alpha Z_d(A_\alpha^{\frac{1}{3}} + A_d^{\frac{1}{3}})} + c + dI + eI^2 \quad \ldots\ldots\ldots (3)$$

where $A = \frac{A_d A_\alpha}{A_d + A_\alpha}$, A_d, A_α represent the mass numbers of daughter nuclei and alpha particle, respectively. Z_α, Z_d are the atomic numbers of alpha particle and daughter nuclei and Q_α denotes the kinetic energy associated with alpha decay. The nuclear isospin asymmetry, denoted as $I = \frac{N-Z}{N+Z}$ is included. The parameters a, b, c, d, and e are the fitting parameters in equation (3), and, according to (Akrawy and Ahmed, 2019), their values are provided in (Table 2). A new set of coefficients (a, b, c, d and e) was obtained by applying a fitting process to equation (3) for the studied nuclei. The new resulting coefficients are provided in (Table 2), which contains the values of coefficients a, b, c, d, and e in both cases.

Table 2: The parameters of the MUDL formula according to (Akrawy and Ahmed, 2019) which are denoted as (a, b, c, d, and e) sub MUDL, and the new parameters of the MUDL formula obtained using Python software are denoted as (a, b, c, d, and e) sub Python.

Types, No Nuclei	a_{MUDL}	a_{Python}	b_{MUDL}	b_{Python}	c_{MUDL}	c_{Python}	d_{MUDL}	d_{Python}	e_{MUDL}	e_{Python}
E-E 152	0.41149	0.5903861	-0.42047	0.61152099	-22.89310	-22.73360	12.13020	9.47471	-44.60575	-35.59474
E-O 120	0.42832	0.626297	-0.44351	-0.6432133	-21.03859	-24.94530	-32.10386	14.98806	157.46876	-22.23498
O-E 118	0.45338	0.5836836	-0.39386	-0.5272918	-28.39745	-24.33619	-1.84615	-13.72705	-3.60637	43.64793
O-O 103	0.43126	0.5601744	-0.43322	-0.5559845	-22.97594	-21.93931	-12.91609	-3.58358	73.36209	33.37491

C. Modified Viola-Seaborg formula (MVS)

Viola and Seaborg introduced a comprehensive Geiger-Nuttall rule, serving as a novel empirical formula for the half-lives of alpha decay events as:

$$log_{10}T_{1/2} = \frac{aZ + b}{\sqrt{Q_\alpha}} + cZ + d \qquad \dots\dots\dots (4)$$

The Viola-Seaborg formula underwent further modification by incorporating of two asymmetry–dependent terms (I and I^2), linearly correlated with the logarithm of α-decay half-lives. The modified Viola –Seaborg formula MVS is given as (Viola and Seaborg, 1966):

$$\log_{10}T_{1/2} = \frac{aZ + b}{\sqrt{Q_\alpha}} + cZ + d + eI + fI^2 \qquad \dots\dots\dots (5)$$

Where $I = \frac{N-Z}{A}$ is the nuclear isospin asymmetry, N and Z are the neutron and proton number of parent nuclei, and Q_α is the decay energy in MeV, the half-lives is given in seconds and the parameters a, b, c, d, e and f are the fitting parameter obtained by fit the experimental data and according to (Akrawy *et al*., 2018) it given in the (Table 3), a new set of parameters for equation (5) will be obtained utilizing the method of least squares using Python software, similar to the procedure employed for equation (1). The parameters outcomes of this analysis are presented in the following (Table 3), which contains the values of parameters.

Table 3: The parameters of the MVS formula according to (Akrawy *et al*., 2018) which are denoted as (a, b, c, d, e, and f) sub MVS, and the new parameters of the MVS formula obtained using Python software are denoted as (a, b, c, d, e and f) sub Python.

Types, No	a_{MVS}	a_{Python}	b_{MVS}	b_{Python}	c_{MVS}	c_{Python}	d_{MVS}	d_{Python}	e_{MVS}	e_{Python}	f_{MVS}	f_{Python}
E-E 152	*1.5261*	*1.5262*	*5.6897*	*8.5123*	*-0.1743*	*-0.1745*	*-36.5424*	*-37.5219*	*6.0806*	*4.7981*	*-39.5819*	*-34.59426*
E-O 120	*1.9289*	*2.4185*	*-22.699*	*-64.2503*	*-0.3160*	*-0.4505*	*-23.7014*	*-14.8396*	*-44.5783*	*1.2927*	*181.8942*	*-4.46070*
O-E 118	*1.8671*	*1.3210*	*-9.2562*	*26.5589*	*-0.2240*	*-0.0797*	*-36.1423*	*-44.5446*	*-6.0006*	*-10.731*	*-5.2040*	*25.17959*
O-O 103	*1.7319*	*1.4346*	*-4.0943*	*9.7607*	*-0.2239*	*-0.1516*	*-33.2668*	*-36.2070*	*-24.0879*	*-7.5616*	*92.6876*	*33.21824*

RESULTS AND DISCUSION

In this research, the theoretically calculated logarithm alpha decay half-lives for a diverse set of 493 nuclei are grouped into the four categories of 152 (E-E), 120 (E-O), 118 (O-E), and 103 (O-O).

We employed three fundamental formulae to compute these theoretical values: The Royer formula, MUDL formula, and MVS formula. The results were meticulously compared to the experimental logarithm half-lives data, demonstrating a strong agreement. In order to improve the accuracy of our computation, we utilized a sophisticated fitting called least square method to adjust the parameter of each formula. This procedure entailed modifying the parameters using experimental data concerning the half-lives of alpha decay and Q_α which represents the energy released during the decay of alpha particle. The adjustment was performed utilizing least square method through the utilization of Python software. The original parameters and the new parameters for the Royer formula, MUDL formula, and MVS formula are specified in (Tables 1, 2, and 3) accordingly. Using recently optimized parameters, we computed the half-lives of alpha decay and compared them to the half-lives computed with parameters found in current literature (Akrawy *et al*., 2018; Akrawy *et al*., b2019; Akrawy and Ahmed, 2019). Notably, our optimized parameters exhibited a significantly improved agreement experimental data compared to the previously established parameters. For a quantitative assessment of this agreement, we computed the standard deviation (σ), for alpha decay half-lives to measure the consistency between theoretical prediction and experimental result.

The Standard Deviation (S.D) σ is given by:

$$\sigma = \sum_{i=1}^{N} \frac{\left|log_{10}T^{i}_{exp.} - log_{10}T^{i}_{theo.}\right|}{N} \quad \dots\dots\dots (6)$$

In the context of this study, N signifies the number of parent nuclei subjected to the emission of alpha particles. For the current investigation, N is equal to152 for (E-E), 120 for (E-O), 118 for (O-E), and 103 for (O-O).

The corresponding calculated values $log_{10}T^{i}_{theo.}$ and experimental. $log_{10}T^{i}_{exp.}$ decay half-lives, along with the Standard Deviation (σ), are represented for each set of (E-E), (E-O), (O-E), and (O-O) in (Table 4). The calculations were carried out using the Royer formula, MVS formula, and MUDL formula. Upon meticulous examination, it is observed that the S.D (σ) obtained from the three formulas, fall within acceptable ranges. Particularly notable is the superior performance of the S.D (σ) calculated with new parameters (S.D.cal), acquired through the least square method employing MATLAB and Python. This improvement is in stark contrast to those computed with parameters according to (Akrawy *et al*., 2018; Akrawy *et al*., b2019; Akrawy and Ahmed, 2019) . The improvement rate of the Standard Deviation can be quantified as follows:

$$Improvement\ Rate = \frac{\mathrm{Sta.re.} - \mathrm{Sta.calc}}{\mathrm{Sta.re}} \times 100 \quad \dots\dots\dots (7)$$

(Table 4) Using the parameters that we've collected, as well as the improvement percentage values for parameters according to (Akrawy *et al*., 2018; Akrawy *et al*., 2019; Akrawy and Ahmed, 2019) a comparison has been made between the Standard Deviations found in the model proposals.

Table 4: An assessment of the values of the standard deviation for the Royer formula, MVS formula, and MUDL formula utilizing the obtained parameters contrast to parameters according to (Akrawy *et al.*, 2018; Akrawy *et al.*, b2019; Akrawy and Ahmed, 2019), along with the corresponding percentage improvement values.

Type	Standard deviation of Royer according to Python			NO. Nuclei
	S.D. Cal.	Royer	Imp. rate	
E-E	0.377	0.378	0.26%	152
E-O	0.65	0.74	11.68%	120
O-E	0.56	0.66	14.66%	118
O-O	0.651	0.656	0.76%	103
Type	Standard deviation of MUDL according to Python			NO. nuclei
	S.D. Cal	MUDL	Imp. rate	
E-E	0.357	0.358	0.28%	152
E-O	0.63	1.25	48.90%	120
O-E	0.56	0.67	15.30%	118
O-O	0.64	0.67	3.84%	103
Type	Standard deviation of MVS according to Python			NO. nuclei
	MVS	S.D. cal	Imp. rate	
E-E	0.358	0.351	2.23%	152
E-O	0.59	1.26	52.74%	120
O-E	0.55	0.69	20.73%	118
O-O	0.63	0.69	7.25%	103

We have also calculated the ΔT difference between experimental and theoretical logarithm alpha-decay half-lives and plot the relationship of ΔT versus the neutron number, ΔT calculated by the following equation:

$$\Delta T = log_{10}T_{\frac{1}{2}}^{exp.} - log_{10}T_{\frac{1}{2}}^{cal.} \qquad \dots\dots\dots\dots (8)$$

The difference (ΔT) between the $experimental$ and theoretical values of alpha decay half-lives against the neutron (N) number for the 152 (E-E), 120 (E-O), 118 (O-E), and 103 (O-O) nuclei will be presented in Fig. (1). According to the Royer formula, MUDL formula, and MVS formula via Python program.

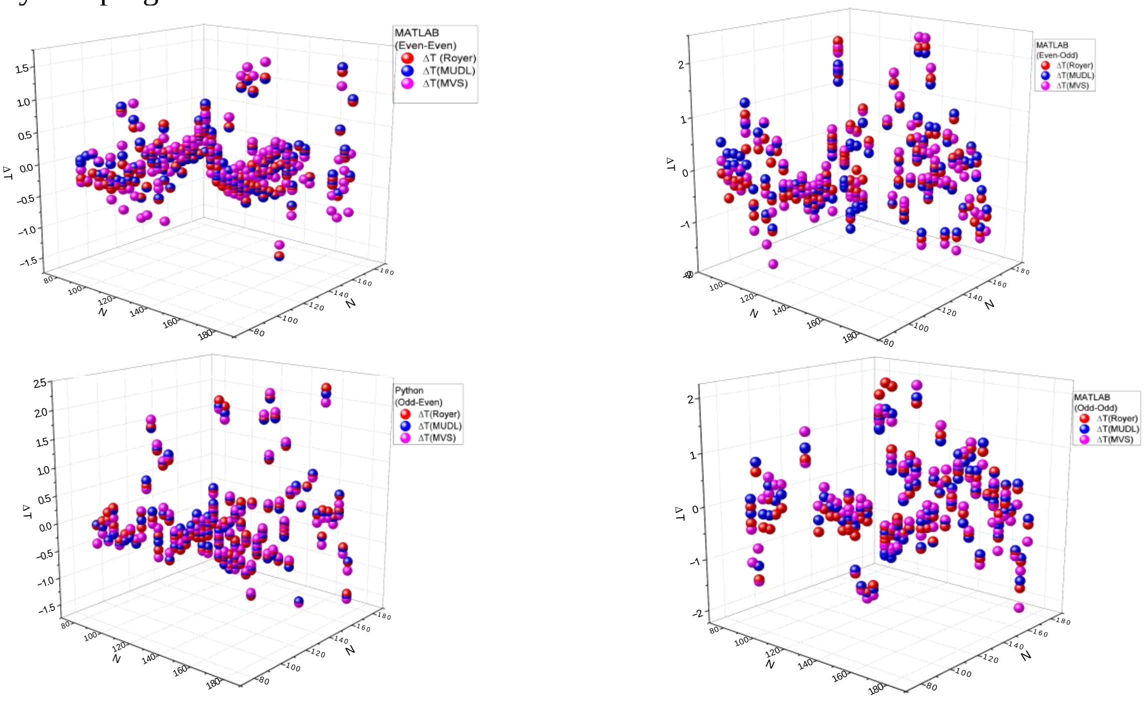

Fig. 1: The difference between experimental and theoretical alpha decay half-lives (ΔT) versus neutron number for the Royer formula, MUDL formula, and MVS formula, respectively, using the parameters obtained by Python software for a set of (E-E), (E-O), (O-E), and (O-O) nuclei.

Fig. (1) shows that for most of the sets of (E-E), (E-O), (O-E), and (O-O) nuclei, the result of ΔT difference between the theoretically calculated and experimental values of alpha decay half-lives shows an acceptable result. Additionally, it is known that the probability of adopting the formula increases with the value of ΔT proximity to zero, as demonstrated by the Royer formula, MUDL formula, and MVS formula.

The fitting curve between the experimental and theoretical values of the logarithm of half-lives for the studied nuclei.

The relationship between the logarithm of the experimental and theoretical values of alpha decay half-lives for the sets of 152 E–E, 120 E-O, 118 O-E, and 103 O-O nuclei will be presented in Fig. (2, 3, and 4) according to the Royer formula, MUDL formula and MVS formula via Python program.

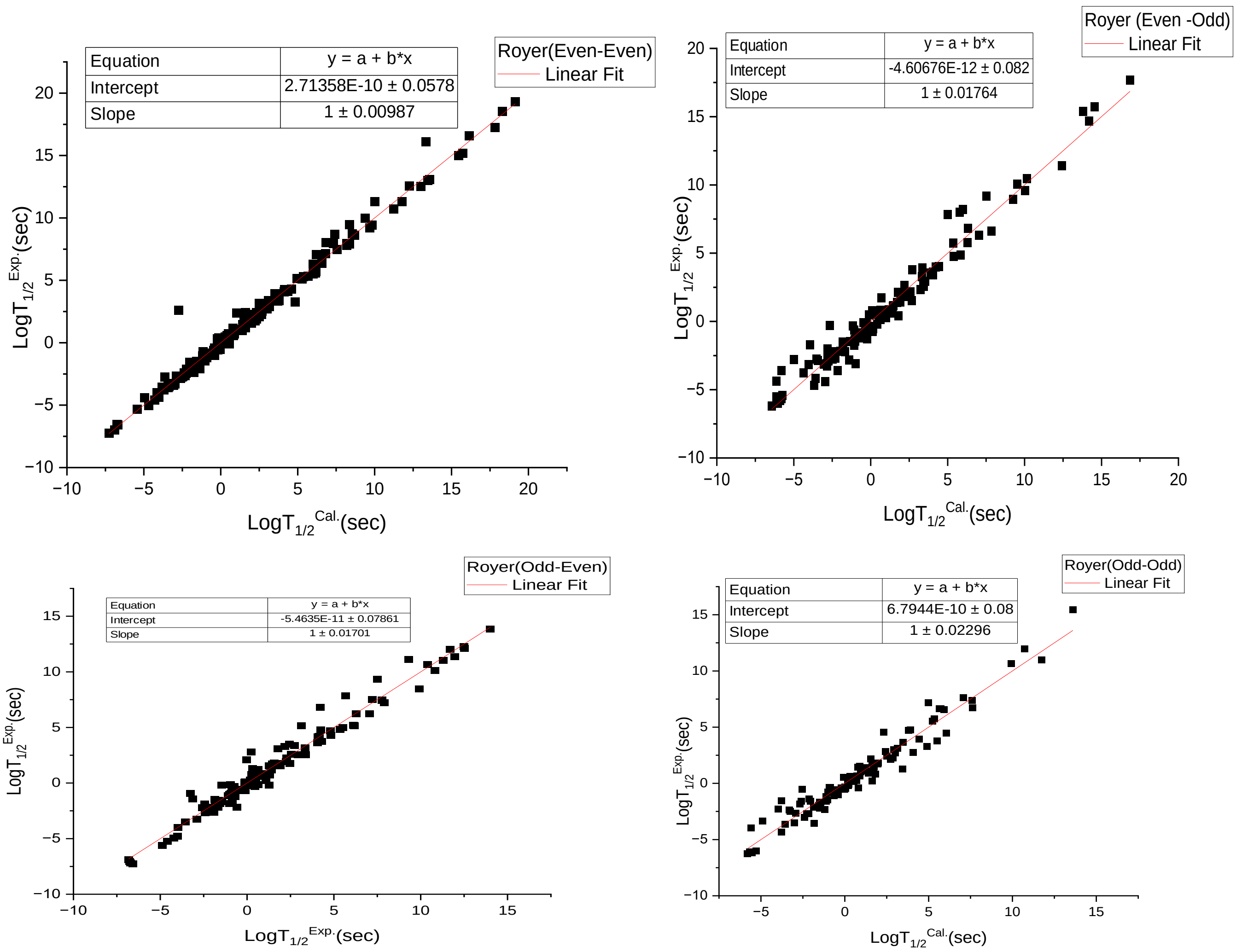

Fig. (2): The relationship between the logarithm of the experimental and theoretical values of alpha decay half-lives for the sets of 152 (E-E), 120 (E-O), 118 (O-E) and 103 (O-O) nuclei according to the Royer formula via Python program.

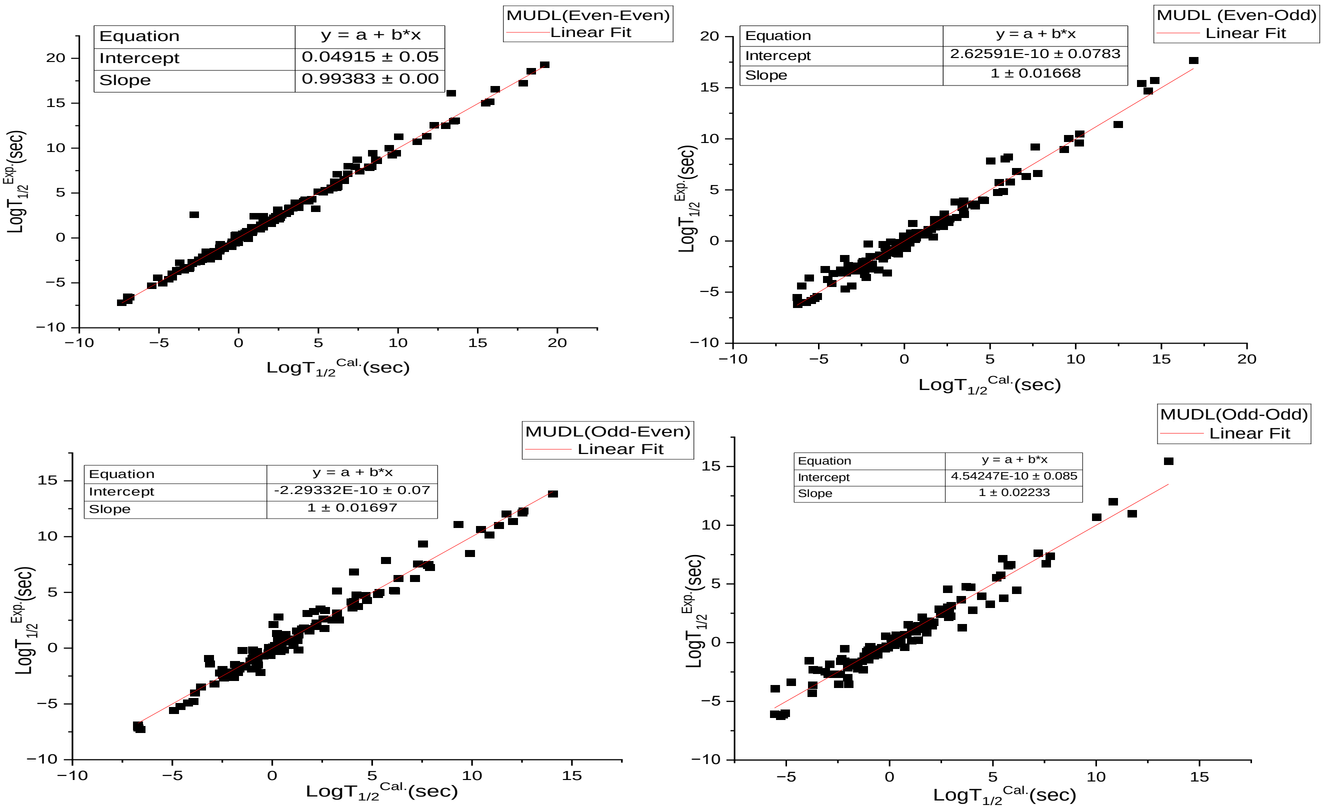

Fig. 3: The relationship between the logarithm of the experimental and theoretical values of alpha decay half-lives for the sets of 152 (E-E), 120 (E-O), 118 (O-E), and 103 (O-O) nuclei according to the MUDL formula via Python program.

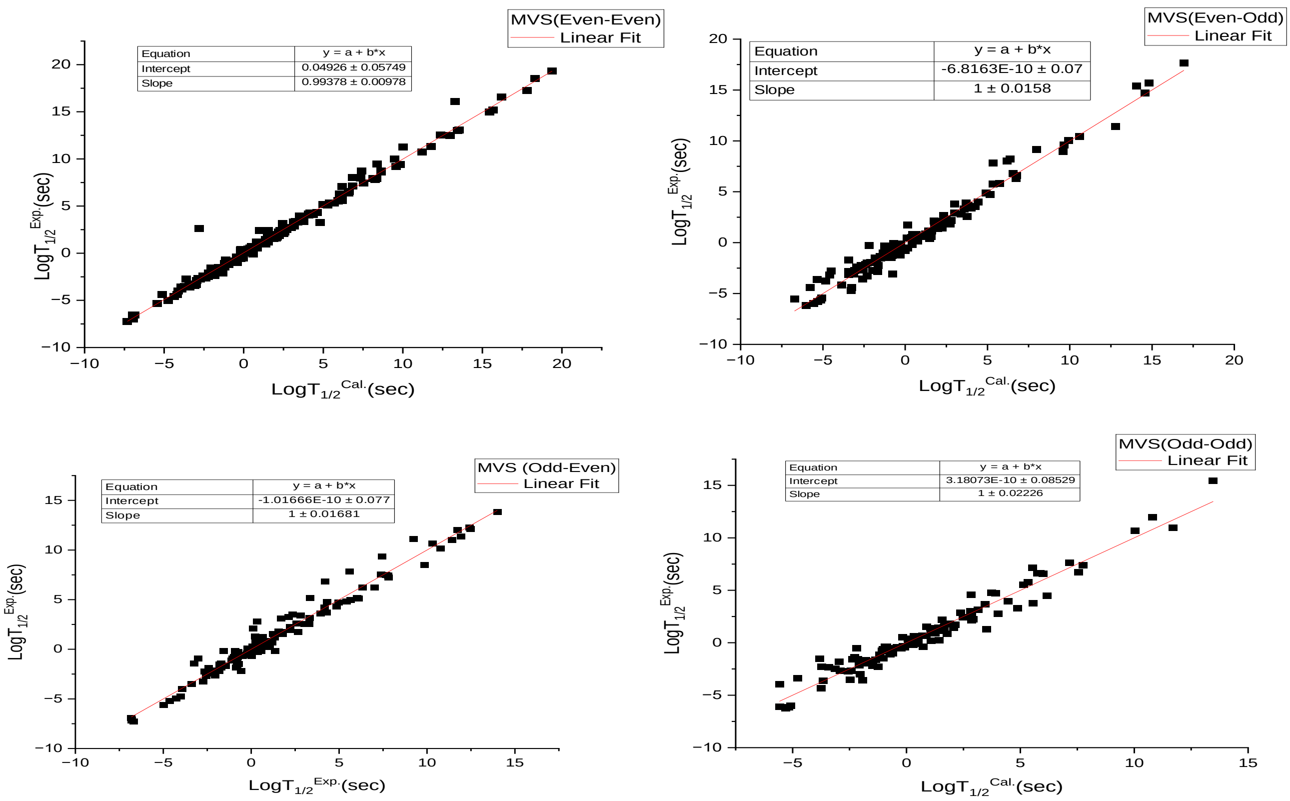

Fig. 4: The relationship between the logarithm of the experimental and theoretical values of alpha decay half-lives for the sets of 152 (E-E), 120 (E-O), 118 (O-E), and 103 (O-O) nuclei according to the (MVS) formula via Python program.

Fig. (2, 3, and 4) shows the relationship between the logarithm of the experimental and theoretical values of alpha decay half-lives for the sets of 152 (E-E), 120 (E-O), 118 (O-E), and 103 (O-O) nuclei according to the Royer formula, MUDL formula, and MVS formula and from the value of slope it is clear that there is a good agreement between the logarithm of the experimental and theoretical values of alpha decay half-lives.

CONCLUSIONS

An improved set of empirical expressions of the Royer formula, MVS formula, and MUDL formula have been established to calculate the alpha decay half-lives for the sets of (E-E), (E-O), (O-E), and (O-O) nuclei through obtained a new fitting parameters by least square fitting method for the 493 nuclei using Python software. The results of the calculated alpha decay half-lives and those of the corresponding experimental ones show a good agreement over the studied sets of nuclei. The standard deviation and improving rate of each formula have been obtained as mentioned previously. It shows that the standard deviation of the logarithmic half-lives obtained with a new fitting parameter is better than that calculated by others. All the standard deviations appear within an acceptable range, and this means that there is a good agreement between experimental and theoretically calculated alpha decay half-lives. Also, we have plotted the difference between experimental and theoretical calculated half-lives (ΔT) versus Neutron number of parent nuclei (N). A closer approach to zero in the difference between the logarithm of the experimental and theoretical half-life is recognized. Additionally, we have plotted the relationship between the logarithm of the experimental and theoretical values of alpha decay half-lives for all sets of nuclei and calculating the slope, which implies a higher likelihood of adopting the formula from the value of slope, as it is known the closer the slope values are to unity, the greater the accuracy of the formula. This means that we can predict values with greater precision using this formula in our scientific calculations. This observation is evident in the Royer and MUDL formulae. Regarding the MVS formula, it has also yielded reasonably acceptable results.

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تحديث لعلاقة كايكر_نوتال لتحديد نصف عمر النوى الثقيلة باستخدام طريقة المربع الأصغر

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الملخص

في هذه الدراسة، تم استخدام مجموعة من الصيغ التجريبية مثل صيغة روير (Royer formula)، وصيغة قانون الانحلال العالمي المعدل (MUDL)، وصيغة فيولا–سيبورغ المعدلة (MVS) لحساب أعمار النصف للنوى الثقيلة وفائقة الثقل التي أعداد البروتونات Z تقع في النطاق $67 \leq Z \leq 118$. تم اقتراح معلمات ملائمة جديدة لهذه الصيغ ووصفها بشكل مثالي للصيغة Royer وMUDL وMVS، على التوالي. تم إيجاد المعلمات باستخدام طريقة المربع الأصغر باستخدام Python. تم بعد ذلك مقارنة نصف عمر انحلال ألفا المحسوب نظريةً بالبيانات التجريبية اظهرت اختلاف بسيط. وتستخدم العمليات الإحصائية، بما في ذلك الانحراف المعياري والمقارنة بين فترات نصف العمر المقدرة نظريًا والمرصودة تجريبيًا، لهذا الغرض. كما يهدف منحنى المعايرة إلى الحصول على دقة القيم التجريبية والنظرية لنصف العمر.

الكلمات الدالة: انحلال ألفا، العمر النصفي، علاقة كايكر_نوتال.