Recalculated Viola-Seaborg Coefficients for Partial Alpha Half-lives Based on AME2016

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1. Introduction

Theoretical models to predict various properties of Super Heavy Elements (SHE) are becoming more and more important as they provide inputs for designing experiments. SHE predominantly undergo alpha decay followed by spontaneous fission (SF). So, properties of alpha decay are studied using various macro-micro methods based on cluster model, generalized liquid drop model (GLDM) and Coulomb and proximity potential model (CPPM) to name a few [1]. It is customary to match the predictions of these models with those of empirical ones such as Viola-Seaborg formula (VSF) [3] and UNIV2 [4]. The main objective of this paper is to recalculate the VSF coefficients using the latest atomic mass evaluation (AME2016) data [5]. The VSF parameters were last calculated by Dong and Ren [6] in 2005 using AME2003, wherein they have not considered the fine-structure of alpha-decay. In this paper, we include the following:

1. Effect of intensity of alpha transitions occurring to various energy levels in the daughter, on determination of experimental partial alpha half-lives.
2. Electron screening correction for determination of alpha-decay energies [7].

2. Background

2.1. Geiger-Nuttel Law

The empirical relationship between partial alpha half-life of isotopic nuclei \( T_{1/2}^a \) and alpha decay energies \( Q_a \) has been established by Geiger-Nuttel (GN) in 1911 as

\[
\log_{10} T_{1/2}^a = \frac{A_Z}{Q_a} + B_Z
\]

where \( T_{1/2}^a \) is determined from experimental data as

\[
T_{1/2}^a = \frac{T_{1/2}}{B.R.}
\]

Here, \( T_{1/2} \) (sec) is total half-life due to all possible decay channels. B.R. is branching ratio for alpha-decay. \( Q_a \) is obtained by taking difference between rest mass of parent and rest masses of daughter and He nuclei. It is expressed in MeV and is given by

\[
Q_a = M(Z, A) - M(Z - 2, A - 4) - M(^4He)
\]

All the half-lives for a given isotopic sequence for different parent nuclei, identified by atomic number \( Z \), are observed to fall on straight lines with slope \( A_Z \) and intercept \( B_Z \).
2.2. Viola-Seaborg Formula

It was observed by Viola and Seaborg that the straight lines resulting from GN-law, when plotted on a single graph, are almost parallel to each other. In 1966, they proposed the Viola-Seaborg formula (VSF), given by

$$\log_{10} T_{1/2} = \frac{aZ+b}{\sqrt{Q_a}} + (cZ + d) + h_{\text{log}} \tag{4}$$

where $h_{\text{log}}$ is a set of constants to compensate for the hindrance factor $HF$. For all odd-A and odd-odd nuclei, the logarithmic partial half-lives calculated using $a$, $b$, $c$, $d$ coefficients of VSF are subtracted from experimental $T_{1/2}$ values to obtain the absolute error. The mean of these absolute errors give the corresponding $h_{\text{log}}$ constants for oddZ-oddN, oddZ-evenN and evenZ-oddN nuclei.

2.3. VSF with Fine-Structure of $\alpha$-Transitions

In case of gs-gs transitions of even-even nuclei, which are considered to be due to barrier penetration without change in angular momentum between parent and the daughter nuclei, the value of $HF = 1$. In case of odd-A and odd-odd nuclei, the favored transition is to one of the excited states of the daughter for which there is no angular momentum change and $HF$ is defined as ratio of experimental partial alpha half-life to that obtained using a semi-empirical formula (SEF) such as VSF without $h_{\text{log}}$.

2.3.1. Contribution from Electron Screening

The VSF is further fine tuned by considering the electron screening correction term which is responsible for the decrease in the alpha-particle energy by about 30 — 40 keV in heavy elements. This electron screening energy could be a result of

a) alpha particle having to do work against Coulomb attractive force due to electrons.

b) loss in total electron binding energy due to reduction of charge of parent nucleus from $Z$ to $Z-2$.

The electron screening energy as discussed in Rasmussen[7], is given by

$$\Delta E_{\text{SC}} = \left(6.5 \times 10^{-5}\right) Z_0^{2/5} MeV \tag{5}$$

where $Z_0 = Z - 2$, is the atomic number of daughter nucleus. $Q_a$ is replaced by effective alpha energy $E_a^*$ which is

$$E_a^* = \frac{A}{A-4} E_a + \Delta E_{\text{SC}} \tag{6}$$

where $E_a$ is the alpha transition energy to a particular level and $A$ is mass number of parent.

2.3.2. Effect of Intensity on $T_{1/2}^\alpha$

The partial alpha half-life needs to be determined accordingly by taking into account intensity of a particular transition. Since intensities of all alpha transitions to various energy levels add up to 1, the partial alpha half-life is determined as

$$T_{1/2}^\alpha = \frac{T_{1/2}}{BR} \left( \frac{I_\alpha}{100} \right) \tag{7}$$

3. Results and Discussion

In this paper, 54 even-even nuclei between $Z = 84$ to 102 with $N > 126$ have been considered to fit parameters $a$, $b$, $c$ and $d$ of Viola-Seaborg formula. To determine $h_{\text{log}}$ constants that improve the estimates for (odd-Z)-(odd-N) and odd-A nuclei, 30(even-odd), 28(odd-even) and 21(odd-odd) nuclei have been selected in the same range $Z = 84-102$. First the constants $A_z$ and $B_z$ have been determined (See Table 1) by plotting the logarithmic partial half-lives w.r.t. $E_a^* / (A-4) MeV$ for each of the isotopic sequences of even-even nuclei from 84-102 and fitting regression lines (See Figure 1).

![Figure 1](image-url)

Figure 1: Plot of $\left( E_a^* \right)^{1/2}$ vs log10($T_{1/2}^\alpha$).

Then, plots of $Z$ vs $A_z$ and $Z$ vs $B_z$, shown in Figure 2, for $Z = 84-102$ are utilised to obtain the VSF coefficients as

$$a = 1.64716, b = -8.13612, c = -0.19889, d = -33.66033 \tag{8}$$
Table 1: The slopes $A_z$ and intercepts $B_z$ of the regression lines for different isotopic sequences for $Z = 84-102$.

| $Z$ | 84  | 86  | 88  | 90  | 92  | 94  | 96  | 98  | 100 | 102 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| $A_z$ | 126.3031 | 134.7425 | 136.7015 | 141.4036 | 145.2525 | 149.3953 | 150.9348 | 152.8324 | 153.1397 | 159.7910 |
| $B_z$ | -48.7407 | -51.3337 | -51.1137 | -52.0811 | -52.7002 | -53.4259 | -53.0363 | -53.0261 | -52.2856 | -53.8316 |

Figure 2: Plot $Z$ vs $A_z$, $Z$ vs $B_z$ to obtain VSF coefficients $a$, $b$, $c$ and $d$.

Then, similar plots (not shown) for $Z = 86-98$ have been used to determine another set of VSF coefficients as

$$a_1 = 1.62014, \quad b_1 = -4.58699,$$

$$c_1 = -0.18335, \quad d_1 = -35.52030. \quad (9)$$

These sets of coefficients are utilised to obtain the logarithmic half-lives of all available even-even nuclei in the test region with $Z = 103-118$ and the data is presented in Table 2.

Table 2: The logarithms of half-lives of 8 even-even nuclei calculated from the Viola-Seaborg formula with new parameters using data set $Z=84-102$. The experimental data is taken from the NUBASE2016 evaluation of nuclear properties by Audi et al. [5].

| Nuclei | $T_{\text{exp.}}^{\text{2016}}$ | $T_{\text{VS}}^{\text{2016}}$ | %error | $T_{\text{VS}}^{\text{2005}}$ | %error |
|--------|-----------------|-----------------|--------|-----------------|--------|
| 256Rf  | -2.1759         | 0.1299          | 105.9699 | 0.126 | 105.7907 |
| 260Sg  | -2.3054         | -1.9594         | 15.0082 | -1.999 | 13.2905 |
| 264Hs  | -3.2676         | -3.0961         | 5.2485  | -3.07  | 6.0473  |
| 266Hs  | -2.52           | -2.4506         | 2.7540  | -2.434 | 3.4127  |
| 270Ds  | -3.6882         | -3.9253         | 6.4286  | -3.906 | 5.9053  |
| 286Fl  | -0.8539         | -0.638          | 25.2840 | -0.576 | 32.5448 |
| 290Lv  | -2.0969         | -1.7027         | 18.7992 | -1.639 | 21.8370 |
| 294Og  | -2.9393         | -3.1717         | 7.9066  | -2.986 | 1.5888  |

Then, using these sets of co-efficients in VSF, the theoretical half-lives for the selected odd-A and odd-odd nuclei have been determined. These were subtracted from the experimental half-lives to determine the error in each case. The mean of these absolute errors have given rise to the constants $h_{\log}$ as follows:

$$h_{\log} = \begin{cases} 0; & \text{(even-Z,even-N)} \\ 0.8054 \pm 0.1872; & \text{(even-Z,odd-N)} \\ 0.5493 \pm 0.1505; & \text{(even-Z,odd-N)} \\ 0.9749 \pm 0.2176; & \text{(even-Z,odd-N)}. \end{cases} \quad (10)$$

Case i Set of parameters considering even-Z, even-N nuclei from $Z = 84-102$

Case ii Set of parameters considering even-Z, even-N nuclei from $Z = 86-98$
Now, these sets of VSFs need to be tested for their effectiveness by determining the logarithmic partial alpha half-lives of nuclei in the region $Z = 103-118$. Further, these formulae are utilised to estimate the half-lives for SHE isotopes of $Z = 121$ and 122. In order to verify the agreement of theoretical half-lives with experimental data, mean deviation and standard deviation are defined as follows:

$$\text{The mean absolute deviation is}$$

$$<\sigma> = \frac{\sum_{i=1}^{N} |\log_{10} \left( \frac{T_{\exp}}{T_{cal}} \right)|}{N}$$  \hspace{1cm} (12)$$

The standard deviation is

$$\sqrt{\sigma^2} = \sqrt{\frac{\sum_{i=1}^{N} \left( \log_{10} \left( \frac{T_{\exp}}{T_{cal}} \right) \right)^2}{N}}$$  \hspace{1cm} (13)$$

The values of mean absolute deviation and standard deviation for data set $Z = 84-102$ ($Z = 86-98$), test data $Z = 103-118$ and estimated half-lives of Superheavy elements ($Z = 121,122$) are listed in Table 3.

Table 3: The mean deviation and standard deviation for data $Z = 84 - 102$ ($Z = 86 - 98$), Test data $Z = 103 - 118$ and for estimated half-lives for Super Heavy Elements ($Z = 121,122$).

| Nuclei type | Sample Data $Z = 84-102$ ($Z = 86-98$) | Test data $Z = 103-118$ using $Z = 84-102$ ($Z = 86-98$) | Estimated half-live for $Z = 121,122$ using $Z = 84-102$ ($Z = 86-98$) |
|-------------|-------------------------------------|-------------------------------------------------|-------------------------------------------------|
|             | $\sigma$ | $\sqrt{\sigma^2}$ | $\sigma$ | $\sqrt{\sigma^2}$ | $\sigma$ | $\sqrt{\sigma^2}$ |
| even Z, even N | 0.1025 (0.0655) | 0.1352 (0.1111) | 0.1913 (0.1920) | 0.2228 (0.2271) | 0.2968 (0.1892) | 0.3229 (0.2280) |
| even Z, odd N | 0.7553 (0.8866) | 0.7875 (0.9332) | 0.5389 (0.5837) | 0.6283 (0.7724) | 0.5786 (0.7899) | 0.5910 (0.7990) |
| odd Z, even N | 0.6088 (0.7320) | 0.7702 (0.8690) | 0.5803 (0.6326) | 0.6236 (0.8184) | 0.3367 (0.5383) | 0.3489 (0.5457) |
| odd Z, odd N | 0.8620 (0.9066) | 0.9109 (0.9516) | 0.6347 (0.6048) | 0.7321 (0.7498) | 0.6889 (0.7762) | 0.6890 (0.7763) |

From Table 3, one can observe that data for 54 even-even nuclei have mean deviation of 0.1025(0.0655) and standard deviation of 0.1352(0.1111), respectively. This means that the VSF with obtained parameters reproduce the experimental data of even-even nuclei on an average within a factor of 1.4 for $Z = 84-102$ set (and 1.3 for $Z = 86-98$ set). For 30 even-odd, 28 odd-even and 21 odd-odd nuclei, on average the half-life from formula agrees with experimental data within a factor of 6.1(8.6), 5.9(7.4) and 8.2(9.0) respectively. The mean deviations and the standard ones of odd-A nuclei are relatively smaller than those of odd-odd nuclei.

Table 4: Number of nuclei in test data ($Z = 103 - 118$) that fall under various %-error regions for half-live obtained using $Z = 84 - 102$ ($86 - 98$).

| Nuclei type | Number | Mean %error 84-102(86-98) |
|-------------|--------|--------------------------|
|             |        | <5% | 5% - 10% | 10% - 20% | >20% |
| E-E         | 8      | 3(1) | 2(3) | 2(1) | 1(3) |
| E-O         | 12     | 2(0) | 2(3) | 0(1) | 8(8) |
| O-E         | 15     | 1(0) | 2(3) | 2(2) | 10(10) |
| O-O         | 30     | 0(1) | 3(1) | 3(4) | 24(24) |
In the last column of Table 3, we have estimated half-lives for Superheavy elements (Z = 121, 122). For even-even nuclei, the mean deviation and standard deviation are 0.2968(0.1892), 0.3229(0.2280), respectively resulting in average deviations with calculated half-lives using theoretical values from CPPM by a factor of 2.1(1.7). In case of odd nuclei, the average deviations range from 0.3367(0.5383) to 0.6889(0.7762). This means that on an average the half-life from formula agree with theoretical results of CPPM within a factor of 2-4(3-6) for odd nuclei. In case of even-odd, odd-even and odd-odd, half-life obtained with VSF parameters reproduce the theoretical values (CPPM) on an average within a factor of 3.9(6.3), 2.2(3.5) and 4.9(6.0) respectively. This clearly shows that parameters from all available even-even nuclei upto Z = 102 perform better.

Finally, we have presented the estimated half-lives in seconds units in comparision to those obtained from Coulomb and proximity potential model. It has been observed that half-life values, for isotopic sequences of Z = 121 and 122, using VSF with recalculated coefficients from AME2016 data are on a higher side as compared to those obtained from AME2003 data. This takes these values even farther away from the theoretical values using CPPM. One has to check how the other empirical formulae such as UNIV2 and GLDM would change with this new evaluation.

Table 5: Comparison of estimated half-lives from Viola-Seaborg with that theoretical results from CPPM [1, 2] (84-102).

| Z = 121 (odd Z-even N) | Z = 121 (odd Z-odd N) | Z = 122 (even Z-even N) | Z = 122 (even Z-odd N) |
|------------------------|------------------------|------------------------|------------------------|
| A(P)                   | T^α_{1/2}              | T^α_{1/2}              | A(P)                   | T^α_{1/2}              | T^α_{1/2}              | A(P)                   | T^α_{1/2}              | T^α_{1/2}              |
| 309                    | 0.0402                 | 0.0402                 | 310                    | 39.9                   | 308                    | 13.4                   | 34.8                   | 307                    | 49.2                   | 11.1                   |
| 311                    | 19.6                   | 10.4                   | 312                    | 80.3                   | 310                    | 45.2                   | 66.1                   | 309                    | 156                    | 35.1                   |
| 313                    | 49.3                   | 26.4                   | 314                    | 378                    | 312                    | 159                    | 238                    | 311                    | 539                    | 121                   |
| –                     | –                      | –                      | –                     | –                      | –                     | –                      | –                      | –                     | –                      | –                     |
| 314                    | 644                    | 1740                   | 313                    | 2030                   | 867                   |

Conclusion

Using least-square fit for logarithmic half-lives w.r.t (E_a)\(^{1/2}\) of even-even nuclei between Z = 84-102 (86-98), we have obtained new parameters for the Viola-Seaborg formula. With these parameters, obtained half-lives match very well with experimental ones for even-even nuclei between Z = 84-102. Then, these parameters are used for test data between Z = 103 - 118 and are found to be in agreement with experimental half-lives. Finally, a comparision of estimated half-lives of SHE (Z = 121,122) with theoretical results obtained by Coulomb and proximity potential model (CPPM) results have been found to be comparable. We hope that these new coefficients would help for making comparisions while proposing new theoretical formulations.

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