NUCL SCI TECH (2020) 31:9
https://doi.org/10.1007/s41365-019-0718-8

Bethe–Weizsäcker semiempirical mass formula coefficients 2019 update based on AME2016

Djelloul Benzaid[1] · **Salaheddine Bentridi**[1] · **Abdelkader Kerraci**[1] · **Naima Amrani**[2]

Received: 26 September 2019 / Revised: 13 November 2019 / Accepted: 18 November 2019 / Published online: 3 January 2020

Abstract In the present work, the classical Bethe–Weizsäcker (BW) mass formula with five energy terms is revisited and updated. We use the least-squares adjustments on the binding energy of 2497 different nuclides from the last update of the atomic mass evaluation, AME2016 published in March 2017, to provide a new set of energy coefficients of the mass formula. The obtained set of formula coefficients allowed us to reproduce most of the experimental values of the binding energies for each nucleus with $A \geq 50$. The comparison between the binding energies provided with updated mass formula and those of AME2016 on the one hand, and those of previous works, on the other hand, yields relative errors that oscillate between less than 0.05% and 1.5%. The revisited BW formula is in very good agreement with the experimental data.

Keywords Binding energy of atomic nuclei · Mass formula coefficients · AME2016 · Least-squares adjustments

✉ Djelloul Benzaid
d.benzaid@univ-dbkm.dz

[1] Laboratory of Energy and Smart Systems, University of Khemis Miliana, Route de Theniet El Had, 44225 Ain Defla, Algeria

[2] Dosing, Analysis and Characterization in High Resolution Laboratory, Physics Department, Faculty of Sciences, Ferhat ABBAS University, 19000 Sétif-1, Algeria

1 Introduction

The semiempirical mass formula (SEMF), usually known as Bethe–Weizsäcker formula, has been developed to most effectively describe the binding energy of any given nucleus at the ground level. In the classical expression, the binding energy is represented as a function of atomic number Z, neutron number N and mass number $A = Z + N$, using five energy coefficients. Each energy coefficient represents an aspect of the binding energy in the liquid-drop model of the nucleus. Considered to be a spherical-like volume with a radius defined as $R = r_0 A^{\frac{1}{3}}$, the stability of the nucleus is based mainly on its volume energy term as a contribution of each nucleon to nuclei cohesion. According to the adopted model, negative contributions should be considered and therefore subtracted from the cohesion component, namely surface tension term, electrical repulsion term (Coulombian term) and asymmetrical term. The contribution of the parity term is given as a delta function of the parity values of both Z and N, and it may be a negative, null or positive contribution. Except for the Coulombian coefficient which may be obtained by analytical calculations ($a_c \approx 0.7$ MeV), the remaining energy coefficients are obtained via experimental data from nuclear reactions, resulting in updated nuclear mass data. Using these data, one may deduce a set of the energy coefficients of the Bethe–Weizsäcker (BW) mass formula using numerical methods. The aim of the present work is to obtain a new set of energy coefficients (including the Coulombian coefficient used as the coherence referring term) based on an update of the nuclear masses table (AME2016), which was processed using numerical code that we developed based on the least-squares adjustments method.

It is evident that the SEMF is attracting research interest in terms of improving the results obtained by the formula given in the next section by Eq. 1. In this work, we have chosen some references based on the same topic. The selection of these references is based mainly on the form of the formula itself. In this regard, we have adopted the classical form to investigate the validity of our results, as well as possible improvements with the evolution of atomic mass evaluation.

Even the classical BW mass formula is not considered as the complete expression to provide the binding energy for a given nucleus. This semiempirical formula is a good indicator for first-level precision of calculations involving binding energy, especially to exclude heavy nuclei stability. In addition, the BW mass formula is still a fundamental keystone in nuclear physics with respect to teaching and research. The update of the energy coefficients for each term may also be adopted for a new BW mass formula with quantum considerations and correction terms.

2 Bethe–Weizsäcker semiempirical mass formula

The first and most important formula for the binding energy of the nucleus was developed by Von Weizsäcker [1] under the main assumption that the nucleus can be considered as a droplet of incompressible matter. The droplet is maintained by the strong nuclear interaction that exists between nucleons. This fundamental short-range force is considered to be spin-independent and charge-independent.

The binding energy B is made up of five terms, each of which describes a particular characteristic of the nucleus [2], namely volume energy, surface energy, Coulomb energy, asymmetry energy and pairing energy. The binding energy formula is given as follows:

$$
\begin{aligned}
{}^{A}_{Z}B = {} & a_v A - a_s A^{2/3} - a_c \frac{Z^2}{A^{1/3}} - a_a \frac{(A-2Z)^2}{A} \\
& + \delta a_p \frac{1}{A^{1/2}},
\end{aligned}
\tag{1}
$$

where a_v, a_s, a_c, a_s, a_a and a_p are taken as constant coefficients of the formula. It should be noted that the pairing term is taken as $a_p/A^{1/2}$ in the present study [3, 4].

3 Least-squares adjustments method

The proposed method involved minimizing the quantity χ^2 given by [5] :

$$
\begin{aligned}
& \chi^2(a_v, a_s, a_c, a_a, a_p) \\
& = \sum_{i=1}^{n} \left[E_i - {}^{A_i}_{Z_i} B(a_v, a_s, a_c, a_a, a_p) \right]^2,
\end{aligned}
\tag{2}
$$

where n is the number of nuclides, E_i are experimental values of binding energy of the nuclei and B_i are the ones given by the mass formula (1).

Let us recall that for a multivariable function such as $f = f(x, y, z\ldots)$ to be at a relative minimum or maximum, three conditions must be met: The first derivative must admit a critical point $(a, b, c\ldots)$; when evaluated at this point, the second-order direct partial derivatives must be positive for a minimum and negative for a maximum.

In our case, the first derivative of χ^2 defined by (2) gives

$$
\frac{\partial \chi^2}{\partial a_v} = 0, \frac{\partial \chi^2}{\partial a_s} = 0, \frac{\partial \chi^2}{\partial a_c} = 0, \frac{\partial \chi^2}{\partial a_a} = 0 \text{ and } \frac{\partial \chi^2}{\partial a_p} = 0. \tag{3}
$$

The second derivative is applied to determine whether the function is concave up (a relative minimum) or concave down (a relative maximum):

$$
\frac{\partial^2 \chi^2}{\partial a^2} > 0 \text{ or } = 0 \text{ or } < 0. \tag{4}
$$

We then obtain:

$$\begin{pmatrix} \sum_{i=1}^{n} A_i^2 & -\sum_{i=1}^{n} A_i^{5/3} & -\sum_{i=1}^{n} Z_i^2 A_i^{2/3} & -\sum_{i=1}^{n} (A_i - 2Z_i)^2 & +\sum_{i=1}^{n} \delta_i A_i^{1/2} \\ \sum_{i=1}^{n} A_i^{5/3} & -\sum_{i=1}^{n} A_i^{4/3} & -\sum_{i=1}^{n} Z_i^2 A_i^{1/3} & -\sum_{i=1}^{n} \frac{(A_i - 2Z_i)^2}{A_i^{1/3}} & +\sum_{i=1}^{n} \delta_i A_i^{1/6} \\ \sum_{i=1}^{n} Z_i^2 A_i^{2/3} & -\sum_{i=1}^{n} Z_i^2 A_i^{1/3} & -\sum_{i=1}^{n} \frac{Z_i^4}{A_i^{2/3}} & -\sum_{i=1}^{n} \frac{Z_i^2 (A_i - 2Z_i)^2}{A_i^{4/3}} & +\sum_{i=1}^{n} \frac{\delta_i Z_i^2}{A_i^{5/6}} \\ \sum_{i=1}^{n} (A_i - 2Z_i)^2 & -\sum_{i=1}^{n} \frac{(A_i - 2Z_i)^2}{A_i^{1/3}} & -\sum_{i=1}^{n} \frac{Z_i^2 (A_i - 2Z_i)^2}{A_i^{4/3}} & -\sum_{i=1}^{n} \frac{(A_i - 2Z_i)^4}{A_i^2} & +\sum_{i=1}^{n} \frac{\delta_i (A_i - 2Z_i)^2}{A_i^{3/2}} \\ \sum_{i=1}^{n} \delta_i A_i^{1/2} & -\sum_{i=1}^{n} \delta_i A_i^{1/6} & -\sum_{i=1}^{n} \frac{\delta_i Z_i^2}{A_i^{5/6}} & -\sum_{i=1}^{n} \frac{\delta_i (A_i - 2Z_i)^2}{A_i^{3/2}} & +\sum_{i=1}^{n} \frac{\delta_i^2}{A_i} \end{pmatrix}$$

$$\begin{pmatrix} a_v \\ a_s \\ a_c \\ a_a \\ a_p \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^{n} A_i E_i \\ \sum_{i=1}^{n} A_i^{2/3} E_i \\ \sum_{i=1}^{n} \frac{Z_i^2 E_i}{A_i^{1/3}} \\ \sum_{i=1}^{n} \frac{(A_i - 2Z_i)^2 E_i}{A_i} \\ \sum_{i=1}^{n} \frac{\delta_i E_i}{A_i^{1/2}} \end{pmatrix} \quad (5)$$

The obtained system is a set of linear equations with five variables a_v, a_s, a_c, a_a and a_p. The system was solved using Gauss's method [6], which was implemented in a proprietary code that we developed. The algorithm consists of three main steps: a. reading the data for the nuclei from a file, b. calculating the different constant parameters of the system and c. solving it using Gauss's method.

4 Nuclear data used in this work

The history of the evaluation of atomic masses [7] over more than 5 decades, particularly from 1983 and 2017, has revealed that data are continuously improved in terms of not only quality and precision but also because the number of new nuclides is increasingly more important day in and day out, and this fact should be exploited by researchers.

The main document of this work is one of three important files, namely "The AME2016 atomic mass evaluation (I)" by W.J. Huang, G. Audi, M. Wang, F.G. Kondev, S. Naimi and X. Xu Chinese Physics C41 030002, March 2017; "The AME2016 atomic mass evaluation (II)" by M. Wang, G. Audi, F.G. Kondev, W.J. Huang, S. Naimi and X. Xu Chinese Physics C41 030003, March 2017 [8, 9], wherein the properties of 2497 nuclides are tabulated, in particular, the number of neutrons N, the number of protons Z, the mass number A and the experimental values of the binding energy EL/A (keV) given in keV. Additional parameters are also tabulated.

5 Results and discussion

The calculations performed using the dedicated code to solve the linear system (5) for all 2497 nuclides yielded the following values for the five coefficients of the mass formula:

$$\begin{aligned} a_v &= 14.9297 \text{ MeV (volume energy coefficient)} \\ a_s &= 15.0580 \text{ MeV (surface energy coefficient)} \\ a_c &= 0.6615 \text{ MeV (Coulomb energy coefficient)} \\ a_a &= 21.6091 \text{ MeV (asymmetry energy coefficient)} \\ a_p &= 10.1744 \text{ MeV (pairing energy coefficient)} \end{aligned} \quad (6)$$

However, if we consider only nuclides with $A \geq 50$, we

then use 2166 different isotopes, and the code gives the following values:

$$\begin{aligned} a_v &= 14.6433 \text{ MeV} \\ a_s &= 14.0788 \text{ MeV} \\ a_c &= 0.6442 \text{ MeV} \quad . \\ a_a &= 21.0680 \text{ MeV} \\ a_p &= 11.5398 \text{ MeV} \end{aligned} \tag{7}$$

Thus, the following empirical mass formula could be proposed:

$$\begin{aligned} {}^{A}_{Z}B = 14.64A - 14.08A^{2/3} - 0.64\frac{Z^2}{A^{1/3}} \\ - 21.07\frac{(A-2Z)^2}{A} \pm 11.54\frac{1}{A^{1/2}} \ . \end{aligned} \tag{8}$$

5.1 Comparison with tabulated data

Figure 1 represents a comparison of the binding energies per nucleon that were calculated using relationship (8) and those given by AME2016 [8, 9]. The calculated results were in good agreement with the data for the mass numbers $A \geq 50$. However, the figure shows some discrepancy for low masses, particularly in the region of $A \leq 20$.

A 3D plot is presented to facilitate a more suitable comparison in Fig. 2.

5.2 Comparison with previous works

Table 1 shows a compilation of different values of the coefficients that were calculated in previous works. An illustration of the most important ones, a comparison of our results with those of Ref. [4], is depicted in Fig. 3. It is

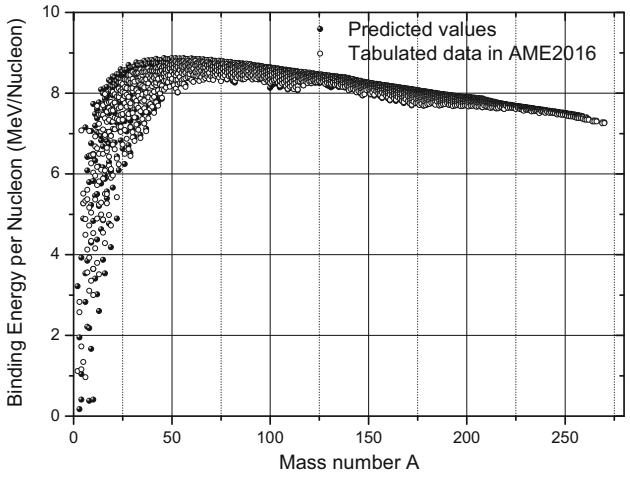

Fig. 1 Comparison of tabulated binding energy per nucleon data given by AME2016 [8, 9] versus those predicted using relationship (8)

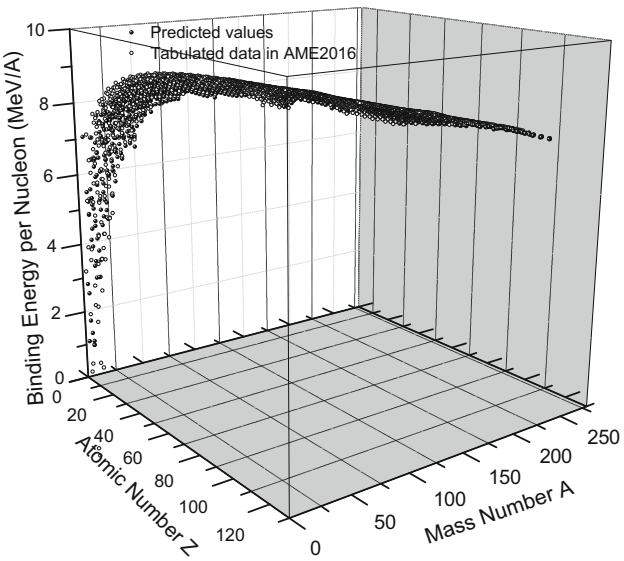

Fig. 2 3D comparison of tabulated binding energy per nucleon data given by AME2016 [8, 9] versus those predicted using relationship (8), as a function of Z and A

Table 1 Comparison of our values to those of previous works

Coefficients (MeV)	Years	a_v	a_s	a_c	a_a	a_p
Present work	2019	14.64	14.08	00.64	21.07	11.54
Ref. [10]	2018	19.12	18.19	00.52	12.54	28.99
Ref. [11]	2007	15.36	16.43	00.69	22.54	–
Ref. [4]	2005	15.78	18.34	00.71	23.21	12.00
Ref. [12]	2004	15.77	18.34	00.71	23.21	12.00
Ref. [13]	1996	16.24	18.63	–	–	–
Ref. [14]	1958	15.84	18.33	00.18	23.20	11.20

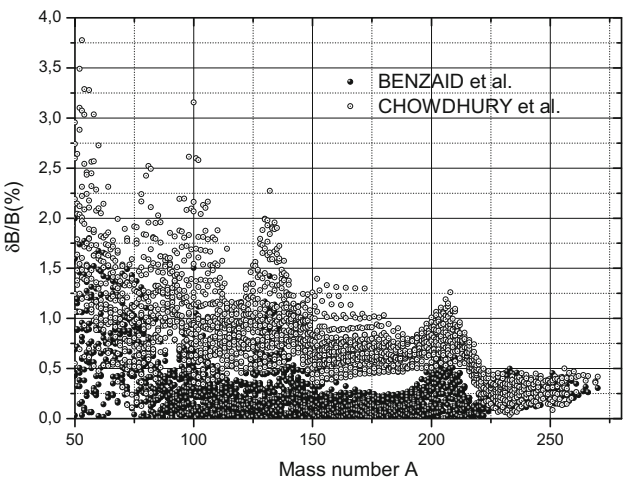

Fig. 3 Comparison of percentage error obtained using coefficients of Ref. [4] versus that obtained using those predicted in this work

Table 2 Different categories of percentage errors

$[A_1, A_2]$	$A < 20$	$20 \leq A \leq 40$	$40 \leq A \leq 50$	$50 \leq A \leq 140$	$140 \leq A \leq 200$	$A \geq 200$
$\frac{\lvert\delta B\rvert}{B}(\%)$	?	11%	4%	$\leq 1.5\%$	0.8%	Around 0.2%

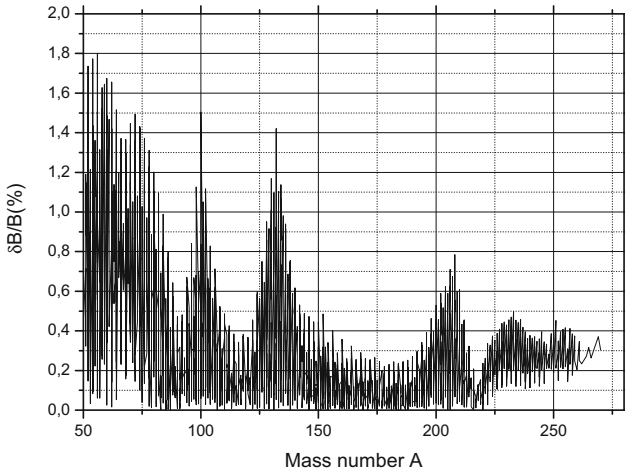

Fig. 4 Percentage error versus A

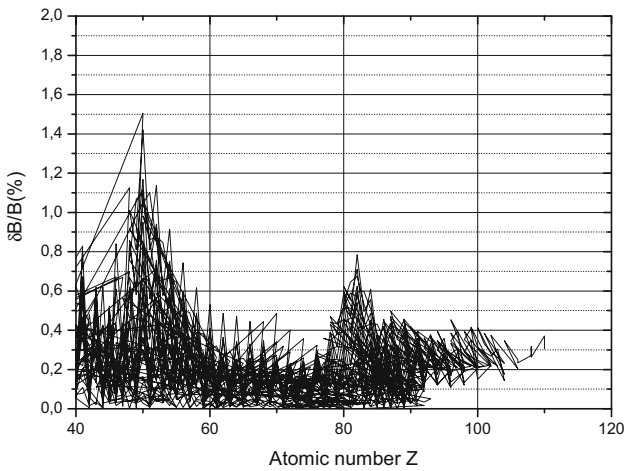

Fig. 5 Percentage error versus Z

important to note that in all references but Ref. [4], the forms of the SEMF that were adopted are slightly different from those that we used and those of Ref. [4], and as such, they cannot be used in the comparison under consideration.

It is evident from Fig. 3 that the binding energies of nuclei that are calculated using relationship (8) and our calculated coefficients are superior to those obtained using the same relationship and the coefficients of the cited references. However, any discrepancies observed in the same figure can be justified by considering that the data used in this work, i.e., AME2016, are more recent than those used in Ref. [4], i.e., AME2013.

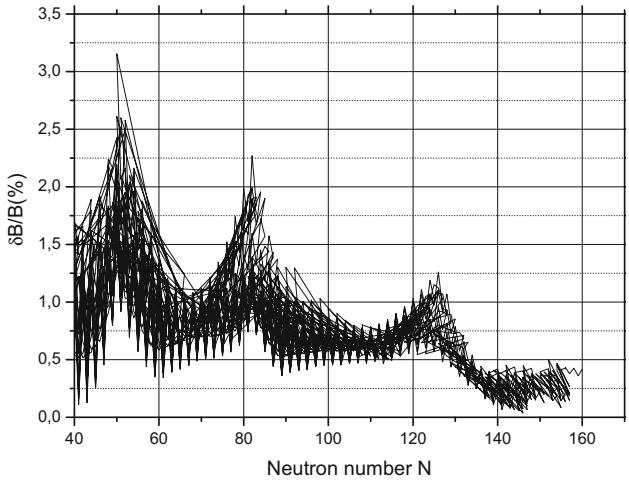

Fig. 6 Percentage error versus N

5.3 A glance at the Coulomb energy coefficient

We can readily demonstrate that the Coulomb energy term can be written as [15]

$$a_c = \frac{3}{5}\frac{e^2}{r_0}, \tag{9}$$

and hence, if we take the mean value of the Coulomb reduced radius $r_0 = 1.2257$ fm [16], the corresponding coefficient as determined analytically is $a_c = 0.705$ MeV. This coefficient is relevant to the binding energy formula because it could be used to control the calculation reliability. However, it should be noted that the value calculated using this approach is only an estimation, given that it depends on modeling considerations.

5.4 Relative error

We will now calculate the percentage error between the predicted and tabulated values:

$$\frac{|\delta B|}{B} = \frac{|B_{\mathrm{AME2016}} - B_{\mathrm{cal}}|}{B_{\mathrm{AME2016}}} \times 100\%, \tag{10}$$

where B_{AME2016} and B_{cal} are the tabulated binding energies and those predicted using relationship (8) with the new set of coefficients, respectively. Table 2 is a resume of six different categories of the percentage errors between the binding energies predicted using relationship (8) and AME2016 data [8, 9]. This can also be illustrated in Fig. 4 where the percentage error is presented versus mass

number A. It is evident that the binding energy calculated using the present set of coefficients has a range of $[0.05\%, 1.5\%]$.

However, the different spikes that appear on the graph should also be considered. This aspect may be understood based on a detailed examination of percentage errors versus atomic number Z and neutron number N, separately, as shown in Figs. 5 and 6, where similar spikes appear. Indeed, the different spikes depend on magic nuclei, three for proton $Z = 50, 82 \& 126$ and two for neutron $N = 50, \& 82$, and the spikes of Fig. 4 are associated with doubly magic nuclei $A = 100, 132 \& 208$ where both protons and neutrons are magic in the same nucleus. It is important to recall that the SEMF as considered in this work using relationship (1) does not take into account the shell corrections, wherein based on the nuclear shell model, the nucleons are arranged in shells so that a filled shell results in greater stability. Thus, an additional term in the formula may considerably reduce or totally remove the effect that causes these spikes to appear in the curves of the percentage errors.

6 Conclusion

The update performed in the present work on the Bethe–Weizsäcker mass formula coefficients yielded a more accurate estimation of their numerical values. The obtained coefficients exhibited excellent agreement with the binding energy of nuclei with $A \geq 50$. The relative error was in the range of $[0.05\%, 1.5\%]$ when the mass formula was applied using the updated coefficients, compared to the AME2016 data. However, the issue of light nuclei is still present with our new set of coefficients.

References

1. C.F. von Weizsäcker, Zur theorie der kernmassen. Z. Phys. A Hadrons Nuclei **96**, 431–458 (1935). https://doi.org/10.1007/BF01337700
2. R.D. Evans, *The Atomic Nucleus* (McGraw-Hill, Bombay, 1955)
3. D.N. Basu, Neutron and proton drip lines using the modified Bethe–Weizsäcker mass formula. Int. J. Mod. Phys. E **13**, 747–758 (2004). https://doi.org/10.1142/S0218301304002491
4. P.R. Chowdhury, C. Samanta, D.N. Basu, Modified Bethe–Weizsacker mass formula with isotonic shift and new driplines. Mod. Phys. Lett. A **20**, 1605–1618 (2005). https://doi.org/10.1142/S021773230501666X
5. N. Piskounov, *Calcul différentiel et intégral*, vol. 1 (MIR, Moscow, 1980), pp. 328–332
6. B. Demidovitch, I. Marov, *Eléments de calcul numérique* (MIR, Moscow, 1973), pp. 272–281
7. G. Audi, The history of nuclidic masses and of their evaluation. Int. J. Mass Spectrom. **251**, 85–94 (2006). https://doi.org/10.1016/j.ijms.2006.01.048
8. W.J. Huang, G. Audi, M. Wang et al., The AME2016 atomic mass evaluation (I). Evaluation of input data; and adjustment procedures. Chin. Phys. C **41**, 030002 (2017). https://doi.org/10.1088/1674-1137/41/3/030002
9. M. Wang, G. Audi, F.G. Kondev et al., The AME2016 atomic mass evaluation (II). Tables, graphs and references. Chin. Phys. C **41**, 030003 (2017). https://doi.org/10.1088/1674-1137/41/3/030003
10. SCht Mavrodiev, M.A. Deliyergiyev, Modification of the nuclear landscape in the inverse problem framework using the generalized Bethe–Weizsäcker mass formula. Int. J. Mod. Phys. E **27**, 1850015 (2018). https://doi.org/10.1142/S0218301318500155
11. M.W. Kirson, Mutual influence of terms in a semi-empirical mass formula. Nucl. Phys. A **798**, 29–60 (2008). https://doi.org/10.1016/j.nuclphysa.2007.10.011
12. C. Samanta, S. Adhikuri, Shell effect in Pb isotopes near the proton drip line. Nucl. Phys. A **738**, 491–494 (2004). https://doi.org/10.1016/j.nuclphysa.2004.04.094
13. W.D. Myers, W.J. Swiatecki MYERS, Nuclear properties according to the Thomas–Fermi model. Nucl. Phys. A **601**, 141–167 (1996)
14. A.H. Wapstra, *Encyclopedia of Physics* (Flügge, Berlin, 1958), pp. 1–37
15. H.A. Bethe, R.F. Bacher, Stationary states of nuclei. Rev. Mod. Phys. **8**, 82–229 (1936). https://doi.org/10.1103/RevModPhys.8.82
16. G. Royer, A. Subercaze, Coefficients of different macro-microscopic mass formulae from the AME2012 atomic mass evaluation. Nucl. Phys. A **917**, 1–14 (2013). https://doi.org/10.1016/j.nuclphysa.2013.09.003