

# DEVELOPMENT OF A SEMI-EMPIRICAL MASS FORMULA BY ADDING AN ISOSPIN TERM

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## Abstract:

We find a new set of Semi-Empirical Mass-Formula coefficients which is  $a_V, a_S, a_C, a_{AS}$  for nuclei with odd mass number using least squares fitting method, and we have also added another term for Semi-Empirical Mass Formula related to isospin  $a_T$  using single-particle model.

When calculating value of standard deviation between values of binding energies of our calculated nuclei and experimental values before and after adding isospin term, we found that adding isospin term to Semi-Empirical Mass Formula lowers the value of standard deviation.

And when comparing values of binding energies of our calculated nuclei with values of previous studies, we found that our calculated values are better than values calculated in these studies.

**Keywords:** Semi-empirical mass formula, Binding energy, Isospin, Least squares fitting method.

## 1. INTRODUCTION

The liquid drop model is considered one of the first and most important nuclear models, it assumes that the nucleus has properties similar to properties of a liquid drop, and by means of this model, the binding energies are calculated according to mass number and atomic number by means of the Semi-Empirical Mass Formula (SEMF) equation, which is known as the equation of Bethe-Weizsäcker[1] .

According to this equation, nuclear binding energy is a set of terms, each of which expresses a distinct characteristic of the nucleus.

This equation consists of five basic terms: volume energy term, surface energy term, Coulomb energy term, asymmetric energy term, and pairing energy term.

Usually, values of coefficients in SEMF are calculated by proportioning to experimental data using Least Square Method, which is considered one of the effective methods for calculations of this type of calculation[2].

The aim of this work is to use the method of least square fitting to find a new set of coefficients of the SEMF for 100 odd-A stable nuclei, that is, they have an odd mass number (odd-even nuclei and even-odd nuclei) using a code designed for this purpose by MATLAB, and we adding isospin term using single-particle model. Then we compare standard deviation between values of binding energies of our calculated nuclei and experimental values before and after adding isospin term.

## 2. NUCLEAR BINDING ENERGY

The sum of the number of protons (which is equal to the atomic number of elements in periodic table) and the number of neutrons within the nucleus is called the mass number  $A = Z + N$  .

Protons and neutrons are bound to each other inside a nucleus by very large and short-term force called nuclear force, and this force differ from other of known forces in nature such as electrical force and gravitational force. As a result of the existence of these large and short-range force, we consider that the nucleus is a bound system, so we need an energy of several million electron volts (order of Megaelectron volts (MeV)) to separate components of the nucleus compared to several electron volts to separate electrons from their atomic orbits (we need an energy of 13.6 eV to separate the hydrogen atom's electron from its orbital)[3].

The least amount of energy needed to separate a components of the nucleus of a proton and a neutron is called binding energy, and this energy is equal to the energy required to form a nucleus consisting of a proton and a neutron separated from each other[3]. Thus, mass of the nucleus is less than sum of masses of its components of protons and neutrons, and therefore we can write mass of the nucleus as follows[3]

$$\Delta M = ZM_H + NM_n - M(A, Z) \quad (1)$$

Where  $M_H$  mass of the hydrogen atom, which is equal to 1.007940u, and  $M_n$  mass of the neutron, which is equal to 1.008665u,  $M$  is mass of the atom, and therefore binding energy of the nucleus is given as

$$E_B = [ZM_H + NM_n - M(A, Z)]c^2 \quad (2)$$

where  $c^2 = 931.494061 \text{ MeV} / u$  the square of speed of light in a vacuum.

### 3. LIQUID DROP MODEL

The liquid drop model is considered one of the most important nuclear models. This model was proposed by Weizacker in 1935 and Bohr developed the basic hypotheses of this model in 1937[1].

In this model, the nucleus was likened to a liquid drop, and this analogy was chosen according to the following three consideration

- Nuclear matter is incompressible, so[4]

$$\left. \begin{array}{l} V \propto R^3 \\ R \propto A^{\frac{1}{3}} \end{array} \right\} V \propto A \quad (3)$$

Where  $R$  is a radius of nucleus and  $A$  is a number of nucleons, so the volume of nucleus proportion with number of nucleons, as in liquid drop.

-The approximate stability of binding energy per nucleon for medium and heavy nuclei, and this indicates that each nucleon interact with a limit number of nucleons, meaning that the nuclear forces are saturated, as the forces acting between the molecules of a liquid.

-The nuclear force are same for nucleons, which means they are not related to the nucleon being a proton or a neutron as in the case of molecules in a liquid drop.

### 4. SEMI-EMPIRICAL MASS FORMULA (SEMF)

This equation was developed in 1935 by C.F. Von Weizacker based on similarity of the nucleus with liquid drop as we mentioned earlier, and this equation is also known as Bethe-Weizacker equation[1]. It is based on consideration that total binding energy of the nucleus is a set of terms, each of term expresses one of characteristics of the nucleus, as follows[1]

$$EB = \sum_{i=1}^n E_i \quad (4)$$

The terms of previous equation are given as following [4]

- The first term is called volume energy term; it was named by this, because size of the nucleus is proportional to number of its nucleons. The interpretation of this term was based on existence of a specific average binding energy per nucleon for all nuclei, and it written as follows

$$E_V = a_v A \quad (5)$$

Where  $E_V$  is volume energy term and  $a_v$  volumetric proportionality coefficient.

- The second term is called surface energy term. This term was found based on phenomenon of surface tension in liquids. In a liquid drop, the molecules on surface of drop are weaker than the molecules inside it, and therefore their energy is greater. The same thing is achieved in the nucleus, where the nucleons located on surface is weaker than the nucleons located deep in the nucleus, and therefore it possesses additional surface energy, because inner nucleon exchanges influence with a greater number of nucleons than in state of outer nucleon located on surface of the nucleus, and this term is written as

$$E_S = -a_s A^{2/3} \quad (6)$$

Where  $E_S$  is surface energy term and  $a_s$  surface proportionality coefficient.

This term is added with a negative sign to binding energy equation because it decreases value of total binding energy.

- The third term is Coulomb energy term, where existence of Coulomb force between protons leads to a decrease in value of binding energy. Coulomb potential is proportional to  $Z(Z - 1)$ , then expression Coulomb energy is written as follows

$$E_C = -a_c \frac{Z^2}{A^{1/3}} \quad (7)$$

where  $E_C$  is surface energy term and  $a_c$  Coulombic proportionality coefficient.

This term is also added with a negative sign to binding energy equation, because repulsion energy decreases value of total binding energy.

The previous three terms are considered classical terms.

- The fourth term is called asymmetric energy term, and this term result from difference between number of protons and neutrons in the nucleus, as this difference leads to a decrease in stability of nucleus and thus a decrease in value of its total binding energy, so this term is also added with a negative sign to binding energy equation, and written as follows

$$E_{AS} = a_{AS} \left( \frac{N - Z}{A} \right)^2 = a_{AS} \left( \frac{A - 2Z}{A} \right)^2 \quad (8)$$

where  $E_{AS}$  is asymmetric energy term and  $a_{AS}$  proportionality coefficient of the asymmetric energy.

- The fifth term is called pairing energy term. This term was added because binding energy does not depend on number of nucleons only, but also on even or odd number of nucleons. It was found that the most stable nucleus in nature are even-even nuclei, and the least stable are odd-odd nuclei, the middle state is odd nuclei (even-odd or odd-even) and these nuclei are called odd nuclei or odd-A nuclei. The number of these nuclei is approximately one hundred nuclei found in nature.

Accordingly, Fermi introduced a correction factor added to binding energy, which takes the following values

- When  $A$  is even,  $N$  and  $Z$  even, the term is  $\delta = +a_p A^{-3/4}$ , thus increases binding energy, because the nucleons are paired with each other.

-When  $A$  is even  $N$  and  $Z$  odd, the term is  $\delta = -a_p A^{-3/4}$ , thus binding energy is reduced.

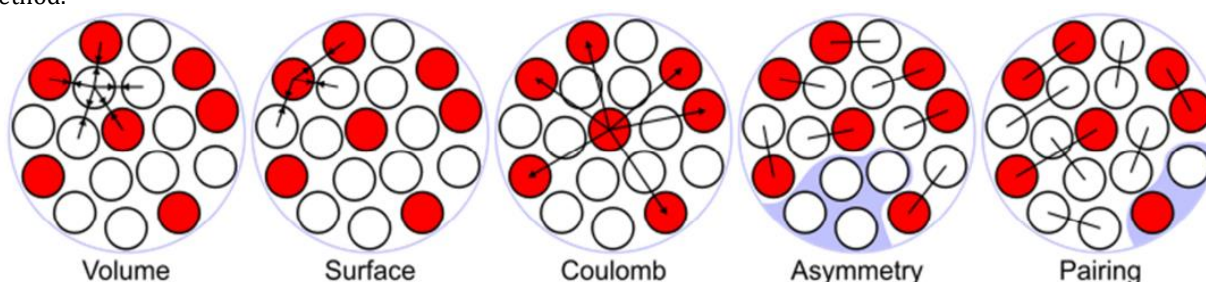
- When  $A$  is odd, this term does not take any value  $\delta = 0$ , and it is the middle state between two previous cases, as this term does not have any contribution to binding energy. This term can be written in abbreviated form as follows

$$\delta = (\pm, 0) a_p A^{-3/4} \quad (9)$$

Where  $\delta$  is pairing energy term and  $a_p$  coefficient of proportionality of pairing energy. An illustration of previous terms is shown in Figure (1). So, SEMF, takes the following form

$$EB = a_v A - a_s A^{2/3} - a_c \frac{Z^2}{A^{1/3}} - a_{AS} \frac{(A - 2Z)^2}{A} + \delta \quad (10)$$

One of the most important methods used to calculate values of coefficients in SEMF is Least Square Fitting method.



Source: [https://commons.wikimedia.org/w/index.php?title=File:Liquid\\_drop\\_model.svg&oldid=74367824](https://commons.wikimedia.org/w/index.php?title=File:Liquid_drop_model.svg&oldid=74367824).

Figure (1): illustration for terms of SEMF in liquid drop model.

## 5. LEAST SQUARES METHOD

The least squares method is a standard method for finding solution to a set of equations that has more than one variable. This allows us to use this method to determine values of coefficients in theoretical formulas by fitting it with experimental values, where fitting is best possible when sum of squares of differences between experimental and theoretical values is smaller, as follows[2]

$$\chi^2 = \sum (y_i - f(x_i))^2 \quad (11)$$

Where  $f(x_i) = \sum_{k=0}^{k=j} a_k x_i^k$  is a polynomial and  $a_k$  is coefficients of polynomial.

Since function  $\chi$  is dependent on several variables, it reaches a local maximum value at the point where all its partial derivatives of first order is zero, that is, when following equations are satisfied

$$\frac{\partial \chi^2}{\partial a_0} = 0, \frac{\partial \chi^2}{\partial a_1} = 0, \frac{\partial \chi^2}{\partial a_2} = 0, \dots, \frac{\partial \chi^2}{\partial a_k} = 0 \quad (12)$$

The set of equations, whose number of variables is equal to number of its equations, is arranged in following matrix form

$$\begin{bmatrix} n & \sum x_i & \sum x_i^2 & \dots & \sum x_i^j \\ \sum x_i & \sum x_i^2 & \sum x_i^3 & \dots & \sum x_i^{j+1} \\ \sum x_i^2 & \sum x_i^3 & \sum x_i^4 & \dots & \sum x_i^{j+2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \sum x_i^j & \sum x_i^{j+1} & \sum x_i^{j+2} & \dots & \sum x_i^{2j} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_j \end{bmatrix} = \begin{bmatrix} \sum y_i \\ \sum (x_i y_i) \\ \sum (x_i^2 y_i) \\ \vdots \\ \sum (x_i^j y_i) \end{bmatrix} \quad (13)$$

By solving these coefficients equations, we get values of  $a_0, a_1, a_2, \dots, a_j$ , and by

substituting them in polynomial  $f(x_i)$ , we get required polynomial.

## 6. ISOSPIN

Heisenberg proposed this idea in 1932, when he considered protons and neutrons to be identical particles, he called nucleons, and assumed the very small difference between two masses resulted from Coulomb interaction between protons. Therefore, neutrons and protons represent two different states of one thing, which called nucleon, and this space is called isospin, and this space is accompanied by isospin operator, which we denote by  $\hat{T}$  and takes following eigen value [5]

$$T = \sqrt{T(T+1)} \quad (14)$$

The algebra of operators in isospin space is developed as in case of spin, isospin operator takes following form[5]

$$T = \frac{1}{2} \tau \quad (15)$$

Where  $\tau$  is Pauli isospin matrix, and accordingly, isospin space (or charge space) for a nucleon has two dimensions, like spin space. The third projection of isospin takes only two values for nucleons, which is [6]

$$T_3 = \frac{1}{2} \tau_3 = \pm \frac{1}{2} \quad (16)$$

The special value of nucleon according to Dirac's representation is  $|T, T_3\rangle$ , the special value of proton is  $\left| \frac{1}{2}, \frac{1}{2} \right\rangle$ , while the special value of neutron is  $\left| \frac{1}{2}, -\frac{1}{2} \right\rangle$ .

The idea of isospin can be generalized for case of a nucleus that has Z protons and N neutrons, where it has a mass number of  $A=Z+N$ . In this case, the third component of isospin is added algebraically to each nucleon (for protons and neutrons) to get this compound for nucleus, as follows [6]

$$T_3 = \sum_i t_{i3} = \sum_i (t_{p3} + t_{n3}) = \frac{Z}{2} - \frac{N}{2} = -\frac{1}{2}(N - Z) = -\frac{1}{2}(A - 2Z) \quad (17)$$

As it is known, value of compounds cannot exceed the value of its vector, so value of isospin vector must be as[6]

$$T \geq \left| \frac{N - Z}{2} \right| \quad (18)$$

The expectation value of two interacting nucleons is calculated from defining equation for total isospin which is equal to vector resultant isospin of each of two interacting nucleons as follows

$$\vec{T} = \vec{t}_a + \vec{t}_b \quad (19)$$

where  $t_a, t_b$  is isospin of two interacting nucleons, by squaring both sides of previous equation, we get

$$T^2 = t_a^2 + t_b^2 + 2t_a t_b \quad (20)$$

Given  $t_a = t_b = \frac{1}{2}$ . So, the expected value  $t_a t_b$  is

$$\langle t_a t_b \rangle = \frac{T(T+1) - t_a(t_a+1) - t_b(t_b+1)}{2} = \frac{2T(T+1) - 3}{4} \quad (21)$$

And since isospin is conserved for strong interactions (which corresponds to fact that the nuclear forces are symmetrical), it is therefore possible to adding a term related to isospin within total binding energy equation form[6], and thus term that can be added to SEMF given by equation (10) takes the following

$$\langle \tau_a \tau_b \rangle = 2T(T+1) - 3 \quad (22)$$

## 7. SINGLE PARTICLE MODEL

This model assumes that the nucleons in the nucleus of a specific type (protons or neutrons) are paired in a basic state with each other in form of pairs to give a total angular moment and a magnetic moment equal to zero, and these paired nucleons form a closed core. According to this, the total angular moment and isospin of even-even nuclei are equal to zero, and this is what we observe in nature, while the properties of odd-A nuclei returns to properties of unpaired nucleon[4].

## 8. CALCULATIONS AND RESULTS

Calculations were made for 100 individual stable nuclei (odd-even and even-odd) located in different area (light-medium-heavy), and they are most of stable nuclei found in nature.

### 8.1. values of coefficients in SEMF

Depending on method of least squares fitting, where fitting is the best possible for binding energy equation given by equation (10) when sum of squares for differences between experimental and theoretical values is smallest, as follows

$$\left. \begin{aligned} \frac{\partial \chi}{\partial a_v} &= -2 \sum_i A_i (y_i - E_{B_{th}}(Z_i, A_i)) = 0 \\ \frac{\partial \chi}{\partial a_s} &= 2 \sum_i A_i^{2/3} (y_i - E_{B_{th}}(Z_i, A_i)) = 0 \\ \frac{\partial \chi}{\partial a_c} &= 2 \sum_i \frac{Z_i(Z_i-1)}{A_i^{1/3}} (y_i - E_{B_{th}}(Z_i, A_i)) = 0 \\ \frac{\partial \chi}{\partial a_{AS}} &= 2 \sum_i \frac{(A_i - 2Z_i)^2}{A_i} (y_i - E_{B_{th}}(Z_i, A_i)) = 0 \end{aligned} \right\} \quad (23)$$

Substituting equation (23) into (10), we get the following matrix equation

$$\begin{bmatrix} a_v \\ a_s \\ a_c \\ a_{AS} \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix} \cdot \begin{bmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\ b_{21} & b_{22} & b_{23} & b_{24} \\ b_{31} & b_{32} & b_{33} & b_{34} \\ b_{41} & b_{42} & b_{43} & b_{44} \end{bmatrix}^{-1} \quad (24)$$

Where values of elements  $[b]$  are given as follows



$$\left. \begin{aligned} b_{11} &= \sum_i A_i^2, b_{12} = b_{21} = -\sum_i A_i^{5/3}, b_{13} = b_{31} = -\sum_i Z_i (Z_i - 1) A_i^{2/3} \\ b_{14} &= b_{41} = -\sum_i (A_i - 2Z_i)^2, b_{22} = \sum_i A_i^{4/3}, b_{23} = b_{32} = \sum_i Z_i (Z_i - 1) A_i^{1/3} \\ b_{24} &= b_{42} = \sum_i \frac{(A_i - 2Z_i)^2}{A_i^{1/3}}, b_{33} = \sum_i \frac{Z_i^2 (Z_i - 1)^2}{A_i^{2/3}} \\ b_{34} &= b_{43} = \sum_i \frac{Z_i (A_i - 2Z_i)^2}{A_i^{4/3}}, b_{44} = \sum_i \frac{(A_i - 2Z_i)^4}{A_i^2} \end{aligned} \right\} \quad (25)$$

The values of elements  $[c]$  are given as follows

$$c_1 = \sum_i y_i A_i, c_2 = -\sum_i y_i A_i^{2/3}, c_3 = -\sum_i y_i \frac{Z_i (Z_i - 1)}{A_i^{1/3}}, c_4 = -\sum_i y_i \frac{(A_i - 2Z_i)^2}{A_i} \quad (26)$$

By solving matrix equation (24), after substituting values of elements given in (25) and (26) with helping of a code designed for this purpose using famous program MATLAB, we get values of coefficients, which are given in units of MeV as follows

$$a_v = 15.8838, a_s = 18.1220, a_c = 0.7279, a_{AS} = 23.2012$$

which is a new set of parameters for odd-A nuclei.

### 8.2. values of coefficients in SEMF after adding isospin

After adding isospin term given by (22), we add to set of equations (23) the following equation

$$\frac{\partial \chi}{\partial a_T} = -2 \sum_i f(T) (y_i - EB_{th}(Z_i, A_i)) = 0 \quad (27)$$

Thus, matrix equation (24) becomes as

$$\begin{bmatrix} a_v \\ a_s \\ a_c \\ a_{AS} \\ a_T \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \end{bmatrix} \cdot \begin{bmatrix} b_{11} & b_{12} & b_{13} & b_{14} & b_{15} \\ b_{21} & b_{22} & b_{23} & b_{24} & b_{25} \\ b_{31} & b_{32} & b_{33} & b_{34} & b_{35} \\ b_{41} & b_{42} & b_{43} & b_{44} & b_{45} \\ b_{51} & b_{52} & b_{53} & b_{54} & b_{55} \end{bmatrix}^{-1} \quad (28)$$

Where values of elements of matrix  $[b]$  are given as follows

$$\left. \begin{aligned} b_{11} &= \sum_i A_i^2, b_{12} = b_{21} = -\sum_i A_i^{5/3}, b_{13} = b_{31} = -\sum_i Z_i (Z_i - 1) A_i^{2/3} \\ b_{14} &= b_{41} = -\sum_i (A_i - 2Z_i)^2, b_{15} = b_{51} = \sum_i A_i [2T(T+1) - 3] \\ b_{22} &= \sum_i A_i^{4/3}, b_{23} = b_{32} = \sum_i Z_i (Z_i - 1) A_i^{1/3}, b_{24} = b_{42} = \sum_i \frac{(A_i - 2Z_i)^2}{A_i^{1/3}} \\ b_{25} &= b_{52} = -\sum_i A_i^{2/3} [2T(T+1) - 3], b_{33} = \sum_i \frac{Z_i^2 (Z_i - 1)^2}{A_i^{2/3}} \\ b_{34} &= b_{43} = \sum_i \frac{Z_i (A_i - 2Z_i)^2}{A_i^{4/3}}, b_{35} = b_{53} = -\sum_i \frac{Z_i (Z_i - 1)^2}{A_i^{1/3}} [2T(T+1) - 3] \\ b_{44} &= \sum_i \frac{(A_i - 2Z_i)^4}{A_i^2}, b_{45} = b_{54} = -\sum_i \frac{(A_i - 2Z_i)^2}{A_i} [2T(T+1) - 3] \\ b_{55} &= \sum_i [2T(T+1) - 3]^2 \end{aligned} \right\} \quad (29)$$

The values of elements of matrix  $[c]$  are given as follows

$$\left. \begin{aligned} c_1 = \sum_i y_i A_i, c_2 = -\sum_i y_i A_i^{2/3}, c_3 = -\sum_i y_i \frac{Z_i(Z_i - 1)}{A_i^{1/3}}, c_4 = -\sum_i y_i \frac{(A_i - 2Z_i)}{A_i} \\ c_5 = -\sum_i [2T(T + 1) - 3] y_i \end{aligned} \right\} \quad (30)$$

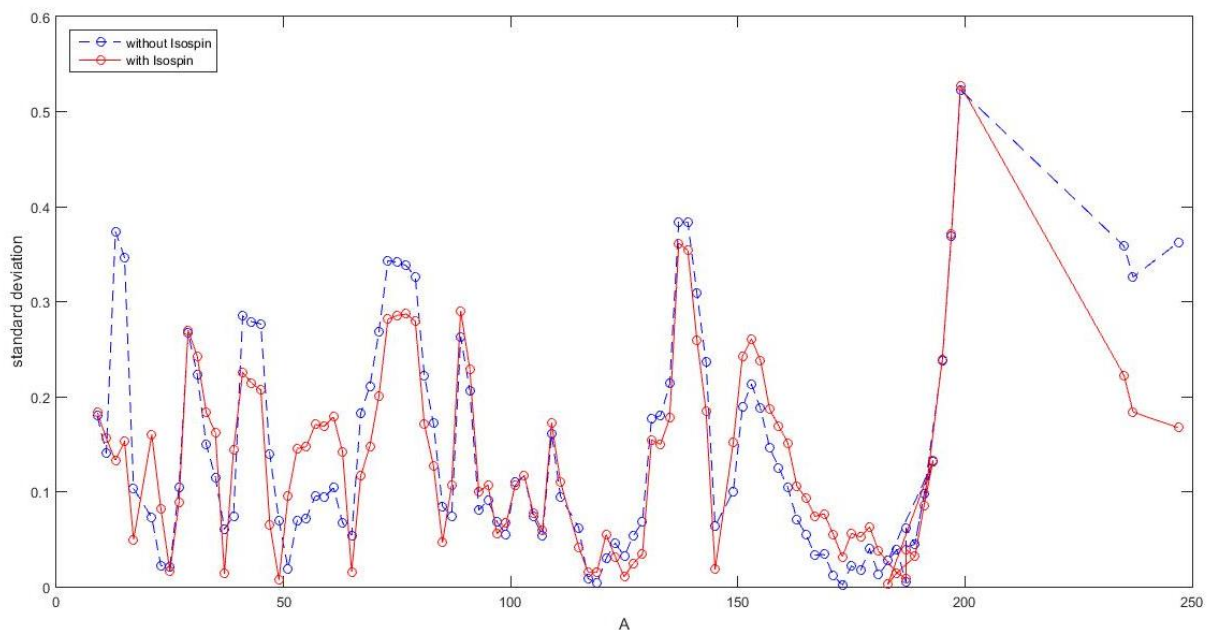
By solving matrix equation (28), after substituting values of elements given in equations (29) and (30), we get values of coefficients  $a_V, a_S, a_C, a_{AS}, a_T$ , which are given MeV as follows

$$a_V = 16.8290, a_S = 22.0231, a_C = 0.7770, a_{AS} = 25.0149, a_T = 8.3892$$

We calculated standard deviation between our calculated binding energy and experimental values for one hundred stable odd-A nuclei, as we use the following standard deviation relation[7]

$$\sigma = \sqrt{\frac{1}{N} \sum_{i=1}^N [E_{B(\text{theo.})}^i - E_{B(\text{exp.})}^i]^2} \quad (31)$$

We found value of standard deviation for these nuclei without adding isospin term is  $\sigma = 1.831(\text{MeV})$ , and we found standard deviation value after adding isospin term is  $\sigma = 1.662(\text{MeV})$ , that is, adding isospin term for SEMF reduces value of standard deviation. And it appears in Figure (2) distribution of standard deviation values of nuclei calculated by us before and after adding isospin in terms of mass number.



**Figure 2: distribution of standard deviation values of our calculated nuclei before adding isospin (dotted line) and after adding it (solid line) in terms of mass number.**

When comparing standard deviation value for calculated nuclei with previous studies, we found value, which we calculated after adding isospin term, is better than values calculated in previous studies mentioned in references[8-10], which depending on different methods and different approximations, and it is better than values calculated in reference[11], which was performed by using coefficients deduced by Evans and Arya, using UAEN method, and these comparisons are shown in table (1).

**Table (1). Comparison between standard deviation value calculated by us with previous studies**

References	[8]	[8]	[9]	[10]	[11] UAEN	[11] Arya	[11] Evans	Present Work Without iso.	Present Work With iso.
$\sigma(MeV)$	4.711	3.888	3.795	1.9307	3.070	2.729	2.412	1.831	1.662

We also found that our standard deviation value is better than study mentioned in reference[12], Which depending on adding different terms to SEMF, which are, exchange Coulomb term, Wigner term, surface symmetry term, pairing term, curvature term and shell effect term, and also calculated with effect of adding all the previous terms. So, we notice adding isospin effect term is great importance compared to adding other terms. These comparisons are shown in table 2.

**Table 2. Comparison of our calculated standard deviation value with values of reference[12]**

Term	Exchange Coulomb	Wigner	Surface symmetry	Pairing	Curvature	Shell effects	All terms	Present Work Without iso.	Present Work With iso.
$\sigma(MeV)$	2.144	1.754	2.121	1.819	1.819	2.389	1.620	1.831	1.662

## 9. CONCLUSION

Using a code designed using MATLAB program, we calculated values of four coefficients of SEMF, which were as follows

$$a_v = 15.8838, a_s = 18.1220, a_c = 0.7279, a_{AS} = 23.2012$$

for one hundred stable nuclei that have an odd mass number (even - odd and odd- even) nuclei, using least squares fitting method. We also added another term to SEMF related to isospin using single-particle model. And we found values of coefficients of SEMF after adding this new term, which were as follows

$$a_v = 16.8290, a_s = 22.0231, a_c = 0.7770, a_{AS} = 25.0149, a_r = 8.3892$$

We found adding isospin term to SEMF reduces value of standard deviation between binding energies of our calculated nuclei and experimental values.

When comparing values of binding energies for studied nuclei with values of previous studies, we found that our calculated values are better than values in these studies.

The addition of isospin to SEMF can be tested for nuclei having an even- even nuclei, at which point calculations must be performed by adding pairing term, and a way to find out isospin of interacting nucleons.

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