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Review Article

Estimation of Semi-Empirical Mass Formula Coefficients

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Abstract: Using linear least squares method and by data of atomic mass, the present study calculates the coefficients of volume, surface, Coulomb, and asymmetry terms in semi-empirical formula. Our findings show that the mass of neutron and hydrogen can be estimated via developing this example. The results of the present calculations are also compared with those of similar previous studies.

Keywords: Liquid Drop Model, Semi Empirical Mass Formula, Least Square Method, Data Fitting, Experimental Data

1. Introduction

In the area of nuclear physics model based on experimental data such as is common to many fields. These models have been confirmed by experimental data and must able to predict some other data. One of the basic and important models in nuclear physics is liquid drop model (LDM). The essential assumptions of this model are

a. The nucleus consists of incompressible matter so that $R \sim A^{1/3}$.
b. The nuclear force is identical for every nucleon and in particular does not depend on whether it is a neutron or a proton.
c. The nuclear force saturates [1].

Semi-empirical mass formula (SEMF), known as Weizsäcker's formula or the Bethe–Weizsäcker formula in nuclear physic [2-3], is used for estimating the atomic mass as a function of mass number and atomic number. As the name implies, SEMF includes both empirical and theoretical parts; the theoretical part of this formula is obtained from the "liquid drop" model as proposed by George Gamow [4] containing some terms which were later developed by Niels Bohr and John Archibald Wheeler [5]. The SEMF is formulated by a German physicist, Carl Friedrich von Weizsäcker, in 1935 [6] [7]. So far, the formula is accepted, giving us an appropriate estimation for atomic masses and other properties of the nuclei, though it does not predict magical numbers. In recent years, newer models have been proposed for nuclear mass [8, 9]. Among these models is Duflo-Zuker's model.

Duflo-Zuker (DZ) shell model mass formulae by fitting to the latest experimental mass compilation AME2012 and analyze the propagation of the uncertainties in binding energy calculations when extrapolated to driplines.

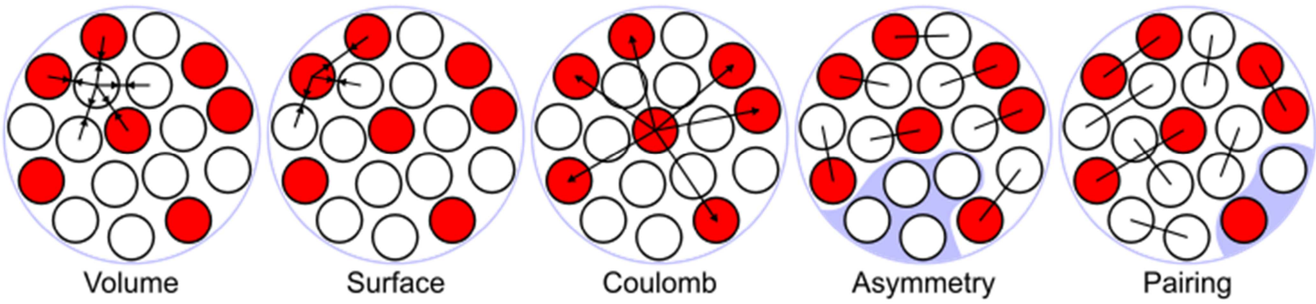
The "liquid drop" model assumes the nucleus as a liquid drop together with its associated properties. According to the model, binding energy (BE) of the nucleus includes Volume Term (the interaction of nucleons with adjacent nucleons regardless of decrease in interaction of surface nucleons), Surface Term (the effect of the decrease in interactions of surface nucleons), Coulomb Term (the interaction of coulomb repulsion among protons), Asymmetry Term (different amount of energy in equal and unequal modes of protons and neutrons numbers), and Parity Term (more stability and resultantly more negative energy of the nucleus for pair-pair nuclei).

Theoretical calculations and data fitness are of the methods to determine coefficient of the terms in the "liquid drop" model [9, 10].

2. About Semi-Empirical Mass Formula

The semi-experimental mass formula (SEMF) is an important formula that roughly gives the relationship between nuclear mass and atomic number as well as neutron numbers. This formula also is called Weizsäcker's formula, or the Bethe–Weizsäcker formula, or the Bethe–Weizsäcker mass formula. According the name of this formula it has two aspects. Theoretical one and experimental one. The theoretical aspect is come from the liquid drop model proposed by George Gamow which it gives the general form of the formula. The values of the coefficients for the first time are presented (in 1935) by German physicist Carl Friedrich von Weizsäcker [2, 3]. The values of the coefficients have been changed over during the time but the original structure of the formula have been remains without changes.

The SEMF gives a good approximation for atomic masses and several other effects, but does not explain the appearance of magic numbers of protons and neutrons, and the extra binding-energy and measure of stability that are associated with these numbers of nucleons. The liquid drop model in nuclear physics treats the nucleus as drop of incompressible nuclear fluid. It was first proposed by George Gamow and then developed by Niels Bohr and John Archibald Wheeler. The nucleus is made of nucleons (protons and neutrons), which are held together by the nuclear force (a residual effect of the strong force). This is very similar to the structure of spherical liquid drop made of microscopic molecules. This is a crude model that does not explain all the properties of the nucleus, but does explain the spherical shape of most nuclei. It also helps to predict the nuclear binding energy and to assess how much is available for consumption. Mathematical analysis of the theory delivers an equation which attempts to predict the binding energy of a nucleus in terms of the numbers of protons and neutrons it contains. This equation has five terms on its right hand side. These correspond to the cohesive binding of all the nucleons by the nuclear force, a surface energy term, the electrostatic mutual repulsion of the protons, an asymmetry term (derivable from the protons and neutrons occupying independent quantum momentum states) and a pairing term (partly derivable from the protons and neutrons occupying independent quantum spin states). If we consider the sum of the following five types of energies, then the picture of a nucleus as a drop of incompressible liquid roughly accounts for the observed variation of binding energy of the nucleus:



Source: https://commons.wikimedia.org/w/index.php?title=File:Liquid_drop_model.svg&oldid=74367824.

Figure 1. *Illustration of the terms of the semi-empirical mass formula in the liquid drop model of the atomic nucleus.*

The volume term is to express the interaction between nucleons which are closest neighbor. This expression means that nuclear energy is proportional to the nucleus volume.

According volume term each nucleons interacts with the closest neighbor. Because of the finite nucleus volume some of nucleons are located on surface of nucleus. These nucleons in analogy to interior nucleons have less interaction. Therefore these nucleons have less interactions which is must reduced from the energy of the volume term. This term is called surface term.

As result of Coulomb repulsion between protons inside the nucleus, the Coulomb term is appeared in semi-empirical mass formula (SEMF). This term is to cause instability of the nucleus.

Asymmetry term which is a result of Pauli exclusion principle says when the difference of the numbers of protons and neutrons increases the nucleus stability decreases.

Pairing term is expressed the fact that in the nucleus systems pairing the protons and neutrons is caused to increasing the stability.

3. The Least Squares Method (LSM)

3.1. History

For the first time least square method is introduced according to needs of astronomy and geodesy as scientists and mathematicians to overcome the navigating the Earth's oceans during the Age of Exploration.

This method was the pick of several advances of eighteenth century [11].

The LSM is one of the methods commonly used for data fitness [12-14].

The method of least squares is a standard approach in regression analysis to the approximate solution of over determined systems, i.e., sets of equations in which there are more equations than unknowns.

This allows us to use least squares method for determining the constants in theoretical formulas which are empirical basis.

"Least squares" means that the overall solution minimizes the sum of the squares of the errors made in the results of every single equation.

Application is in data fitting. Least square method is used in two categories: the first one is linear or ordinary least square which applicable for linear sets of data. The linear least-squares method is used in statistical regression analysis. The second one is non-linear least square method. In this category the approach of the problem solving is iterative. As is clear from the name this category is used for non-linear data [15].

Legendre in 1805 was the first scientist who published a paper of the application of the least square method [16]. He was used this method for data fitting of linear data. In fact Legendre was presented a new method for the data fitting of the same data as Laplace for the shape of the earth.

Another research in this method was published by Carl Friedrich Gauss in 1809. In this research using least square method he was calculated the orbits of celestial bodies [17, 18]. He had managed to complete Laplace's program of specifying a mathematical form of the probability density for the observations, depending on a finite number of unknown parameters, and define a method of estimation that minimizes the error of estimation. Gauss showed that arithmetic mean is indeed the best estimate of the location parameter by changing both the probability density and the method of estimation. He then turned the problem around by asking what form the density should have and what method of estimation should be used to get the arithmetic mean as estimate of the location parameter. In this attempt, he invented the normal distribution [19, 20].

3.2. The Method

General term for each error in the LSM of linear type is a function as:

$$\mathrm{err} = \sum(d_i)^2 = \sum\big(y_i - f(x_i)\big)^2 \tag{1}$$

If it is assumed that fit a polynomial function, then:

$$\mathrm{err} = \sum_i\Big(y_i - \sum_{k=0}^{k=j} a_k x_i^k\Big)^2 \tag{2}$$

For example, with two columns of data (x, y), the objective is to minimize the error in equation (2), thus:

$$\begin{cases} \frac{\partial \mathrm{err}}{\partial a_0} = -2\sum_i\big(y_i - \sum_{k=0}^{k=j} a_k x_i^k\big) = 0 \\ \frac{\partial \mathrm{err}}{\partial a_1} = -2\sum_i\big(y_i - \sum_{k=0}^{k=j} a_k x_i^k\big)x_i = 0 \\ \frac{\partial \mathrm{err}}{\partial a_2} = -2\sum_i\big(y_i - \sum_{k=0}^{k=j} a_k x_i^k\big)x_i^2 = 0 \\ \vdots \\ \frac{\partial \mathrm{err}}{\partial a_j} = -2\sum_i\big(y_i - \sum_{k=0}^{k=j} a_k x_i^k\big)x_i^j = 0 \end{cases} \tag{3}$$

rewriting of equation (3) results in the following:

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

Where i=1, 2,…, n.a_k coefficients are indeterminate of the problem in equation (4). Assuming the data in Table 1 to be related to a polynomial with degree of 5, the objective would be to find the coefficients with the best data fitness for a polynomial with degree of 5.

Table 1. *Pair of data related to polynomial with degree of 5.*

x_i	y_i
-1.4833	39.0336
-1.0667	12.2011
-0.6500	3.5372
-0.2333	1.3652
0.1833	0.8807
0.6000	1.1373
1.0167	2.03245
1.4333	1.2934
1.8500	-8.5361
2.2667	-43.1118

The related matrix equation was changed into the equation (5) after calculation of entries proportionate to equation (4).

$$\begin{bmatrix} 10. & 3.9 & 15. & 17. & 49. & 80. \\ 3.9 & 15. & 17. & 49. & 80. & 197. \\ 15. & 17. & 49. & 80. & 197. & 377. \\ 17. & 49. & 80. & 197. & 377. & 878. \\ 49. & 80. & 197. & 377. & 878. & 1823. \\ 80. & 197. & 377. & 878. & 1823. & 4140. \end{bmatrix} = \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{bmatrix} \begin{bmatrix} 9.83 \\ -182. \\ -144. \\ -693. \\ -1025. \\ -3052. \end{bmatrix} \tag{5}$$

The results were a_5=-2.0001, a_4=3.0002, a_3=-0.9998, a_2=1.9994, a_1=-1.0001, a_0=1.0002. Therefore, the best data fitness for polynomial with degree of 5 for data in Table 1 was equation (6):

$$f(x) = -2.x^5 + 3.x^4 - 0.99x^3 + 1.99x^2 - 1.x + 1 \tag{6}$$

The atomic mass of elements in terms of the energy stored in the nucleus (BE) written in SEMF as below:

$$m\big({}_Z^AX\big) = Zm\big({}_1^1H\big) + Nm_n - \frac{1}{c^2}B(Z, A) \tag{7}$$

and

$$B(Z, A) = a_v A - a_s A^{\frac{2}{3}} - a_c \frac{Z(Z-1)}{A^{\frac{1}{3}}} - a_a \frac{(A-2Z)^2}{A} \tag{8}$$

where in (8), A, Z, m(^{1}H) and m_n are mass number, atomic number, mass of hydrogen atom, and neutron mass respectively. B(Z,A) is binding energy for a nucleus with mass number A and atomic number Z [equation (8) is just applied and valid for BE of those nuclei with odd mass number in which their numbers of protons or neutrons is none of 2, 8, 20, 28, 50, 82, 126, and 184. These numbers are called "magical numbers" in nuclear Physics, including volume, surface, coulomb, and asymmetry terms respectively. Coefficient of volume term (a_y), surface term (a_s), coulomb term (a_c), and asymmetry term (a_a) were calculated by LSM (Table 2).

Generalizing LSM to this problem results in definition of function (9):

$$\mathrm{err} = \sum_i \left(y_i - B(Z_i, A_i)\right)^2 = \sum_i \left(\begin{array}{c} y_i - a_v A_i + a_s A_i^{\frac{2}{3}} + \\ a_c \frac{Z_i(Z_i-1)}{A_i^{\frac{1}{3}}} + a_a \frac{(A_i-2Z_i)^2}{A_i} \end{array} \right)^2 \quad (9)$$

If the above-mentioned function is minimized, then the coefficient of volume, surface, coulomb, and asymmetry terms are obtained; in other words, partial derivative of function err in proportion to coefficient of volume term (a_v), surface term(a_s), coulomb term(a_c), and asymmetry term (a_a) should equal zero.

$$\begin{cases} \frac{\partial err}{\partial a_v} = -2\sum_i A_i\left(y_i - B(Z_i, A_i)\right) = 0 \\ \frac{\partial err}{\partial a_s} = 2\sum_i A_i^{\frac{2}{3}}\left(y_i - B(Z_i, A_i)\right) = 0 \\ \frac{\partial err}{\partial a_c} = 2\sum_i \frac{Z_i(Z_i-1)}{A_i^{\frac{1}{3}}}\left(y_i - B(Z_i, A_i)\right) = 0 \\ \frac{\partial err}{\partial a_a} = 2\sum_i \frac{(A_i-2Z_i)^2}{A_i}\left(y_i - B(Z_i, A_i)\right) = 0 \end{cases} \quad (10)$$

In equation (10), y_i is binding energy of i-th special nucleus obtained from equation (8) when mass of hydrogen atom and neutron be given.

Data of Table 2 was selected in a way that the share of parity term equals zero.

Table 2. *Symbol, atomic number, mass number, and atomic mass of some special nucleus [12].*

atomic mass (m) in terms of u	mass number	atomic number	Nucleus symbol
13.003355	13	6	C
20.993843	21	10	Ne
20.997651	21	11	Na
26.986704	27	14	Si
34.969032	35	16	S
34.975256	35	18	Ar
40.961825	41	19	K
44.958124	45	22	Ti
52.944340	53	23	V
50.948213	51	25	Mn
60.933461	61	29	Cu
80.923270	81	38	Sr
102.906323	103	44	Ru
116. 908630	117	52	Te
142.910930	143	61	Pm
182.950817	183	75	Re
182.953290	183	76	Os
192.966560	193	80	Hg
206.980456	207	84	Po
215.000310	215	87	Fr
235.043924	235	92	U
251.079580	251	98	Cf

System of equation (10) results in matrix equation 11:

$$\begin{bmatrix} b_1 & b_2 & b_3 & b_4 \\ b_5 & b_6 & b_7 & b_8 \\ b_9 & b_{10} & b_{11} & b_{12} \\ b_{13} & b_{14} & b_{15} & b_{16} \end{bmatrix} \begin{bmatrix} a_v \\ a_s \\ a_c \\ a_a \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix} \quad (11)$$

where,

$$\begin{cases} c_1 = \sum_i y_i A_i \\ c_2 = -\sum_i y_i A_i^{\frac{2}{3}} \\ c_3 = -\sum_i y_i \frac{Z_i(Z_i-1)}{A_i^{\frac{1}{3}}} \\ c_4 = -\sum_i y_i \frac{(A_i-2Z_i)^2}{A_i} \end{cases} \quad (12)$$

and

$$\begin{cases} b_1 = \sum_i A_i^2 \\ b_2 = b_5 = -\sum_i A_i^{\frac{5}{3}} \\ b_3 = b_9 = -\sum_i Z_i(Z_i-1)A_i^{\frac{2}{3}} \\ b_4 = b_{13} = -\sum_i (A_i - 2Z_i)^2 \\ b_6 = \sum_i A_i^{\frac{4}{3}} \\ b_7 = b_{10} = \sum_i Z_i(Z_i-1)A_i^{\frac{1}{3}} \\ b_8 = b_{14} = \sum_i \frac{(A_i-2Z_i)^2}{A_i^{\frac{1}{3}}} \\ b_{11} = \sum_i \frac{Z_i^2(Z_i-1)^2}{A_i^{\frac{2}{3}}} \\ b_{12} = b_{15} = \sum_i \frac{Z_i(Z_i-1)(A_i-2Z_i)^2}{A_i^{\frac{4}{3}}} \\ b_{16} = \sum_i \frac{(A_i-2Z_i)^4}{A_i^2} \end{cases} \quad (13)$$

The required determinants were c^2=931.494061 MeV/u, mass of hydrogen atom=1.007940u, and neutron mass=1.008665u. The results obtained through the LSM for volume, surface, coulomb, and asymmetry coefficients were a_v=15.519MeV ، a_s=17.476MeV ، a_c=0.674MeV and a_a=24.576MeV respectively.

4. Conclusion and Recommendation

Comparing the results obtained for volume, surface, coulomb, and asymmetry terms with those of other studies showed an appropriate compatibility. It is recommended to use more input data with higher accuracy obtained from more recent references, so as to increase the accuracy of the results. An estimation of neutron and hydrogen atom masses can be presented if their masses in equation (7) are regarded indeterminate.

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