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ESTIMATION OF NUCLEAR MASS FORMULAS COEFFICIENTS USING LEAST-SQUARES METHOD BASED ON GAUSS-SEIDEL SCHEME: A COMPARATIVE STUDY BETWEEN THREE MODELS

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This paper presents the analysis and implementation of the least-squares method based on the Gauss-Seidel scheme for solving nuclear mass formulas. The least-squares method leads to the solution of the system by iterations. The main advantages of the discussed method are simplicity and high accuracy. Moreover, the method enables us to process large data quickly in practice. To demonstrate the effectiveness of the method, implementation using the FORTRAN language is carried out. The steps of the algorithm are detailed. Using 2331 nuclear masses with $Z \geq 8$ and $N \geq 8$, it was shown that the performance of the liquid drop mass formula with six parameters improved in terms of root mean square (r.m.s. deviation equals 1.28 MeV), compared to the formula of liquid drop mass with six parameters without microscopic energy, deformation energy and congruence energy (r.m.s. deviation equals 2.65 MeV). The nuclear liquid drop model is revisited to make explicit the role of the microscopic corrections (shell and pairing). Deformation energy and the congruence energy estimate have been used to obtain the best fit. It is shown that the performance of the new approach is improved by a model of eight parameters, compared to the previous model of six parameters. The obtained r.m.s. result for the new liquid drop model in terms of masses is equal to 1.05 MeV.

Keywords: *Nuclear masses; Numerical methods; Binding energy; Shell correction; Pairing correction*

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1. INTRODUCTION

The determination of nuclear masses is one of the most crucial tools for accessing the binding energy within the nucleus, and therefore the total of all forces affecting the interior of the nucleus. Experimentally, there are a number of techniques for measuring masses in the fundamental as well as the excited state. When discussing the mass models, we're interested exclusively in theoretical models intended to calculate the nuclear masses of all bonded nuclei. At different levels, these models require experimental values for their calculations. The purpose of these models is to predict all quantities related to the nucleus: mass, binding energy or deformation energy, separation energy....etc. The three most common categories of existing models are: semi-empirical, macroscopic-microscopic and microscopic, plus two models of a different type [1]. These models have a property that applies to all nuclei globally with $Z, N \geq 8$. Among the models there are: SEMF: The Semi-Empirical Mass Formula and the LDM: Liquid-Drop Model. The macroscopic-microscopic models include the MS-LD: Myers and Świątecki model [2], a Strutinsky-type approach [3], the FRDM: Finite-Range Droplet Model, the FRLDM: Möller's Finite-Range Liquid-Drop Model [4], the TF: Thomas-Fermi nuclear model [5] or the ETFSI: Extended Thomas-Fermi plus Strutinsky Integral [6], and the LSDM: Lublin-Strasbourg Drop Model [7]. The models that are only microscopic are: Hartree-Fock-Bogoliubov (HFB21) approach [8], that employs Skyrme interactions, and the HFB strategy, utilizing the advantage of Gogny forces (GHFB) [9]. With the existence of two other models proving its effectiveness in nuclear mass calculations: the model of DZ: Duflo and Zuker [10] and that of KTUY: Koura et al. [11].

In nuclear physics, the first SEMF, known as the Weizsäcker formula or the Bethe-Weizsäcker formula [12], is used to estimate atomic mass in relation to mass number A and atomic number Z. The SEMF was proposed

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by Carl Friedrich Von Weizsäcker, in 1935 [13], [14], where the nucleus is seen as a liquid droplet containing protons and neutrons moving in a disorderly fashion. SEMF's reference formula for all macroscopic approaches has been able to retrieve a large number of nucleus properties such as nuclear masses, binding energies, separation energies, nuclear fission, although it does not provide for magic numbers. Next, a significant improvement in the LDM liquid droplet model was made after the incorporation of phenomenological microscopic corrections to the macroscopic terms. In fact, Myers and Świątecki took (made) the first step in this approach in 1966, who added layer correction and pairing corrections to the binding energy of the liquid drop [2]. This new microscopic-macroscopic model was very successful in reproducing nuclear data (masses, quadrupole moments, heights of fission barriers, ... etc.), when the layer corrections were more precisely evaluated using a method proposed by Strutinsky [15], [16], and the matching correction obtained in the Bardeen-Cooper-Schrieffer (BCS) approximation [2], [17], this introduced a simple algebraic layer correction, plus an attribution to a "clustering" effect of the novel equidistant distribution of individual particle levels, subsequently generating a series of gap band intervals at the observed magic numbers. In addition to this microscopic addition, Myers-Świątecki's final mass formula featured an empirical odd-even correction (pairing coefficient), and diverged from spherical symmetry through the incorporation of a shape dependence into the surface and Coulomb terms of Von Weizsäcker's semi-empirical equation.

Later, Strutinsky's theorem [3] appeared, that can be seen as an approximation of the Hartree-Fock (HF) approach [18], which offers an even more stringent microscopic formulation of Strutinsky's layer correction method [19]. Total binding energy is now decomposed into a macroscopic term and a microscopic term (denoting the layer and the pairing corrections), both of which are a function not only of A and Z, it also depends on a set of deformation parameters β, featuring the shape of the core. The significance of these upgrades was astonishing since the squared deviation (r.m.s) between theory and experiment decreased [20].

Recently years, a significant number of studies have been published on the subject of nuclear masses such as the published papers [21]–[27]. Interestingly, to date no researcher has discussed the proposed LDM formula of eight parameters with making a comparison between three models. Hence this work aim to presents the LDM formula of six parameters, the LDM formula of six parameters without (microscopic energy, deformation energy, and congruence energy), and the proposed LDM formula of eight parameters. The idea is based on adding two coefficients to the six-parameter LDM formula, which are the shell correction coefficient and the pairing correction coefficient. Correction coefficients are added to improve the root mean square value. Then, the Least Squares Method (LSM) is implemented to determine the parameters of the theoretical formulas. LSM is one of the widely employed methods for data fitting [24], where the method for different experimental cases is detailed in [28]. Two categories of least-squares problems can be distinguished: linear and non-linear, based on whether all unknown residuals are linear or non-linear. In statistical regression analysis, the linear least-squares problem has a closed-form solution.

The non-linear problem is generally solved by iterative refinement, where each iteration approximating the system by a linear system, so the basic calculation is similar in both cases [29]. This work is very significant considering the following merits: (1) an improved LDM formula of eight parameters is proposed. (2) A comparison between three liquid-drop models and comparison with other previous works are discussed. (3) A step-by-step tutorial for determining the parameters of nuclear masses formulas is presented using the least squares method. This paper will add to the information contained in the previous studies and give a new perspective about the application of the LSM with improved nuclear masses formulas.

This paper is divided into five sections, the second of which describes the implemented three liquid drop mass formulas. Next, principle of the least squares method is presented. In the fourth section, the theoretical and experimental results are shown and compared. Finally, the fifth section provides the conclusions of the study.

2. DESCRIPTION OF THE LIQUID DROP MASS MODELS

In this section, three LDM models are detailed; the six parameters LDM formula, the six parameters LDM formula without (microscopic energy, deformation energy, and congruence energy), and the proposed eight parameters LDM formula.

2.1. The six parameters liquid drop mass formula

In nuclear physics, the liquid drop mass formula is well known. LDM sometimes called the Liquid Drop Model, or Myers-Świątecki Liquid Drop (MS-LD) formula, it was developed by Von Weizsäcker [12], [30]. In accordance with the usual rules of the liquid drop model approaches, the mass of an atom with Z protons and N neutrons is described by the following relation [2], [5].

$$\begin{aligned} M_{theo}(Z,N,def) &= ZM_H + NM_n - 0.00001433Z^{2.39} \\ &+ b_{vol}\left(1 - k_{vol}I^2\right)A \\ &+ b_{surf}\left(1 - k_{surf}I^2\right)A^{2/3} \\ &+ b_{coul}\,Z^2/A^{1/3} \;-\; f_pZ^2/A \\ &+ E_{shell}(Z,N) + \; E_{pair}(Z,N) + \; E_{def}(Z,N) + E_{cong}(Z,N) \end{aligned} \tag{1}$$

Where:
A, Z and N: are the numbers of atoms, protons and neutrons, respectively (A = Z + N).
M_H is the hydrogen-atom mass excess, $M_H = 7.288970613$ MeV
M_n is the neutron mass excess, $M_n = 8.071317133$ MeV.
$Z^{2.39}$: is the binding energy of electrons.
$b_{vol}(1 - k_{vol}I^2)A$: is the volume energy term.
$b_{surf}(1 - k_{surf}I^2)A^{2/3}$: is the surface energy term.
$b_{coul}(Z^2/A^{1/3})$: is the Coulomb energy term.
$f_p(Z^2/A)$: is the Proton form-factor correction to the Coulomb energy term.
b_{coul}, R_0, e^2: are quantities defined by:

$$b_{coul} = \frac{3}{5}\frac{e^2}{R_0} \tag{2}$$

R_0: is the nuclear-radius constant, its value $R_0 = 1.16$ fm.
e^2: electronic charge squared, its value $e^2 = 1.4399764$ MeV.fm.
I: is the relative neutron excess, defined by:

$$I = \frac{N - Z}{N + Z} \tag{3}$$

$E_{def}(Z,N)$: is the deformation energy, the difference between a nucleus's macroscopic energy at equilibrium deformation and its energy if it were spherical [7]. The deformation energy is given by:

$$E_{def}(Z,N) = \; E(\beta) \; - \; E(\beta \; = \; 0) \tag{4}$$

β: is a set of parameters defining the deformation of the nucleus, $\beta = 0$ representing the spherical deformation (undeformed nucleus).
$E_{cong}(Z,N)$: is the congruence energy is described as:

$$E_{cong}(Z,N) = \; -10\exp\left(-4.2\;|I|\right) \tag{5}$$

$E_{shell}(Z,N)$, and $E_{pair}(Z,N)$: are the corrections of shell and pairing, respectively.
The microscopic energy is given by:

$$E_{micro}(Z,N) = \; E_{shell}(Z,N) \; + \; E_{pair}(Z,N) \tag{6}$$

E_{micro} containing the contributions from shell and paring effects coming from the protons and neutrons.
For simplifying the calculation, we put:

$$\begin{aligned} U(Z,N,def) &= E_{shell}(Z,N) + \; E_{pair}(Z,N) + \; E_{def}(Z,N) + E_{cong}(Z,N) \\ &+ ZM_H + NM_n - 0.00001433\,Z^{2.39} \end{aligned} \tag{7}$$

So, the model of the standard liquid drop can be expressed as follows:

$$\begin{aligned} M_{theo}(Z,N,def) &= b_{vol}\left(1 - k_{vol}I^2\right)A \\ &+ b_{surf}\left(1 - k_{surf}I^2\right)A^{2/3} \\ &+ b_{coul}\,Z^2/A^{1/3} \;-\; f_pZ^2/A \\ &+ U(Z,N,def) \end{aligned} \tag{8}$$

In literature, the least squares method is one of the best methods for solving the liquid drop model Eq. (1) in order to find the six parameters (b_{vol} , k_{vol}, b_{surf}, k_{surf}, b_{coul}, f_p), the steps of the method are illustrated in the next section, and results are discussed in the 4th section.

2.2. The six parameters liquid drop mass formula without (microscopic energy, deformation energy, and congruence energy)

In this part, we eliminate microscopic energy (the corrections of shell and pairing), deformation energy, and congruence energy to observe their impact on the root-mean-square value. So, the new liquid drop model can be expressed as follows:

$$\begin{aligned} M_{theo}(Z,N,def) &= ZM_H + NM_n - 0.00001433Z^{2.39} \\ &+ b_{vol}\left(1 - k_{vol}I^2\right)A \\ &+ b_{surf}\left(1 - k_{surf}I^2\right)A^{2/3} \\ &+ b_{coul}\,Z^2/A^{1/3} \; - \; f_pZ^2/A \end{aligned} \tag{9}$$

In order to find the six parameters (b_{vol} , k_{vol}, b_{surf}, k_{surf}, b_{coul}, f_p), the Least Squares Method (LSM) is used. The steps of the method are illustrated in the next section, and results are discussed in the 4th section.

2.3. The proposed eight parameters liquid drop mass formula

In this part, we add two coefficients to the previous equation Eq.1, which are the shell correction coefficient b_{sh} and the pairing correction coefficient b_{pa}. The microscopic corrections for pairing and shell effects treated as in Ref. [23]. Correction coefficients are added to improve the root mean square value. So, the new liquid drop model is described by the following relation:

$$\begin{aligned} M_{theo}(Z,N,def) &= ZM_H + NM_n - 0.00001433Z^{2.39} \\ &+ b_{vol}\left(1 - k_{vol}I^2\right)A \\ &+ b_{surf}\left(1 - k_{surf}I^2\right)A^{2/3} \\ &+ b_{coul}\,Z^2/A^{1/3} \; - \; f_pZ^2/A \\ &+ b_{sh}\,E_{shell}(Z,N) + \; b_{pa}\,E_{pair}(Z,N) + E_{def}(Z,N) + E_{cong}(Z,N) \end{aligned} \tag{10}$$

The Least Squares Method (LSM) is used to find the eight parameters (b_{vol} , k_{vol}, b_{surf}, k_{surf}, b_{coul}, f_p, b_{sh}, b_{pa}). The steps of the method are illustrated in the next section, and results are discussed in the 4th section.

3. THE LEAST SQUARES METHOD

The Least Squares Method is traditionally credited to Carl Friedrich Gauss, with origins dating back to 1795 [31], [32]. LSM finds utility across a range of scientific disciplines including statistics, geodesy, economics, optimization and more. The current study suggests utilizing LSM for optimizing the semi-empirical mass formula, or formulas with similar characteristics. Examples of models in this category include: (a) The FRDM and the FRLDM, which involve comprehensive calculations of shell and pairing corrections, along with consideration of various nuclear deformations [33], (b) The "Pomorski-Dudek Model" with shell and pairing corrections [7], (c) The "Royer Model" with shell and pairing corrections but no nuclear deformation [34], and (d) The "Myers Droplet Model based on the Thomas-Fermi Approximation" with or without shell correction [35]. These nuclear mass formulas play a vital role in assessing certain ground-state properties, nuclear reactions, and predicting the neutron/proton drip lines. All these formulas can be optimized using the same method, which is described by the following procedure.

A) **Define the root mean square deviation (R.M.S).**

The root mean square deviation (R.M.S) is defined by:

$$R.M.S = err(b_{vol},k_{vol},b_{surf},k_{surf},b_{coul},f_p) = \frac{1}{n}\sum_{i=1}^{i_{\max}}\left[M_{\exp}(i) - M_{theo}(i)\right]^2 \tag{11}$$

where:

n: is the total number of nuclides.

$M_{theo}(i)$: are the mass computed at a specific value of Z and N.

$M_{exp}(i)$: are experimental values of nuclear mass that calculated using the mass excess values found in on the recent updated Atomic Mass Evaluation, i.e. AME table, published in [36]. $M_{exp}(i)$ are given with MeV by the following formula:

$$M_{\exp}(i) = Mass\,excess \; + \; A\,.\,u \tag{12}$$

u: The atomic mass unit, $1u = 931.49410242$ MeV.

B) **Replacing the $M_{theo}(i)$ by its expression in the RMS deviation formula.**
In this step, we calculate $M_{theo}(i)$ by the given Eq.8, and replace results in Eq. 11. So, the root mean square deviation is described by:

$$R.M.S = \frac{1}{n}\sum_{i=1}^{i_{\max}} \begin{pmatrix} M_{\exp}(i) - b_{vol}\left(1 - k_{vol}I_i^2\right)A_i - b_{surf}\left(1 - k_{surf}I_i^2\right)A_i^{2/3} - \\ b_{coul}\, Z_i^2/A_i^{1/3} \quad + \; f_p Z_i^2/A_i \; - U_i\left(Z_i, N_i, def\right) \end{pmatrix}^2 \tag{13}$$

C) **Define the objective.**
According to LSM, the goal is to reduce the error in Eq. 11 to a minimum, thus:

$$\frac{\partial err\left(b_{vol}, k_{vol}, b_{surf}, k_{surf}, b_{coul}, f_p\right)}{\partial \chi|_{\chi = b_{vol},\, \cdots, f_p}} = 0 \tag{14}$$

D) **Construction of the model.**
The equations of model are given by:

$$\begin{cases} \frac{\partial err}{\partial b_{vol}} &= -2\sum\limits_{i=1}^{i_{\max}}\left(M_{\exp}(i) - M_{theo}(i)\right)\frac{\partial M_{theo}(i)}{\partial b_{vol}} &= 0 \\ \frac{\partial err}{\partial k_{vol}} &= -2\sum\limits_{i=1}^{i_{\max}}\left(M_{\exp}(i) - M_{theo}(i)\right)\frac{\partial M_{theo}(i)}{\partial k_{vol}} &= 0 \\ \frac{\partial err}{\partial b_{surf}} &= -2\sum\limits_{i=1}^{i_{\max}}\left(M_{\exp}(i) - M_{theo}(i)\right)\frac{\partial M_{theo}(i)}{\partial b_{surf}} &= 0 \\ \frac{\partial err}{\partial k_{surf}} &= -2\sum\limits_{i=1}^{i_{\max}}\left(M_{\exp}(i) - M_{theo}(i)\right)\frac{\partial M_{theo}(i)}{\partial k_{surf}} &= 0 \\ \frac{\partial err}{\partial b_{coul}} &= -2\sum\limits_{i=1}^{i_{\max}}\left(M_{\exp}(i) - M_{theo}(i)\right)\frac{\partial M_{theo}(i)}{\partial b_{coul}} &= 0 \\ \frac{\partial err}{\partial f_p} &= -2\sum\limits_{i=1}^{i_{\max}}\left(M_{\exp}(i) - M_{theo}(i)\right)\frac{\partial M_{theo}(i)}{\partial f_p} &= 0 \end{cases} \tag{15}$$

Where:

$$\begin{cases} \frac{\partial M_{\text{theo}}(i)}{\partial b_{\text{vol}}} = \sum_{i=1}^{i_{\max}}\left(A_i\left(1 - k_{\text{vol}}I_i^2\right)\right) \\ \frac{\partial M_{\text{theo}}(i)}{\partial k_{\text{vol}}} = -\sum_{i=1}^{i_{\max}}\left(b_{\text{vol}}A_iI_i^2\right) \\ \frac{\partial M_{\text{theo}}(i)}{\partial b_{\text{surf}}} = \sum_{i=1}^{i_{\max}}\left(A_i^{2/3}\left(1 - k_{\text{surf}}I_i^2\right)\right) \\ \frac{\partial M_{\text{theo}}(i)}{\partial k_{\text{surf}}} = -\sum_{i=1}^{i_{\max}}\left(b_{\text{surf}}A_i^{2/3}I_i^2\right) \\ \frac{\partial M_{\text{theo}}(i)}{\partial b_{\text{coul}}} = \sum_{i=1}^{i_{\max}}\left(Z_i^2/A_i^{1/3}\right) \\ \frac{\partial M_{\text{theo}}(i)}{\partial f_p} = -\sum_{i=1}^{i_{\max}}\left(Z_i^2/A_i\right) \end{cases} \tag{16}$$

E) **Solve the equations of model.**
Solutions of the model given by Eq. (15) are determined as follow:

$$b_{\text{vol}} = \frac{\begin{pmatrix} \sum_i A_iM_{\exp}(i) - b_{\text{surf}}\sum_i A_i^{5/3} + k_{\text{surf}}b_{\text{surf}}\sum_i A_i^{5/3}I_i^2 - \\ b_{\text{coul}}\sum_i A_i^{2/3}Z_i^2 + f_p\sum_i Z_i^2 - \sum_i A_iU_i - k_{\text{vol}}\sum_i A_iI_i^2M_{\exp}(i) + \\ k_{\text{vol}}b_{\text{surf}}\sum_i A_i^{5/3}I_i^2 - k_{\text{vol}}k_{\text{surf}}b_{\text{surf}}\sum_i A_i^{5/3}I_i^4 + \\ k_{\text{vol}}b_{\text{coul}}\sum_i A_i^{2/3}I_i^2Z_i^2 - k_{\text{vol}}f_p\sum_i I_i^2Z_i^2 + k_{\text{vol}}\sum_i A_iI_i^2U_i \end{pmatrix}}{\sum_i A_i^2 - 2k_{\text{vol}}\sum_i A_i^2I_i^2 + k_{\text{vol}}^2\sum_i A_i^2I_i^4} \tag{17}$$

$$k_{\text{vol}} = \frac{\begin{pmatrix} -\sum_i A_iI_i^2M_{\exp}(i) + b_{\text{vol}}\sum_i A_i^2I_i^2 + b_{\text{surf}}\sum_i A_i^{5/3}I_i^2 - k_{\text{surf}}b_{\text{surf}}\sum_i A_i^{5/3}I_i^4 + \\ b_{\text{coul}}\sum_i A_i^{2/3}I_i^2Z_i^2 - f_p\sum_i I_i^2Z_i^2 + \sum_i A_iI_i^2U_i \end{pmatrix}}{b_{\text{vol}}\sum_i A_i^2I_i^4} \tag{18}$$

$$b_{\text{surf}} = \frac{\left(\begin{array}{l} \sum_i A_i^{2/3} M_{\exp}(i) - b_{\text{vol}} \sum_i A_i^{5/3} + k_{\text{vol}} b_{\text{vol}} \sum_i A_i^{5/3} I_i^2 - b_{\text{coul}} \sum_i A_i^{1/3} Z_i^2 + \\ f_p \sum_i A_i^{-1/3} Z_i^2 - \sum_i A_i^{2/3} U_i - k_{\text{surf}} \sum_i A_i^{2/3} I_i^2 M_{\exp}(i) + \\ k_{\text{surf}} b_{\text{vol}} \sum_i A_i^{5/3} I_i^2 - k_{\text{surf}} k_{\text{vol}} b_{\text{vol}} \sum_i A_i^{5/3} I_i^4 + k_{\text{surf}} b_{\text{coul}} \sum_i A_i^{1/3} I_i^2 Z_i^2 - \\ k_{\text{surf}} f_p \sum_i A_i^{-1/3} I_i^2 Z_i^2 + k_{\text{surf}} \sum_i A_i^{2/3} I_i^2 U_i \end{array}\right)}{\sum_i A_i^{4/3} - 2k_{\text{surf}} \sum_i A_i^{4/3} I_i^2 + k_{\text{surf}}^2 \sum_i A_i^{4/3} I_i^4} \tag{19}$$

$$k_{\text{surf}} = \frac{\left(\begin{array}{l} -\sum_i A_i^{2/3} I_i^2 M_{\exp}(i) + b_{\text{vol}} \sum_i A_i^{5/3} I_i^2 - k_{\text{vol}} b_{\text{vol}} \sum_i A_i^{5/3} I_i^4 + \\ b_{\text{surf}} \sum_i A_i^{4/3} I_i^2 + b_{\text{coul}} \sum_i A_i^{1/3} I_i^2 Z_i^2 - f_p \sum_i A_i^{-1/3} I_i^2 Z_i^2 + \sum_i A_i^{2/3} I_i^2 U_i \end{array}\right)}{b_{\text{surf}} \sum_i A_i^{4/3} I_i^4} \tag{20}$$

$$b_{\text{coul}} = \frac{\left(\begin{array}{l} \sum_i A_i^{-1/3} Z_i^2 M_{\exp}(i) - b_{\text{vol}} \sum_i A_i^{2/3} Z_i^2 + k_{\text{vol}} b_{\text{vol}} \sum_i A_i^{2/3} I_i^2 Z_i^2 - b_{\text{surf}} \sum_i A_i^{1/3} Z_i^2 + \\ k_{\text{surf}} b_{\text{surf}} \sum_i A_i^{1/3} I_i^2 Z_i^2 + f_p \sum_i A_i^{-4/3} Z_i^4 - \sum_i A_i^{-1/3} Z_i^2 U_i \end{array}\right)}{\sum_i A_i^{-2/3} Z_i^4} \tag{21}$$

$$f_p = \frac{\left(\begin{array}{l} -\sum_i A_i^{-1} Z_i^2 M_{\exp}(i) + b_{\text{vol}} \sum_i Z_i^2 - k_{\text{vol}} b_{\text{vol}} \sum_i Z_i^2 I_i^2 + b_{\text{surf}} \sum_i A_i^{-1/3} Z_i^2 - \\ k_{\text{surf}} b_{\text{surf}} \sum_i A_i^{-1/3} I_i^2 Z_i^2 + b_{\text{coul}} \sum_i A_i^{-4/3} Z_i^4 + \sum_i A_i^{-1} Z_i^2 U_i \end{array}\right)}{\sum_i A_i^{-2} Z_i^4} \tag{22}$$

The Gauss-Seidel approach involves performing successive calculations of $(b_{vol}, k_{vol}, b_{surf}, k_{surf}, b_{coul}, f_p)$. At each iteration, the new value supersedes the previous one. Use Eq. (17) to determine the unknowns by an iterating sequence, where we choose the initial values $(b_{vol}^0, k_{vol}^0, b_{surf}^0, k_{surf}^0, b_{coul}^0, f_p^0)$ appropriately, the steps are as follows:

$$\left\{\begin{array}{ll} \left(b_{vol}^0, k_{vol}^0, b_{surf}^0, k_{surf}^0, b_{coul}^0, f_p^0\right) & \rightarrow \quad b_{vol}^1 \\ \left(b_{vol}^1, k_{vol}^0, b_{surf}^0, k_{surf}^0, b_{coul}^0, f_p^0\right) & \rightarrow \quad k_{vol}^1 \\ \left(b_{vol}^1, k_{vol}^1, b_{surf}^0, k_{surf}^0, b_{coul}^0, f_p^0\right) & \rightarrow \quad b_{surf}^1 \\ \left(b_{vol}^1, k_{vol}^1, b_{surf}^1, k_{surf}^0, b_{coul}^0, f_p^0\right) & \rightarrow \quad k_{surf}^1 \\ \left(b_{vol}^1, k_{vol}^1, b_{surf}^1, k_{surf}^1, b_{coul}^0, f_p^0\right) & \rightarrow \quad b_{coul}^1 \\ \left(b_{vol}^1, k_{vol}^1, b_{surf}^1, k_{surf}^1, b_{coul}^1, f_p^0\right) & \rightarrow \quad f_p^1 \\ \\ \left(b_{vol}^1, k_{vol}^1, b_{surf}^1, k_{surf}^1, b_{coul}^1, f_p^1\right) & \rightarrow \quad b_{vol}^2 \\ \left(b_{vol}^2, k_{vol}^1, b_{surf}^1, k_{surf}^1, b_{coul}^1, f_p^1\right) & \rightarrow \quad k_{vol}^2 \\ \left(b_{vol}^2, k_{vol}^2, b_{surf}^1, k_{surf}^1, b_{coul}^1, f_p^1\right) & \rightarrow \quad b_{surf}^2 \\ \left(b_{vol}^2, k_{vol}^2, b_{surf}^2, k_{surf}^1, b_{coul}^1, f_p^1\right) & \rightarrow \quad k_{surf}^2 \\ \left(b_{vol}^2, k_{vol}^2, b_{surf}^2, k_{surf}^2, b_{coul}^1, f_p^1\right) & \rightarrow \quad b_{coul}^2 \\ \left(b_{vol}^2, k_{vol}^2, b_{surf}^2, k_{surf}^2, b_{coul}^2, f_p^1\right) & \rightarrow \quad f_p^2 \\ \\ \left(b_{vol}^2, k_{vol}^2, b_{surf}^2, k_{surf}^2, b_{coul}^2, f_p^2\right) & \rightarrow \quad b_{vol}^3 \\ \quad \vdots & \quad \vdots \quad \vdots \\ \cdots & \quad \cdots \quad \cdots \end{array}\right. \tag{23}$$

F) **Update the values.**
The process is repeated till convergence is reached, i.e. until a stable set $(b_{vol}^k, k_{vol}^k, b_{surf}^k, k_{surf}^k, b_{coul}^k, f_p^k)$ after a sufficient number k of rounds, where k is a whole number.

4. RESULTS AND DISCUSSION

The LSM is made with FORTRAN code to solve the equations systems Eq. 8, Eq. 9, and Eq. 10 for 2331 nuclides. The achieved results are discussed in this section. Table 1 demonstrates the coefficients obtained using LSM for the discussed three models. $(SP-LDM)_1$: The Six Parameters LDM formula. $(SP-LDM)_2$: The Six Parameters LDM formula without (microscopic energy, deformation energy, and congruence energy. $(EP-LDM)$: The proposed Eight Parameters LDM formula.

Table 1. The coefficients obtained using LSM for the discussed three models.

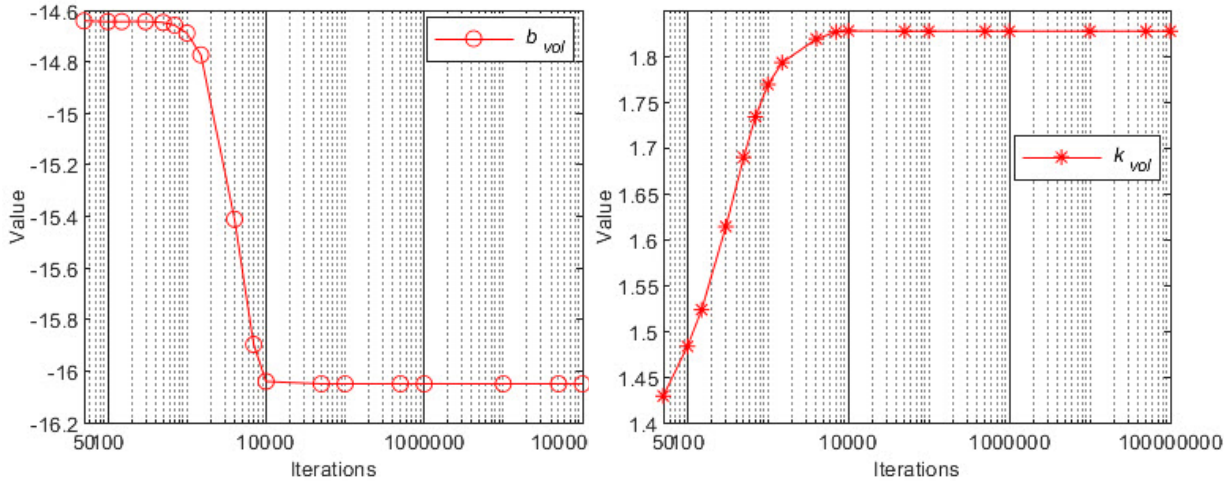
Coefficients (MeV)	$(SP-LDM)_1$	$(SP-LDM)_2$	$(EP-LDM)$
b_{vol}	-15.9727	-15.5986	-16.0498
k_{vol}	1.8397	1.6954	1.8272
b_{surf}	19.8832	18.9262	20.3437
k_{surf}	1.9206	1.5061	1.8925
b_{coul}	0.7327	0.7231	0.7390
f_p	1.2344	2.0543	1.4446
b_{sh}	-	-	0.7275
b_{pa}	-	-	0.6637
RMS	**1.28**	**2.65**	**1.05**

Table 2 demonstrates the obtained values versus iterations for the proposed eight parameters LDM Formula. Figures 1a, 1b, 2a, 2b, 3a, 3b, 4a, 4b depict the convergence of the eight coefficients $b_{vol}, k_{vol}, b_{surf}, k_{surf}, b_{coul}, f_p, b_{sh}, b_{pa}$, respectively.

Table 2. Iterations and convergence of the eight coefficients formula.

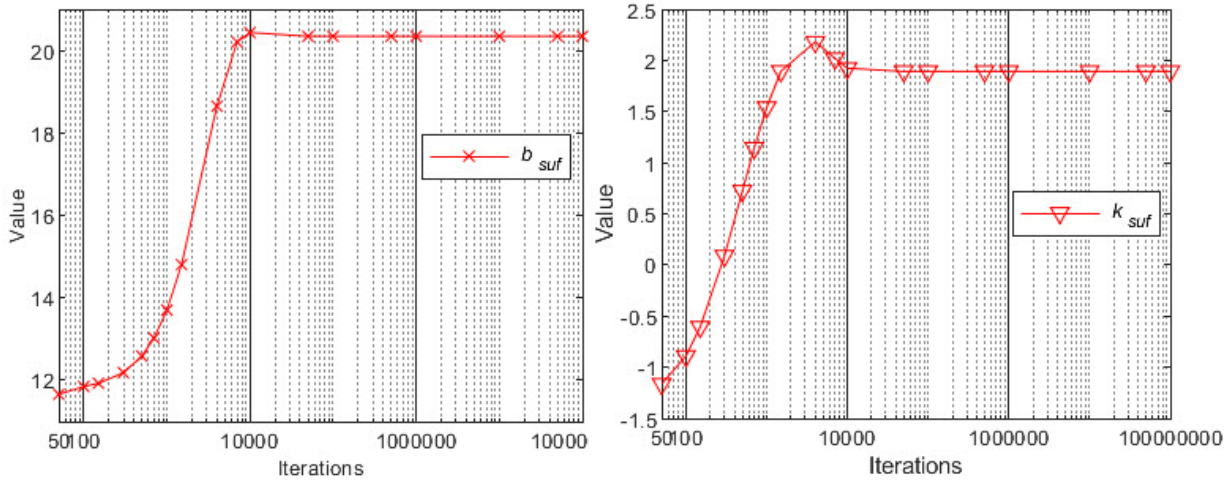
Iterations	b_{vol}	k_{vol}	b_{surf}	k_{surf}	b_{coul}	f_p	b_{sh}	b_{pa}
50	-14.641376	1.428979	11.660317	-1.163253	0.615636	-3.215885	1.174006	1.226985
100	-14.644251	1.483173	11.849770	-0.891092	0.600652	-3.450187	1.040020	0.985133
150	-14.644095	1.523160	11.929214	-0.605908	0.598580	-3.431418	1.030725	0.960194
300	-14.643833	1.613897	12.185625	0.088771	0.596867	-3.240858	1.021870	0.929168
500	-14.647650	1.689492	12.587653	0.723691	0.598327	-2.852138	1.005048	0.896717
700	-14.658353	1.733695	13.025564	1.143882	0.602349	-2.394916	0.985021	0.870226
1000	-14.688660	1.768886	13.703765	1.541319	0.610902	-1.689191	0.953279	0.837541
1500	-14.773100	1.792807	14.806025	1.893609	0.627683	-0.629695	0.903030	0.794445
4000	-15.410877	1.818667	18.649300	2.180657	0.698445	1.792211	0.757456	0.683832
7000	-15.896930	1.826270	20.206447	2.018919	0.733131	1.874165	0.720209	0.657450
10000	-16.040475	1.827507	20.432650	1.922742	0.740038	1.596387	0.721804	0.659292
50000	-16.049779	1.827150	20.343749	1.892542	0.739009	1.444598	0.727491	0.663692
100000	-16.049779	1.827150	20.343749	1.892542	0.739009	1.444598	0.727491	0.663692
500000	-16.049779	1.827150	20.343749	1.892542	0.739009	1.444598	0.727491	0.663692
1000000	-16.049779	1.827150	20.343749	1.892542	0.739009	1.444598	0.727491	0.663692
10000000	-16.049779	1.827150	20.343749	1.892542	0.739009	1.444598	0.727491	0.663692
50000000	-16.049779	1.827150	20.343749	1.892542	0.739009	1.444598	0.727491	0.663692
100000000	-16.049779	1.827150	20.343749	1.892542	0.739009	1.444598	0.727491	0.663692

The experimental values of nuclear mass are calculated using the mass excess equation given by Eq. 12. The experimental masses values are taken from the recently updated Atomic Mass Evaluation, i.e. AME table, published in [36]. The number of total iterations was set at 100,000,000 (100 million of iterations) to illustrates the convergence of parameters. However, despite the number of iterations, the execution time is of the order



(a) **(b)**

Figure 1. Convergence of b_{vol}, and k_{vol} coefficients versus iterations.



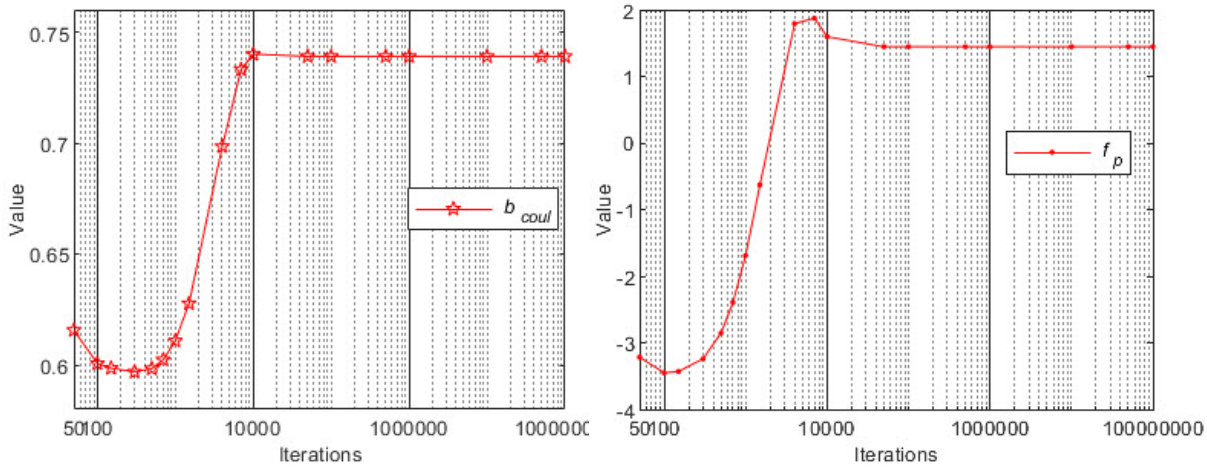
(a) **(b)**

Figure 2. Convergence of b_{surf}, and k_{surf} coefficients versus iterations.

of a few seconds for this case where only eight quantities varied. Coefficient values were recorded for a certain number of iterations (see Table 1). Results for all the eight coefficients are stable from 50,000 iterations onwards. Here, stability is defined by requiring that the 6 digits after the decimal point no longer change. With these stabilized values, we obtain a root-mean-square deviation given by Eq. 11, i.e. 1.05 MeV in the nuclear mass. As a result, shell and pairing corrections are necessary in these kinds of formulas. Root mean square deviation of 0.864 MeV has been achieved in our improved equation, published in [27], (which is not the subject of our study in this paper). On the other part, it should be pointed out that the direct comparison between the different types of mass formulas proposed in the literature is only a relative significance, as very often the "basis", i.e. the set and number of nuclei aren't the same. Other factors come into consideration, such as the fact that microscopic corrections are model-dependent. What's more, in some serious calculations, the root mean square deviation is weighted by a measurement error,... etc. The root mean square deviation can be improved by increasing the number of corrective terms and the introduction of the shell and pairing corrections.

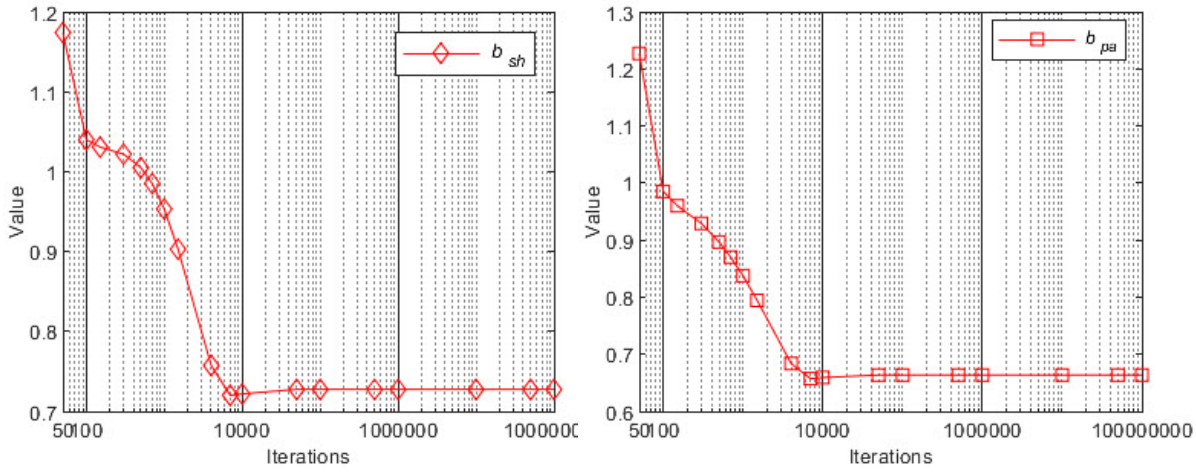
5. CONCLUSION

A new liquid drop model of eight parameters has been proposed in this paper. The main advantage of this proposed model is adding only two coefficients to the common six parameters model to improve the root mean square value. A comparative analysis of the proposed model with some proposed models in literature have been presented. A simple and fast algorithm based on the least squares method is used to find the eight



(a) **(b)**

Figure 3. Convergence of b_{coul}, and f_p coefficients versus iterations.



(a) **(b)**

Figure 4. Convergence of b_{sh}, and b_{pa} coefficients versus iterations.

parameters. The steps of the method are described in detail, where it is characterized by the maximum of simplicity in the procedure. The performance of the proposed model was verified using developed FORTRON program and checked with experimental nuclear DATA from Atomic Mass Data Center. A close concordance between theoretical and experimental values has been obtained. The results demonstrate that r.m.s. value for the new liquid drop model in terms of masses is equal to 1.05 MeV. Also, finding a mathematical formula for a liquid drop model that is close to reality is still a good problem for research because this will open way to new perspectives in the study of nuclei. The results of the present work join a growing body of literature in the field of theoretical physics, and the information presented opens new avenues for further studies on other models.

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ОЦІНКА КОЕФІЦІЄНТІВ ЯДЕРНОЇ МАСИ ЗА ДОПОМОГОЮ МЕТОДУ НАЙМЕНШИХ КВАДРАТІВ НА ОСНОВІ СХЕМИ ГАУССА-ЗЕЙДЕЛЯ: ПОРІВНЯЛЬНЕ ДОСЛІДЖЕННЯ МІЖ ТРЬОМА МОДЕЛЯМИ

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У цій статті представлено аналіз та реалізацію методу найменших квадратів на основі схеми Гаусса-Зейделя для розв'язування формул ядерної маси. Метод найменших квадратів приводить до розв'язку системи шляхом ітерацій. Основними перевагами розглянутого методу є простота і висока точність. Крім того, метод дозволяє нам швидко обробляти великі дані на практиці. Для демонстрації ефективності методу виконано реалізацію на мові FORTRAN. Деталізовано кроки алгоритму. Використовуючи 2331 ядерну масу з $Z \geq 8$ і $N \geq 8$, було показано, що продуктивність формули маси рідкої краплі з шістьма параметрами покращилася в термінах середньоквадратичного кореня (середньоквадратичне відхилення дорівнює 1,28 МеВ), порівняно з формулою маси краплі рідини з шістьма параметрами без мікроскопічної енергії, енергії деформації та енергії конгруентності (середньоквадратичне відхилення дорівнює 2,65 МеВ). Модель краплі ядерної рідини переглянуто, щоб чітко виявнити роль мікроскопічних поправок (оболонка та спарення). Енергія деформації та оцінка енергії конгруентності були використані для отримання найкращої відповідності. Показано, що ефективність нового підходу покращується за допомогою моделі восьми параметрів порівняно з попередньою моделлю шести параметрів. Отримане середньоквадратичне значення Результат для нової моделі рідкої краплі в термінах мас дорівнює 1,05 МеВ.

Ключові слова: *ядерні маси; чисельні методи; енергія зв'язку; корекція оболонки; виправлення пар*