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**Mémoire**

Présenté pour obtenir le diplôme de :

**Master En Physique**

**Spécialité : Physique Théorique**

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**Thème :**

Calculation of the coefficients of the Bethe-Weizsäcker Semi-Empirical Formula.

Soutenu publiquement/ le :26 /06 /2022, devant le jury composé de :

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Année universitaire : 2021/2022

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## Abstract

In our work, a numerical method optimizing the five energy coefficients of the semi empirical mass formula is presented. This method is based on the least-squares adjustments method on the atomic masses of 2550 different nuclides from the last update of the atomic mass evaluation, AME2020 published in February 2021. This lead to the resolution of a linear system which is solved by iterations according to the Gauss-Seidel method.

The obtained set of formula coefficients allowed us to reproduce most of the experimental values with a very good agreement for  $A > 50$ , yielding relative errors that oscillate between less than 0.05% and 1.5%.

**Keywords:** Semi Empirical Mass Formula, AME2020, Least-squares adjustment, Gauss-Seidel, Data Fitting.

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## Résumé

Dans notre travail, une méthode numérique optimisant les cinq coefficients d'énergie de la formule semi-empirique de masse est présentée. Cette méthode est basée sur la méthode des ajustements des moindres carrés sur les masses atomiques de 2550 différents nucléides de la dernière mise à jour de l'évaluation de la masse atomique, AME2020 publiée en février 2021. Cela conduit à un système linéaire qui était résolu par itérations selon à la méthode de Gauss-Seidel.

L'ensemble de coefficients de formule obtenu nous a permis de reproduire la plupart des valeurs expérimentales avec un très bon accord pour  $A > 50$ , donnant des erreurs relatives qui oscillent entre moins de 0.05% et 1.5%.

**Mots clés :** La formule semi-empirique de masse, AME2020, l'ajustement des moindres carrés, Gauss-Seidel, ajustement des données.

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## ملخص

في عملنا هذا، تم تقديم طريقة عددية لتحسين معاملات الطاقة الخمسة لصيغة الكتلة شبه التجريبية. تعتمد هذه الطريقة على تعديل المربعات الصغرى على الكتل الذرية لـ 2550 نويدات مختلفة مأخوذة من التحديث الأخير لتقييم الكتلة الذرية، AME2020 المنشور في فبراير 2021. أدى ذلك إلى حل نظام خطي عن طريق التكرارات وفق طريقة غوس-زايدل Gauss-Seidel.

سمحت لنا معاملات الصيغة التي تم الحصول عليها بإعادة إنتاج معظم القيم التجريبية باتفاق جيد جدًا من أجل  $A > 50$ ، ونتج عنها أخطاء نسبية تتأرجح بين أقل من 0.05% و 1.5%.

**كلمات مفتاحية:** صيغة الكتلة شبه التجريبية، AME2020، تعديل المربعات الصغرى، غوس-زايدل، توفيق البيانات.

## **Acknowledgement**

I wish to extend my special thanks to my supervisor, **Dr. MEKHTICHE Abdelhalim**, for his patience, guidance, and support.

Another big thank you to the members of the jury, the president **Dr. BOUCHACHIA Karim** and the examiners **Dr. DEKAR Liès** and **Dr. DAHMANE Djamilia**, to have accepted the evaluation of this work.

## **Dedication**

This submission is dedicated to my best friend, **ARKATI Anfel**, who has been there for me through my darkest times.

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## Introduction

One of the main aims of researches in nuclear physics is to describe the ground-state properties of all nuclei. A variety of models hence were introduced to study nuclear structure. These models with certain validity, can explain a limited number of certain properties. Between those theories, the liquid drop model (LDM) has been used with success despite its simplicity; it can describe for example the fission, fusion and  $\alpha$  decay potential barriers quite well.

Based on the LDM with some modifications, the Semi-Empirical Mass Formula (SEMF), usually known as Bethe–Weizsäcker formula has been developed as a good tool to describe the binding energy of any given nucleus at the ground level. By combining physical hypotheses with experimental data, the SEMF consists of different terms with specific coefficients. The accurate determination of these coefficients can provide theoretical predictions concerning a number of features of nuclei and their behaviors.

The aim of this work is to adjust the masses of 2550 nuclides using the latest update of the nuclear masses table (AME2020), to obtain a new set of the SEMF energy coefficients. A numerical code based on the least squares adjustments method was developed.

In the first chapter, we will explain the most fundamental nuclear properties, such as mass, binding energy and radii. We will focus on the atomic mass for being one of the most decisive factors governing nuclear stability, presenting the different methods used for accurate mass measurements, and then the Atomic Mass Evaluation AME; one of the most trusted resource for the experimented atomic mass values of all known nuclei today.

The second chapter will be devoted to present the Liquid Drop Model, then derive the Semi-Empirical Mass Formula with its five terms, giving an explanation to each of them. We will briefly talk about the limits of the SEMF and some other models as well.

In the third chapter, we will present the results of the five coefficients obtained after the adjustment of the experimental data by the least squares method. After that, an analysis, interpretation and comparison of the results obtained with the experimental ones will also be presented.

## Chapter 1

### Nuclear structure

One of the central challenges in nuclear physics is to come to a basic understanding of the structure and dynamics of nuclei. It is the key to understand the universe.

Nuclear structure studies the properties of nuclei in isolation such as nuclear mass, characteristic energy levels, and radioactive decay modes. This chapter aims to present a brief description of the general aspects of nuclear structure, particularly describing the most fundamental properties of a nucleus: nuclear mass and binding energy and how we can measure it.

#### 1.1. Atomic nuclei

Atomic nuclei are quantum bound states of particles called nucleons of which there are two types, the positively charged proton  $p$  and the uncharged neutron  $n$  [1]. Their main properties are summarized in Table 1.1.

A nucleus is therefore characterized by  $N$  number of neutrons, and by  $Z$  number of protons. The mass number  $A$  is the total number of nucleons, i.e.  $A = Z + N$ . A nucleus can be denoted as:

$${}^A X \leftrightarrow {}^A_Z X \leftrightarrow {}^A_Z X_N.$$

Where  $X$  is the chemical symbol.

Some particular sequences of nuclei have special names:

- **Isotopes:** have the same charge  $Z$ , but different  $N$ . The corresponding atoms have practically identical chemical properties, but very different nuclear properties.
- **Isobars:** have the same mass number  $A$ . Different isobars frequently have similar nuclear properties.
- **Isotones:** for nuclei of the same  $N$ , but different  $Z$ .
- **Isomers:** two nuclei are isomeric if they contain the same number of protons  $Z$  and the same number of neutrons  $N$ , but they are in different energy states.

Property	Proton $p$	Neutron $n$
Mass ( $kg$ )	$1.67262192369(51)\times 10^{-27}$	$1.67492749804(95)\times 10^{-27}$
Mass ( $MeV/c^2$ )	938.27208816(29)	939.56542052(54)
Method of mass measurement	Mass spectroscopy	n-p difference from nuclear reactions
Electric charge ( $C$ )	$1.602176634\times 10^{-19}$	0
Spin	1/2	1/2
Composition	uud	udd
Magnetic moment ( $J\cdot T^{-1}$ )	$1.4106067873(97)\times 10^{-26}$	$-9.6623647(23)\times 10^{-27}$

**Table 1.1.** The main properties of the nucleons [2].

## 1.2. Nuclear mass

The mass is a fundamental property of atomic nuclei and it reflects directly so many other properties. In general, the nuclear mass  $M\left({}_Z^A X\right)$  can be calculated from the atomic one  $M_A$ ; the mass of an atom at rest.

### 1.2.1. Mass units

#### 1.2.1.1. The Unified atomic mass unit

The atomic mass unit is a purely microscopic unit defined, since 1960 [3], as one twelfth of the mass of one free atom of  $^{12}C$  in its atomic and nuclear ground state and in its rest coordinate system [4]:

$$1u = M(^{12}C)/12.$$

Before 1960, there were two mass units: the physical one  $M(^{16}O)/16$ , and the chemical one, which considered one sixteenth of the average mass of a standard mixture of the three stable isotopes of oxygen [3]. Physicists could not convince the chemists to drop their unit because the change meant millions of dollars lost in sales. Joseph H. E. Mattauch, Truman P. Kohman and Aaldert H. Wapstra then calculated that, if  $M(^{12}C)/12$  was chosen, the change would be ten times smaller for them. That led to unification. 'u' stands therefore, officially, for 'unified mass unit' [5].

It is worth mentioning that the chemical mass-spectrometry community (e.g. biochemistry, polymer chemistry) widely uses the Dalton unit (symbol  $Da$ , named after John Dalton) which is an alternative name for the same unit and allows to express the number of nucleons in a molecule [4].

### 1.2.1.2. The electron volt

Mass measurement can be obtained by establishing an energy relation between the mass we want to determine and a well-known mass; as we will explain later. This energy relation is then expressed in electron-volts ( $eV$ ). The  $eV$  is defined as the kinetic energy of an electron after being accelerated from rest through a potential difference of one volt [1].

The choice of the volt in the unit is not evident: it can be expressed in  $V_{SI}$ , which is based on the internationally accepted definition (SI) or the one as *maintained*  $V_{90}$  by the Bureau International de Poids et Mesures (BIPM) [6];  $V_{90}$  was defined in 1990 by  $2e/h = 483597.9GHz/V_{90}$  [4].

It was demonstrated [4], that the energy would be expressed more precisely in the *maintained* volt than in the standard volt [5]. The relation between the two defined volts and their relations with the atomic mass unit can be expressed as:

$$V_{90} = 1.000\ 000\ 106\ 66\ V_{SI} [4]$$

$$1u = 931494.10242 \pm 0.0002\ keV_{SI} [4]$$

$$1u = 931494.0038 \pm 0.0004\ keV_{90} [5]$$

### 1.2.1.3. The kilogram

The kilogram is a macroscopic unit, being defined as the mass of a certain Platinum-Iridium bar housed in Sevres, a suburb of Paris. Atomic masses on the kilogram scale can be found by assembling a known (macroscopic) number of atoms and comparing the mass of the assembly with that of the bar [1].

In the current SI, the kilogram is defined by taking the fixed numerical value of the Planck constant  $h$  to be  $6.62607015 \cdot 10^{-34}\ J.s$ , which is equal to  $Kg.m^2.s^{-1}$ , where the meter and the second are defined by the fixed values of the speed of light in vacuum and frequency of

the ground-state Cesium hyperfine splitting [6]. With the new SI definition, the mass of an atom can be expressed in 'Kg' with higher precision [4].

### 1.2.2. Mass Defect

The actual nuclear mass is less than the masses of its components, because when a nucleus is formed, some of the mass is converted to energy and this results in the mass defect. The mass defect  $\Delta M$  is thus defined as the difference between the actual nuclear mass and the predicted mass calculated by adding the mass of protons and neutrons present in the nucleus:

$$\Delta M = Zm_p + (A - Z)m_n - M({}_Z^A X) \quad (1.1)$$

### 1.2.3. Mass Excess

The Mass excess  $\delta M$  of a nuclide is defined as the difference between its actual mass and its mass number in atomic mass units ( $u$ ).

$$\delta M = M({}_Z^A X) - A \quad (1.2)$$

The nuclear masses in atomic mass units are very close to the mass number  $A$ . This is the reason why usually the mass excess is used.

### 1.2.4. Atomic mass measurement

The history of atomic-mass measurements is as old as nuclear physics. We can consider that this activity began with *J.J. Thomson's* studies on nuclei, when in 1897, he measured the charge-to-mass ratio using electric and magnetic fields by tracking the trajectories of cathode rays containing electrical charges. Soon after by 1907 *Thomson* built what is considered the first spectrograph, and by 1918, *Arthur Jeffrey Dempster*, at the University of Chicago, built the first mass spectrometer [3]. Thanks to the constant developments of mass spectrometry and spectrographs, the experimental knowledge of atomic masses is rapidly expanding.

Two methods are used in atomic mass measurements: the "direct method" where the inertial masses are determined by means of mass spectrometry, and the "indirect method" where a reaction energy, is determined using a nuclear reaction or a decay process.

### 1.2.4.1. Direct Methods

The mass (expressed in  $u$ ) can be measured directly from its movement in an electromagnetic field; mass spectrometry. Using techniques based on the measurement of quantities proportional to the mass/charge ( $m/q$ ) ratio of ions [3]:

$$\frac{B\rho}{v} = \gamma \frac{m}{q} \quad (1.3)$$

Where  $B\rho$  is the magnetic rigidity of the charged ion,  $v$  the velocity,  $\gamma$  the Lorentz factor,  $m$  the rest mass and  $q$  the charge state.

However, such absolute measurements are limited by the precision of the devices and are usually not practical. To avoid the direct measurements of the absolute values of the apparatus, a delicate calibration is imperative [5].

#### a) Time of flight

The atomic mass of an ion can be deduced from the equation (1.3) by measuring the time of flight ( $TOF$ ); the time it takes to travel a fixed distance [7]:

$$B\rho = \gamma \frac{m}{q} \left( \frac{L}{TOF} \right) \quad (1.4)$$

where  $L$  is the flight length. Usually, the time of flight can be measured precisely while the magnetic rigidity and flight length are unknown. The mass of an ion of interest can be determined by using well-known masses as calibrants [5].

This technique offers a good opportunity to map a wide range of exotic and short-lived nuclides (down to  $1\mu s$ ) [7]. However, it cannot in most cases separate a ground state from an eventual (long-lived) isomeric state of a nuclide. Moreover, neither the magnetic rigidity nor the flight length can be measured with sufficient precision, which means that an unknown mass is usually deduced from a complex calibration function using as many reference nuclides as possible. This could lead to erroneous results [5].

### b) Cyclotron frequency

This technique is used especially in a Penning trap spectrometry. The principle of Penning-trap mass spectrometry is to measure the cyclotron angular frequency  $\omega_c$  of an ion in a magnetic field  $B$ , which is related to its mass-to-charge ratio by the following equation [5]:

$$\omega_c = \frac{q}{m} B \quad (1.5)$$

For better precision, high cyclotron frequency caused by highly charged state or strong magnetic field, and long observation time are desirable [5].

Nowadays this method, provides the most accurate and precise data in atomic mass measurements:  $7 \times 10^{-12}$  for stable nuclei [8], and up to  $10^{-7}$  for short-lived nuclides [5].

#### 1.2.4.2. Indirect methods

These methods establish an energy relation between two or more nuclides through reactions or decays, expressed in electron-volt ( $eV$ ).

However, the indirect methods are much useful in the case of stable nuclei than for exotic nuclei with short life-times because the information on their structure (energy levels, decay modes, etc.) is often scarce [3].

### a) Nuclear reaction energy [5]

From Einstein's Mass-Energy Equation  $E = mc^2$ , we know that the released energy in a reaction is directly related to the involved masses. For a nuclear reaction type  $A(a,b)B$ , the released (absorbed) energy is defined as:

$$Q = M_A + M_a - M_b - M_B \quad (1.6)$$

Where the masses of the target  $A$ , the projectile  $a$ , and the ejectile  $b$  are well known. Hence the mass of the fragment  $B$  can be derived by the measured  $Q$ -value based on reaction kinematics. Generally, the target, the projectile, and the ejectile are stable or very close to stability, and the fragment will not be very exotic.

## b) Nuclear decay energy

In nuclear-decay experiments, the decay energy is often measured to determine an unknown mass if the mass of its decay-companion is known.

- **$\beta$ -decay:** Since The  $\beta$ -decay spectrum has continuous distribution, the decay energy is obtained from the maximum energy so-called the *endpoint* energy. This spectrometry has long been used as a powerful tool to study the properties of nuclei not too far from stability [5].
- **$\alpha$ -decay:** The measurement of the  $\alpha$ -decay energy  $Q_\alpha$  yields the mass of a heavy nuclide. If the  $\alpha$ - decay chain ends up with a nuclide with known mass, then we can deduce all the masses along the chain from the succession of  $\alpha$  lines. For even-even nuclei, ground state to ground state transitions dominate and the assignment is usually reliable. For odd-odd nuclei, on the contrary, their  $\alpha$  decay does not go directly to the ground state for most of the cases [9].
- **proton radioactivity:** The masses of nuclides between  $Z = 50$  and  $Z = 80$  have been obtained mainly from proton radioactivity [10]. This special decay mode allows to investigate the properties of proton-rich nuclei.

Type of decay	$Q$ -value
$\beta^-$	$Q_{\beta^-} = M({}_Z^A X) - M({}_{Z+1}^A X)$
$\beta^+$	$Q_{\beta^+} = M({}_Z^A X) - M({}_{Z-1}^A X) - 2m_e c^2$
Electronic capture $EC$	$Q_{EC} = M({}_Z^A X) - M({}_{Z-1}^A X)$
$\alpha$	$Q_\alpha = M({}_Z^A X) - M({}_{Z-2}^{A-4} X) - M({}_2^4 He)$

**Table 1.2:**  $Q$ -value calculations of common types of decay [5].



### 1.3. Mass Evaluation

Scientists have accumulated a huge amount of data on a large number of nuclides. These nuclear data are of two classes [11]: one class is for data related to nuclides at rest (*static*) such as nuclear ground-state masses, radii, magnetic moments...etc. Whereas the other class is for those related to nuclidic dynamics, e.g. reaction properties and mechanisms.

The evaluation of atomic masses is subject to special ways of treating data because, as explained before, all mass measurements are relative measurements, which makes obtaining the best value for masses from numerous data hard [5]. For this purpose, several collections were published, each with specific data treatment.

1935	H. Bethe	Evaluation and table $^1_0n$ - $^{17}_8O$
1937	M.S. Livingston and H.A. Bethe	Combined evaluation: energies +masses
1946	G. Seaborg	The plutonium project table
1948	A.H. Wapstra	Table of atomic nuclei
1955	A.H. Wapstra and J.R. Huizenga	Isotopic masses
1960	F. Everling et al.	Relative nuclidic masses
1971	A.H. Wapstra and M.B. Gove	The 1971 atomic mass evaluation
1977	A.H. Wapstra and K. Bos	The 1977 atomic mass evaluation
1993	G. Audi and A.H. Wapstra	The 1993 atomic mass evaluation
2003	G. Audi <i>et al.</i>	The AME 2003 atomic mass evaluation
2016	G. Audi <i>et al.</i>	The AME 2016 atomic mass evaluation
2021	G. Audi <i>et al.</i>	The AME 2020 atomic mass evaluation

**Table 1.3:** Different evaluations of atomic masses throughout nuclear history [3].

#### 1.3.1. The Atomic Mass Evaluation

In the early 1950's it was found that the many mass measurement techniques (direct and indirect) overdetermined the mass value of many nuclides. *Aaldert H. Wapstra* established a procedure using a least-squares method to solve the problem of over-determination [3]. Since then, *Wapstra* has carried on the evaluation of the experimental masses of nuclei in what we call the *Atomic Mass Evaluation AME* [5].

AME is a horizontal evaluation; it means a unique nuclear property is being considered across the whole chart of nuclides, here the ground-state masses. Only such a structure allows to encompass all types of connections among nuclides [12].

The AME evaluators work primarily on three steps:

- The first step is to make a compilation, i.e., collect all available data. Up to the publication of AME2016, 24 different kinds of physics journals and conference proceedings were scanned [5].
- The second step is the critical reading process by making judgment on several parts [12]: calibration procedure, spectra examination and comparing the new results with the previous ones.
- The last step is to enter the new data in the AME database.

### 1.3.2. NUBASE evaluation

AME faced a problem of identifying - in some difficult cases - which state is the ground-state [4]. Up to the 1993 mass table, the AME was not concerned with all known cases of isomerism, but only in those that were relevant to the determination of the ground state masses. In AME 95 it was decided, to include all isomers. This was one of the main reasons for setting up a collaboration with NUBASE evaluation, leading to a thorough examination and evaluation of those ground state and isomeric properties that can help in identifying which state is the ground state and which states are involved in a mass measurement [12].

By evaluating all available experimental mass data, AME together with NUBASE serves the research community with the most reliable source for comprehensive information related to the atomic masses. For this reason, we will be using the latest *AME2020* (published in February 1st, 2021 [4]) together with the *NUBASE2020* in our work instead of other evaluations.

## 1.4. Stability of Nuclei

Nuclear stability means that the nucleus of an element is stable and thus it does not decay spontaneously emitting any kind of radioactivity.

### 1.4.1. Binding energy

As we have mentioned before, when a nucleus is formed, some of its mass is converted into energy. This energy is the binding energy  $BE$ , also defined as the energy that must be supplied to a nucleus at rest to dissociate it into its constituent nucleons.

The binding energy of a given nucleus is obtained based on Einstein's mass-energy equation  $\Delta E = \Delta mc^2$ :

$$BE({}_Z^A X) = (Zm_p + Nm_n - M({}_Z^A X)) \times c^2 \quad (1.7)$$

Where  $m_p$ ,  $m_n$  denote the proton and neutron mass respectively, and  $M({}_Z^A X)$  is the actual nuclear mass.

Since the binding energy is responsible for holding the nucleons in the nucleus. Nuclear stability is proportional to the nuclear binding energy. The more the binding energy per nucleon the greater is the nuclear stability.

**Note:** We often talk about the binding energy per nucleon which is the binding energy of the nucleus divided by its mass number  $BE/A$ .

### 1.4.2. Separation energy

In the nucleus, nucleons pile up according to the laws of quantum physics in quantum layers (energy levels). The energy needed to remove a nucleon (the least bound one) is called separation energy and can be calculated as follows:

$$S_n({}_Z^A X) = (M({}_Z^{A-1} X) + m_n - M({}_Z^A X)) \times c^2 \quad (1.8)$$

$$S_p({}_Z^A X) = (M({}_{Z-1}^{A-1} X) + M_p - M({}_Z^A X)) \times c^2 \quad (1.9)$$

Or by using binding energies as:

$$S_n \left( {}^A_Z X \right) = BE \left( {}^A_Z X \right) - BE \left( {}^{A-1}_Z X \right) \quad (1.10)$$

$$S_p \left( {}^A_Z X \right) = BE \left( {}^A_Z X \right) - BE \left( {}^{A-1}_{Z-1} X \right) \quad (1.11)$$

### 1.4.3. Stability criteria

Out of all the currently identified nuclides, only 252 are known to be stable. we can add 34 very long-lived nuclides to it. We then got 286 stable or practically stable nuclei [13]. The two main factors that determine nuclear stability are the neutron/proton ratio and the total number of nucleons  $A$  in the nucleus:

- For light elements the ratio of neutrons to protons is approximate to unity, therefore light elements are much more stable than heavy ones.
- Nuclides of even number of protons and/or neutrons are much more stable than those of odd  $Z$  and/or  $N$ . This was first pointed out by *Harkin* and has been confirmed by X-ray analysis [14].
- It was observed that the most stable nuclei have a number of protons or neutrons equal to: 2, 8, 20, 50, 82 or 126. These numbers are called *magic numbers*. Similarly, nuclei with 14, 28, & 40 nucleons are slightly less stable but more stable than the rest. These numbers are called *semi magic numbers*.

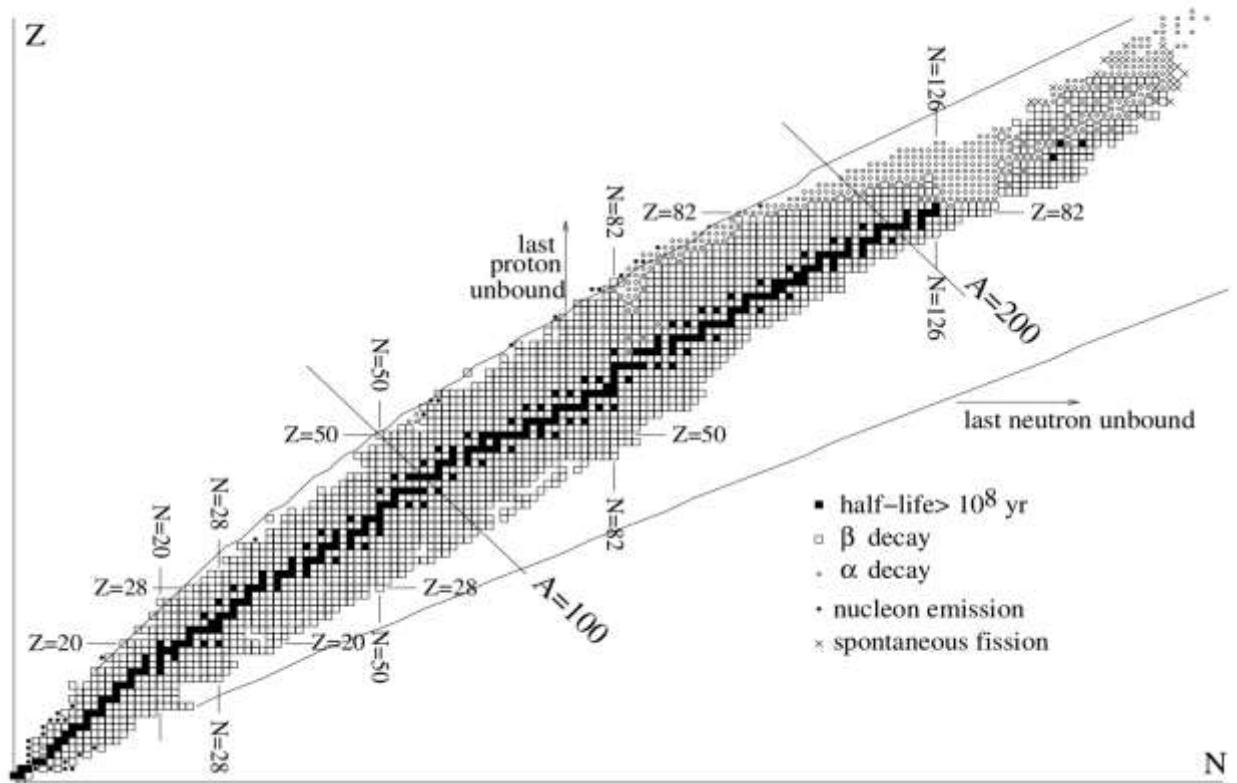


Figure 1.1: Band of stability [1].

## 1.5. Other properties

### 1.5.1. Radii

The volume  $V$  of a nucleus is, to a good approximation, proportional to the number of nucleons  $A$ , with each nucleon occupying a volume of the order of:

$$V_0 \approx 7.2 \text{ fm}^3 \quad (1.12)$$

In approximation, stable nuclei are spherical, so a volume of  $V = AV_0$  implies a radius:

$$r = r_0 A^{1/3} \quad (1.13)$$

with  $r_0 \approx 1.2 \text{ fm}$  [1].

The experimental access to obtain information on nuclear radii comes from scattering particles off the atomic nucleus with appropriate energy to map out the nuclear matter

distributions. Electron scattering off nuclei is, for example, one of the most appropriate methods to deduce radii [15].

nucleus	$r$ fm	$r/A^{1/3}$ fm	nucleus	$r$ fm	$r/A^{1/3}$ fm
$^1H$	1.0	1.0	$^{12}C$	3.04	1.33
$^4He$	2.08	1.31	$^{16}O$	3.41	1.35
$^6Li$	2.8	1.56	$^{24}Mg$	3.84	1.33
$^7Li$	2.8	1.49	$^{40}Ca$	4.54	1.32
$^9Be$	2.84	1.37	$^{122}Sb$	5.97	1.2

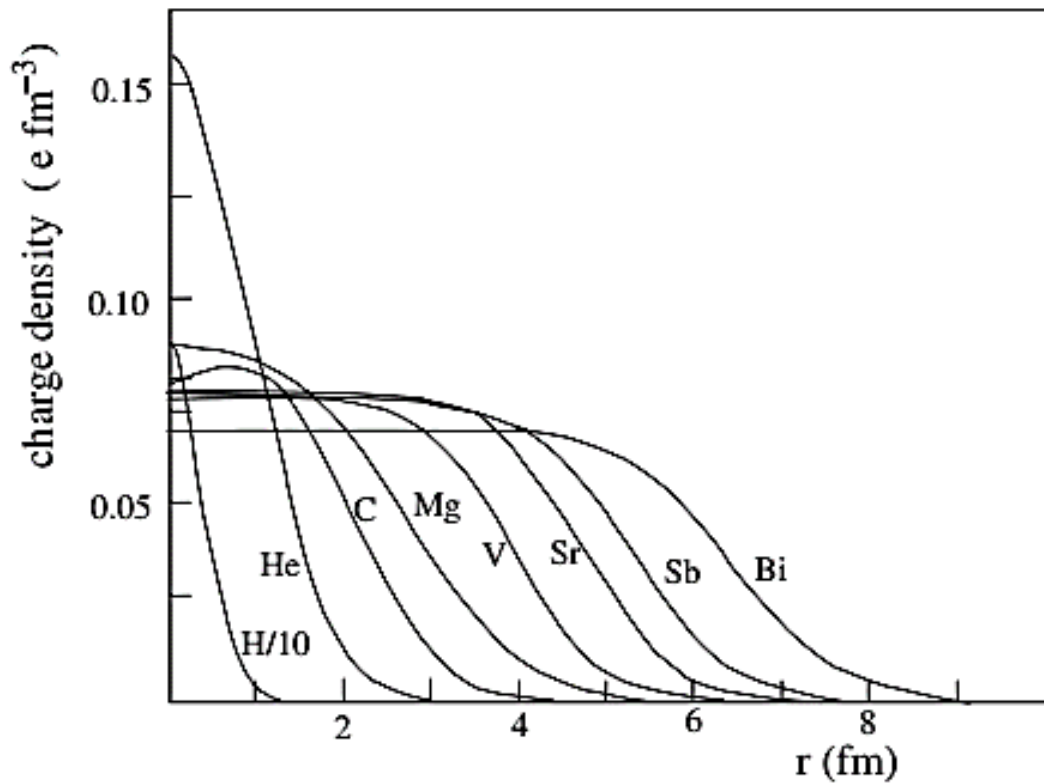
**Table 1.4:** Radii of selected nuclei as determined by electron–nucleus scattering [1].

### 1.5.2. Density [1]

We can determine the spatial distribution of nucleons inside a nucleus by scattering electrons off the nucleus. Electrons can penetrate inside the nucleus so their trajectories are sensitive to the charge distribution. This allows one to reconstruct the proton density. Assuming the neutron and proton densities are the same, we find a nucleon density inside nuclei of  $\rho_0 \approx 0.15 \text{ nucleons. fm}^{-3}$ .

As shown in figure 1.2:

- For  $A > 40$  the charge density, therefore the proton density, is roughly constant inside these nuclei. It is independent of the nucleus under consideration and it is roughly  $0.075$  protons per  $\text{fm}^3$ .
- Nuclear densities do not increase with increasing  $A$ , implying that a nucleon does not interact with all the others inside the nucleus, but only with its nearest neighbours. This phenomenon is the first aspect of a very important property called the saturation of nuclear forces.
- For nuclei with  $A < 20$ , charge densities are not flat but rather peaked near the centre. For such light nuclei, there is no well-defined radius and eq.(1.13) does not apply.



**Figure 1.2:** Experimental charge density ( $e \text{ fm}^{-3}$ ) according to  $r$  (fm) as determined in elastic electron–nucleus scattering [1].

## Conclusion

In this chapter we have presented the most fundamental nuclear properties that are needed for understanding the nuclear structure, focusing mostly on the nuclear mass: mass measurement, mass evaluation and its relation to the binding energy and the stability of nuclei.

## Chapter 2

### The Liquid Drop Model (LDM) and the Semi-Empirical Mass Formula (SEMF)

It is impossible to obtain the properties of nuclei starting from its constituents and their interactions alone. Therefore, there is a need to use models that represent their structure and internal motion.

Current models are essentially of two classes:

- **Collective models:** these models assume that the nucleons interact strongly with each other and thus they study phenomena that involve the nucleus as a whole [16]. The Liquid Drop model belongs to this first class.
- **Independent particle models [16]:** on the other hand, the models belonging to this class assume that the nucleons move independently in an overall potential, because the Pauli principle restricts the collisions of the nucleons inside the nuclear matter. The several forms of Shell models belong to this class.

In this chapter we will present the Liquid Drop Model: a collective model that represents the nucleus as a charged spherical drop. Then show how it was applied to formulate a semi-empirical mass formula that is successfully used to determine several properties of nuclei with good estimations.

#### 2.1. The Liquid Drop Model

The Liquid Drop Model (LDM) was historically the first model to describe nuclear properties. It was first proposed by *George Gamow* and then developed by *Niels Bohr* and *John Archibald Wheeler* [15] [17].

This model is based on the hypothesis that the nucleus has behaviour identical to that of a liquid, due mainly to the fact of the occurrence, in both cases, of saturation of forces between its constituents [16]. And therefore it assimilates the nucleus to an incompressible charged liquid drop based on the following assumptions [1]:

- 1) The nucleus is a sphere of radius  $r$ , such that:  $r = r_0 A^{1/3}$ ,  $r_0$  is the length of the order of average inter-particle distance.



- 2) The density of all nuclei is constant.
- 3) The volumetric charge density is constant: the protons are evenly distributed in the volume of the nucleus.
- 4) The nuclear force is identical for each nucleon. It does not depend on the nature of the nucleon (proton or neutron).
- 5) The Nuclear forces are short-range.

### 2.1.1. Saturation density [18]

The nuclear radius observed in various experiments is found to be proportional to the cube root of the mass number i.e.  $r = r_0 A^{1/3}$ , which implies that the nuclear volume  $V = \frac{4}{3} \pi r^3$  is proportional to  $A$  and, hence, the average nucleon density in the nucleus is approximately constant, irrespective of the mass number  $A$  of the nucleus for all stable nuclei:

$$\rho_0 = \frac{A}{V} = \frac{3}{4\pi r_0^3} \approx 0.17 \text{ fm}^{-3} \quad (2.1)$$

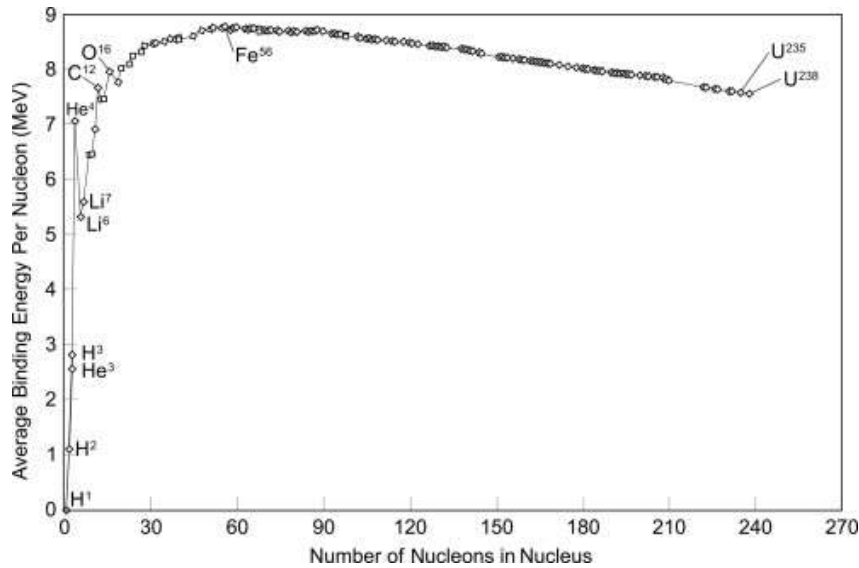
$\rho_0$  is called the *saturation density*.

### 2.1.2. Saturation of the binding energy

If the nucleon-nucleon interaction were the same for all possible nucleon pairs, the total binding energy would be proportional to the total number of pairs, which is equal to  $A(A-1)/2 \cong A^2/2$ . Therefore, the binding energy per nucleon would be proportional to  $A$ . The fact that this energy is constant is due to the short range of nuclear force, leading to the interaction of a nucleon with its neighbours [16].

$$\bar{E} = \frac{BE}{A} \approx 8 \pm 0.5 \text{ MeV} \quad (2.2)$$

$\bar{E}$  is called the saturation of binding energy in atomic nuclei [18].



**Figure 2.1.** Binding energy per nucleon of each isotope according to the mass number  $A$ . [19]

The figure above shows that the  $A$ -dependence is not really negligible. However, this dependence is smooth almost everywhere except for the region of the lightest nuclei [20].

## 2.2. The Semi-Empirical Mass Formula

There are many elaborate fits to the binding energies that use a large number of parameters [20]. An excellent parametrization of the binding energies of nuclei in their ground state was proposed in 1935 by *Bethe* and *Weizsäcker*. It is known as the Bethe-Weizsäcker Semi-Empirical Mass Formula (SEMF) [17]. The SEMF is reasonably successful in describing data around the line of stability and in predicting binding energies of new isotopes away from this line (although not very far away) [21].

As the name suggests, this formula is based partly on theory and partly on empirical measurements. The theory is based on the LDM which can account for most of the terms in the formula [17], but it also incorporates two quantum ingredients [1]. Although refinements have been made to the coefficients over the years, the structure of the formula remains the same today [21] [22].

The current formula which we will use in the next chapter is written as:

$$BE(A, Z) = a_v A - a_s A^{2/3} - a_c Z(Z-1) / A^{1/3} - \frac{a_a (A - 2Z)^2}{A} / A + \begin{cases} +a_p A^{-1/2}, & \text{for both } A \text{ and } Z \text{ even} \\ 0 & \text{,for } A \text{ odd and } Z \text{ even} \\ -a_p A^{-1/2}, & \text{for } A \text{ even and } Z \text{ odd} \end{cases} \quad (2.3)$$

Where  $a_v, a_s, a_c, a_a, a_p$  are the coefficients of the mass formula with dimension of energy contributing in: a volume term, a surface term, an electrostatic coulomb term, an asymmetry term and a pairing term.

### 2.2.1. The volume term

This volume term (or volume energy) expresses the fact that the nuclear force is saturated and thus, a certain part of the nuclear interior represents a given binding energy contribution [15]. Therefore, it is of the form:

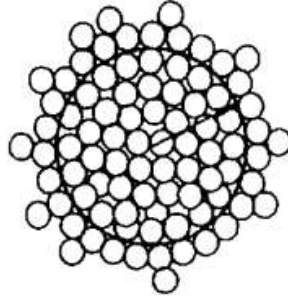
$$E_v = a_v A \quad (2.4)$$

### 2.2.2. The surface term

The following term was a correction since a deficit of binding energy for surface nucleons is expected, due to the fact that those nucleons have fewer near neighbours than deep within the nuclear matter [23].

This surface energy term takes that into account and is therefore negative and is proportional to the surface area [17]:  $4\pi r^2 = 4\pi r_0^2 A^{2/3}$ . The surface energy is therefore written as:

$$E_s = -a_s A^{2/3} \quad (2.5)$$



**Figure 2.2.** Pictorial representation of nuclear surface effects on binding energy. [15]

This energy gives the largest correction for the smallest  $A$ .

### 2.2.3. The Coulomb term

The electric repulsion between each pair of protons in a nucleus contributes toward decreasing its binding energy [17]. This force is long range and so every proton affects every other proton in the nucleus. We can evaluate this contribution as follows [15]:

We calculate the Coulomb energy using the assumption that the total nuclear charge  $Ze$  is spread uniformly throughout the spherical nuclear volume:

$$\rho_c = \frac{Ze}{\frac{4}{3}\pi r^3} \quad (2.6)$$

The Coulomb energy needed to add a spherical shell, to the outside of the sphere with radius  $r'$ , to give an increment  $dr'$  becomes:

$$E'_c = \frac{1}{4\pi\epsilon_0} \int_0^r \frac{\frac{4}{3}\pi r'^3 \rho_c 4\pi r'^2 \rho_c}{r'} dr' \quad (2.7)$$

Using the charge density (2.6), the integral becomes:

$$E'_c = \frac{3}{5} \frac{e^2}{4\pi\epsilon_0} \frac{Z^2}{r} \quad (2.8)$$

Above we have smoothed out the charge of  $Z$  nucleons over the whole nucleus, however the single proton should not have any contribution to the Coulomb energy and hence Coulomb self-energy contribution by each of  $Z$  protons should be removed:

$$\rho_p = \frac{e}{\frac{4}{3}\pi r^3} \quad (2.9)$$

And a self-Coulomb energy for  $Z$  protons is;

$$E_c'' = \frac{3}{5} \frac{e^2}{4\pi\epsilon_0} \frac{Z}{r} \quad (2.10)$$

The total coulomb energy correction becomes:

$$E_c = E_c' - E_c'' = \frac{3}{5} \frac{1}{4\pi\epsilon_0} \frac{Z(Z-1)}{r} \quad (2.11)$$

Thus, the third term is:

$$E_C = -a_c \frac{Z(Z-1)}{A^{1/3}} \quad (2.12)$$

With the coefficient is :  $a_c = \frac{3}{20\pi\epsilon_0 r_0}$  .

**Note:** The Coulomb energy correction is relatively weak but its influence grows very fast for heavy nuclei [20].

#### 2.2.4. The asymmetry term

The fourth term also called *Pauli Energy* is an empirical quantum mechanical term that accounts for the fact that if  $N \neq Z$ , the energy of the nucleus increases and the binding energy decreases because of the exclusion principle. We can explain that as follows [15]:

- a. The binding energy of nuclei is maximum when nucleons occupy the lowest possible orbitals. The Pauli principle, however, prevents the occupation of a certain orbital by more than two identical nucleons with opposite intrinsic spin orientations. The symmetric distribution  $Z = N = A/2$  proves be the energetically most favoured but is impossible due to the Coulomb energy. Any other repartition,  $N = A/2+n$  and  $Z = A/2-n$  will involve

lifting particles from occupied into empty orbitals. If the average energy separation between adjacent orbitals amounts to  $\Delta$ , replacing  $n$  nucleons will cost an energy loss of:

$$\Delta BE = n \left( \Delta \frac{n}{2} \right) \quad (2.13)$$

and with  $n = (N - Z) / 2$ , this becomes:

$$\Delta BE = \frac{1}{8} (N - Z)^2 \Delta \quad (2.14)$$

- b.** The potential depth describing the nuclear well does not vary much with changing mean number and thus, the average energy spacing between the single particles, delta, should vary inversely proportionally to  $A$ .

The final result becomes:

$$E_a = -a_a \frac{(N - Z)^2}{A} = -a_a \frac{(A - 2Z)^2}{A} \quad (2.15)$$

### 2.2.5. The pairing term

The last term is an empirical one as well, that arises from the tendency of the nucleons to form pairs (proton pairs, neutron pairs) in the nucleus under the influence of the short-range nucleon-nucleon attractive force.

This occurs because of the different overlap of wave functions for pairs of nuclei in various states. For two identical nucleons in the same spatial state, with opposite spins to be antisymmetric as required, then the spatial wave functions are effectively identical and have maximal overlap. Because of the short range force, this gives more of a binding energy for this particular pair. This effect occurs for all nucleons except potentially the ones in the highest occupied energy level for each type of nucleon, where there is either one or two nucleons of that type. Hence, the nucleus will be more strongly bound for ones with an even number of nucleons of either type [17] [23]. We introduce the pairing term as follows:

$$E_p = \begin{cases} +\delta & \text{for even-even nuclei,} \\ 0 & \text{for odd nuclei,} \\ -\delta & \text{for odd-odd nuclei.} \end{cases} \quad (2.16)$$

Chapter 2 The Liquid Drop Model (LDM) and the Semi-Empirical Mass Formula (SEMF).

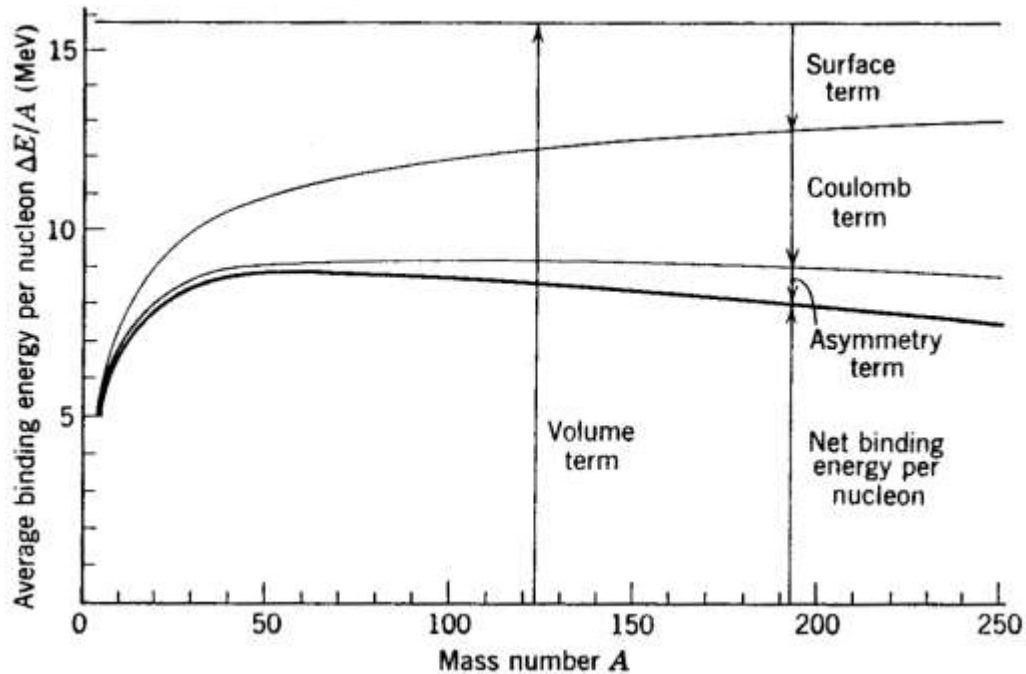
- *Even-even* meaning an even number of both protons and neutrons, and hence even  $A$ . This has both pairs strongly bound.
- *Odd-odd* meaning an odd number of both protons and neutrons, and hence also even  $A$ . This is the least strongly bound.
- *Even-odd* meaning an even number of one type and an odd number of the other, and hence odd  $A$ . This has one strongly bound pair and so should be half way in between the previous two; equalling to zero.

Empirically it was found  $\delta \cong a_p A^{-1/2}$ .

The following table gives the number of stable nuclei classified according to the parity or the oddness of  $Z$  and  $N$ :

<b>Z-N</b>	<b>E-E</b>	<b>O-O</b>	<b>E-O</b>	<b>O-E</b>	<b>Total</b>
Stable	146	5	53	48	252
Long-lived	21	4	4	5	34
All primordial	167	9	57	53	286

**Table 2.1:** Number of stable nuclei according to the parity or oddness of their  $Z$  and  $N$  [13].



**Figure 2.3.** Contributions to the binding energy per nucleon according to  $A$ , from each term in the semi-empirical mass formula. [15].

### 2.3. Determining the SEMF coefficients

The coefficients of the terms in the SEMF can be evaluated using theoretical calculations and hundreds of experimental data fitness that is obtained by various methods such as:

- The measurement of atomic masses by the mass spectrometer
- The balance measurement of nuclear reactions.
- The study of the stability of nuclei vis-à-vis.
- Beta radioactivity.

In the next chapter we will show how we can use theoretical calculations to fit hundreds of experimental mass data to calculate these coefficients with a good precision.



## 2.4. The limits of the SEMF and the LDM and their improvements

So far the current SEMF is accepted, giving us not only an appropriate estimation for atomic masses and the binding energies, but also providing theoretical predictions concerning a number of features of nuclei and their behaviour. However, as we will see in the third chapter, this model does not perform well with light nuclei. It also fails to explain the appearance of magic numbers and the extra binding energy and measure of stability that are associated with these numbers of nucleons.

For these reasons, many papers and research has been dedicated to the improvement of the SEMF. Some terms have been extended or modified over the years and new terms have been proposed using different methods of corrections such as [24]: microscopic corrections for shell behaviour, deformation, nuclear incompressibility, nucleon pairing... etc. We will mention some of the most important corrections.

### 2.4.1. Surface and Coulomb energy corrections [15].

For nuclei, which deviate from a spherical shape, both the surface and Coulomb energy corrections will change in a specific way. If we denote the nucleus with its lowest deformation multipoles via the  $(\theta, \varphi)$  expansion:

$$r = r_0 (1 + \alpha_2 P_2 \cos \theta + \alpha_4 P_4 \cos \theta) \quad (2.17)$$

Where  $P_2, P_4$  are Legendre's polynomials.

Correction functions for surface energy  $g(\alpha_2, \alpha_4)$  and for Coulomb energy  $f(\alpha_2, \alpha_4)$  appear in the expression for the BE i.e. we obtain a result :

$$E_s + E_c = -a_s g(\alpha_2, \alpha_4) A^{2/3} - a_c f(\alpha_2, \alpha_4) Z(Z-1) A^{-1/3} \quad (2.18)$$

A simple illustration of the above modification is obtained for an ellipsoidal deformation and, retaining a constant volume for the deformation, we get the major axis  $a = r(1 + \epsilon)$  and the

minor axis  $b = r(1 + \epsilon)^{-1/2}$  where  $\epsilon = \sqrt{1 - \left(\frac{b^2}{a^2}\right)}$  is the deformation parameter .

Using the parameter of deformation  $\epsilon$ , the surface and Coulomb energy terms become:

$$\begin{aligned} E_s &= a_s A^{2/3} \left(1 + \frac{2}{5\epsilon^2}\right) \\ E_C &= a_c Z(Z-1)A^{-1/3} \left(1 - \frac{1}{5\epsilon^2}\right) \end{aligned} \quad (2.19)$$

$\epsilon=0$  corresponds to the spherical nucleus.

### 2.4.2. Shell corrections

There exist different ways of implementing shell corrections to the LDM, with large differences between the shell correction energy in various approaches (closed-shell nuclei, mid-shell...) [25].

A simple method was proposed based on counting the number of valence nucleons, as suggested by the interacting boson model (IBM) [26]. This “shell” correction is linear and quadratic in the total number of valence nucleons [25]:

$$E_{shell}(N, Z) = b_1(n_v + z_v) + b_2(n_v + z_v)^2 \quad (2.20)$$

where  $n_v$  and  $z_v$  are the numbers of valence neutrons and protons and  $b_i$  are parameters.

Inclusion of these two terms in the LDM mass formula reduces the *rms* deviation [25].

### 2.4.3. Corrections on the radii [25]

In addition to the binding energies, charge radii of nuclei provide valuable information on how ground-state properties of nuclei vary with  $N$  and  $Z$ . The simple parametrization  $r = r_0 A^{1/3}$  provides only a very rough and qualitative description of charge radii. To obtain a quantitative description in a generalized LDM approach, one needs to take into account an isovector term; furthermore, it is necessary to include shell effects.

A good fit to charge radii of closed shell nuclei was obtained with:

$$r_p = r_0 A^{1/3} \left(1 - \nu \frac{(N-Z)}{A^{4/3}} - \omega \frac{(N-Z)^2}{A^2}\right) e^{g/A} \quad (2.21)$$

Where  $\nu$  and  $\omega$  are parameters. The small correction  $e^{g/A}$  (with  $g \approx 1.04$ ) accounts for the larger radii of light nuclei.

For open shell nuclei the inclusion of a shell correction was found to be necessary. Assuming charge symmetry, we find it convenient to decompose the radius into an isoscalar part  $R_0$  (representing the mass radius) and an isovector part  $R_1$ , which changes sign under the interchange of neutrons and protons. If one allows in addition for a small charge symmetry-breaking Coulomb correction, the following parametrization results:

$$R_i(N, Z) = R_0(N, Z) \pm \frac{N-Z}{2A} R_1(N, Z) \pm \frac{1}{2} \delta R_c(N, Z) \quad (2.22)$$

where  $i = n, p$  and the upper (lower) sign applies to neutrons (protons). The explicit dependence of  $R_i(N, Z)$  on  $N$  and  $Z$  will be suppressed in the following. We parametrize the mass radius,  $R_0 = (R_n + R_p)/2$ , in the following simple way:

$$R_0 = r_0 A^{1/3} + a A^{-2/3} + c(N-Z)^2 / A^2 \quad (2.23)$$

## 2.5. Other Models

Today we have a clear notion that the nucleus can exhibit both collective and independent particle phenomena, and therefore each class of models finds its usefulness in the explanation of a specific group of properties. There exist other models as well that treat the nucleus as a quantum system which are the only ones capable of giving a justification to some specific quantum problems [21].

Among these models we mention:

- **The Infinite Nuclear Matter (INM) model:** in which the ground-state energy of a nucleus is considered to be equal to the energy of a perfect sphere made up of infinite nuclear matter plus the residual characteristic energy called the local energy [27]. This model has much better ability for predicting masses of nuclei in the unknown region far from stability [28].
- **Duflo-Zuker's model [29]:** this model is based on the sequential filling of a pre-assumed shell structure where the monopole Hamiltonian represents an averaged mean field extracted from the interacting shell model.

- **The Garvey-Kelson model (GK) [30]:** The formalism of this model is based on local mass relations that are derived from a few simple physical principles (such as isospin symmetry) and a central assumption of a nuclear mean field and residual interaction that vary slowly with atomic number.
- **The Relativistic Mean Field theory (RMF):** Relativistic mean-field theory is used to describe ground-state deformations of nuclei. The relativistic Hartree equations are solved by expansion of the nucleon wave functions and the meson field in a harmonic-oscillator basis [31]. RMF received wide attention due to its many successes in describing lots of nuclear phenomena as well as successful applications in astrophysics [21].

We should note that these models and many others undergo constitutive corrections to improve their predictions.

## **Conclusion**

In this chapter we have presented the Bethe-Weizsäcker Semi-Empirical Mass Formula that was based on the Liquid Drop Model of the nucleus. This formula has five terms with five coefficients that can be determined in a semi empirical method and therefore can be used to predict many nuclear properties.

## Chapter 3

### Estimation of the Semi-Empirical Mass Formula Coefficients

This chapter is devoted to obtain a new set of the SEMF coefficients based on an update of the nuclear masses table AME2020, which was processed using a numerical code that we have developed based on the least squares adjustments method. The obtained set of coefficients allowed us to reproduce the values of the atomic masses and the binding energies for each nucleus. Then we perform a comparison with those of the AME2020 on one hand, and those of previous works on the other hand. Finally, relative errors were calculated to confirm that the revisited formula is in good agreement with the experimental data.

#### 3.1. The Least Squares adjustment

##### 3.1.1. The method of the Least Squares

As the name implies the method of Least Squares (LS) minimizes the sum of the squares of the estimated errors, frequently called *residuals*. It can be applied either in a simple form where all errors equally affect the solution or in an extended form when the contribution of each error is counted regarding its importance, this is called *weight*. The concept of weight is proportionally related to the precision of the corresponding measurement or inversely proportional to its uncertainty; larger weights are associated with more precise measurements [29].

This method can be expressed in mathematical terms as follows:

The residual  $r_i$  is the difference between the actual value of a measurement  $y_i$  and the predicted value using the theoretical model  $f(x_i)$ :

$$r_i = (y_i - f(x_i)) \quad (3.1)$$

The sum of the squares residuals is thus:

$$S = \sum_{i=1}^N r_i^2 = \sum_{i=1}^N (y_i - f(x_i))^2 \quad (3.2)$$

The function  $S$  can be thought of as a measure of the distance between the experimental data and the theoretical model that predicts this data for  $N$  number of measurements [32].

The standard deviation  $\sigma$  of the uncertainty is therefore:

$$\sigma^2 = \frac{S}{N} = \frac{1}{N} \sum_{i=1}^N (y_i - f(x_i))^2 \quad (3.3)$$

To be at a minimum, the first derivative must admit a critical point, and the second-order direct partial derivatives must be positive [33]:

$$\frac{\partial \sigma^2}{\partial x_i} = 0 \quad \text{and} \quad \frac{\partial^2 \sigma^2}{\partial x_i^2} > 0 \quad (3.4)$$

## 3.2. Calculation of the Semi-Empirical Mass Formula Coefficients

In this section, we aim to calculate the five coefficients of the SEMF using the LS adjustment. The standard deviation previously defined becomes:

$$\sigma^2 = \frac{1}{N} \sum_{i=1}^N (M_{ex}^i - M_{th}^i)^2 \quad (3.5)$$

where  $N$  is the number of nuclides,  $M_{ex}^i$  is the experimental atomic mass value of the nuclide  $i$  and  $M_{th}^i$  is the theoretical one obtained by the SEMF.

The set of experimental nuclear masses are obtained from *AME2020*, the most recent evaluation database. Only measured nuclei are included into our consideration. The masses extrapolated from systematics and marked with the symbol # in the error column are not taken into account here. Therefore, we use only 2550 experimental nuclear masses, excluding the Hydrogen atom; The LDM cannot describe the binding energy of a nucleus with one nucleon, although including the Hydrogen atom does not influence the obtained values much.

### 3.2.1. The theoretical atomic mass using the SEMF

The atomic mass of an element is the sum of the masses of its nucleus  $M\left({}_Z^A X\right)$  and its electrons:

$$M_{th} = M\left({}_Z^A X\right) + Z m_e - \frac{B_e}{c^2} \quad (3.6)$$

Where  $B_e$  is the electronic binding energy.

An approximate formula for  $B_e$  can be found in the review of Lunney, Pearson and Thibault [4]:

$$B_e = 14.4381 \times 10^{-6} Z^{2.39} + 1.55468 \times 10^{-12} Z^{5.35} \quad (MeV) \quad (3.7)$$

Using the binding energy eq (2.3), we get therefore the theoretical atomic mass of the SEMF:

$$M_{th} = Z(m_p + m_e) + (A - Z)m_n - \frac{1}{c^2} \left( a_v A - a_s A^{\frac{2}{3}} - a_c \frac{Z(Z-1)}{A^{\frac{1}{3}}} - a_a \frac{(A-2Z)^2}{A} \pm a_p A^{\frac{1}{2}} - 14.4381 \times 10^{-6} Z^{2.39} + 1.55468 \times 10^{-12} Z^{5.35} \right) \quad (3.8)$$

### 3.2.2. The linear equations

By minimizing  $\sigma^2$  for each coefficient we obtained a set of linear equations with five variables  $a_v$ ,  $a_s$ ,  $a_c$ ,  $a_a$  and  $a_p$ :

$$\frac{\partial \sigma^2}{\partial a_v} = 0 \Rightarrow \frac{2}{N} \sum_{i=1}^N A_i (M_{ex}^i - M_{th}^i) = 0 \quad (3.9)$$

$$\frac{\partial \sigma^2}{\partial a_s} = 0 \Rightarrow \frac{2}{N} \sum_{i=1}^N A_i^{\frac{2}{3}} (M_{ex}^i - M_{th}^i) = 0 \quad (3.10)$$

$$\frac{\partial \sigma^2}{\partial a_c} = 0 \Rightarrow \frac{2}{N} \sum_{i=1}^N Z_i (Z_i - 1) A_i^{\frac{1}{3}} (M_{ex}^i - M_{th}^i) = 0 \quad (3.11)$$

$$\frac{\partial \sigma^2}{\partial a_a} = 0 \Rightarrow \frac{2}{N} \sum_{i=1}^N \frac{(A_i - 2Z_i)^2}{A_i} (M_{ex}^i - M_{th}^i) = 0 \quad (3.12)$$

$$\frac{\partial \sigma^2}{\partial a_p} = 0 \Rightarrow \frac{2}{N} \sum_{i=1}^N \pm A_i^{-\frac{1}{2}} (M_{ex}^i - M_{th}^i) = 0 \quad (3.13)$$

The system formed by the five linear equations (3.9-3.13), can be writing in a matrix form as:

$$A\vec{X} = \vec{B} \quad (3.14)$$

Where

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25} \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} \\ a_{51} & a_{52} & a_{53} & a_{54} & a_{55} \end{pmatrix} \begin{pmatrix} a_v \\ a_s \\ a_c \\ a_a \\ a_p \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \end{pmatrix} \quad (3.15)$$

The coefficients  $a_{ij}$  and  $b_i$  are defined by:

$$a_{11} = -\sum_{i=1}^N A_i^2, a_{12} = \sum_{i=1}^N A_i^{5/3}, a_{13} = \sum_{i=1}^N Z_i (Z_i - 1) A_i^{2/3}, a_{14} = \sum_{i=1}^N (A_i - 2Z_i)^2, a_{15} = \sum_{i=1}^N \mp A_i^{1/2}$$

$$a_{21} = -a_{12}, a_{22} = \sum_{i=1}^N A_i^{4/3}, a_{23} = \sum_{i=1}^N Z_i (Z_i - 1) A_i^{1/3}, a_{24} = \sum_{i=1}^N (A_i - 2Z_i)^2 A_i^{-1/3}, a_{25} = \sum_{i=1}^N \mp A_i^{1/6}$$

$$a_{31} = -a_{13}, a_{32} = a_{23}, a_{33} = \sum_{i=1}^N (Z_i (Z_i - 1))^2 A_i^{-2/3}, a_{34} = \sum_{i=1}^N Z_i (Z_i - 1) (A_i - 2Z_i)^2 A_i^{-4/3},$$

$$a_{35} = \sum_{i=1}^N \mp Z_i (Z_i - 1) A_i^{-5/6}$$

$$a_{41} = -a_{14}, a_{42} = a_{24}, a_{43} = a_{34}, a_{44} = \sum_{i=1}^N (A_i - 2Z_i)^4 A_i^{-2}, a_{45} = \sum_{i=1}^N \mp (A_i - 2Z_i)^2 A_i^{-3/2}$$

$$a_{51} = a_{15}, a_{52} = -a_{25}, a_{53} = -a_{35}, a_{54} = -a_{45}, a_{55} = \sum_{i=1}^N A_i^{-1}$$

$$b_1 = \sum_{i=1}^N A_i C_i, b_2 = \sum_{i=1}^N A_i^{2/3} C_i, b_3 = b_1 = \sum_{i=1}^N Z_i (Z_i - 1) A_i^{1/3} C_i, b_4 = \sum_{i=1}^N \frac{(A_i - 2Z_i)^2}{A_i} C_i,$$

$$b_5 = \sum_{i=1}^N \pm A_i^{-1/2} C_i$$

With

$$C_i = \left( M_{ex}^i - Z_i (m_p + m_e) - (A_i - Z_i) m_n + 14.4381 \times 10^{-6} Z_i^{2.39} + 1.55468 \times 10^{-12} Z_i^{5.35} \right)$$



### 3.2.3. Solution of the system of linear equations

To solve a system of linear equations, it exists different *direct* methods or *iterative* methods. The efficiency of each method depends on the size and the structure of the coefficients of the matrix  $A$ .

Compared to direct solution methods, iterative methods become indispensable when the size of the system becomes large. Indeed, direct methods require a number of floating point operations of the order of  $n^3$  ( $n$  is the size of the system, i.e. the number of equations) tends to infinity which makes them slow for large values of  $n$ . In this case direct methods must be avoided and methods such as *Jacobi's*, *Gauss-Seidel* and *conjugate gradient* must be preferred. For simplicity of programming, the Jacobi and Gauss-Seidel methods prevail over the conjugate gradient method. Compared to the method of Jacobi, the Gauss-Seidel method converges faster than that of Jacobi. [34]

Our system of linear equations was thus solved using Gauss Seidel's iterative method.

The previous linear equations can be written as:

$$\begin{aligned}
 a_v &= \frac{1}{a_{11}} \left[ b_1 - (a_{12}a_s + a_{13}a_c + a_{14}a_a + a_{15}a_p) \right] \\
 a_s &= \frac{1}{a_{22}} \left[ b_2 - (a_{21}a_v + a_{23}a_c + a_{24}a_a + a_{25}a_p) \right] \\
 a_c &= \frac{1}{a_{33}} \left[ b_3 - (a_{31}a_v + a_{32}a_s + a_{34}a_a + a_{35}a_p) \right] \\
 a_a &= \frac{1}{a_{44}} \left[ b_4 - (a_{41}a_v + a_{42}a_s + a_{43}a_c + a_{45}a_p) \right] \\
 a_p &= \frac{1}{a_{55}} \left[ b_5 - (a_{15}a_v + a_{52}a_s + a_{53}a_c + a_{54}a_a) \right]
 \end{aligned} \tag{3.16}$$

The Gauss-Seidel method consists of successive calculations and in each iteration the new value replaces the old value of the previous.

In general, for  $k+1$  iteration:

$$a_i = \frac{1}{a_{ii}} \left[ b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(k+1)} - \sum_{j=i+1}^5 a_{ij} x_j^{(k)} \right]; 1 \leq i \leq 5; k = 0, 1, 2, \dots \tag{3.17}$$

### 3.2.4. Calculation of the coefficients of the SEMF

In order to apply the previous method on the system of equation (eq.3.16) we have developed a computer code. Its algorithm is based of three main steps: reading the atomic mass data for the nuclei from a file, calculating the different constant parameters of the system and finally solving the system using the Gauss Seidel's method.

The calculations performed using the dedicated code yielded the following values for the five coefficients of the mass formula in *MeV*:

$$a_v = 15.24658$$

$$a_s = 16.32495$$

$$a_c = 0.68485$$

$$a_a = 22.09792$$

$$a_p = 10.60849$$

#### 3.2.4.1. Comparison with previous work

Table 3.1 shows a compilation of different values of the coefficients that were calculated in previous works and our results.

Compilation year	Ref	Atoms number	Coefficients ( <i>MeV</i> )				
			$a_v$	$a_s$	$a_c$	$a_a$	$a_p$
2022	Present work	2550	15.247	16.325	0.685	22.098	10.608
2020	[33]	2497	14.930	15.058	0.661	21.609	10.174
2018	[25]	2496	19.12	18.19	00.52	21.54	28.99
2005	[35]	-	15.78	18.34	00.71	23.21	12.00
1958	[36]	-	15.84	18.33	00.18	23.20	11.20

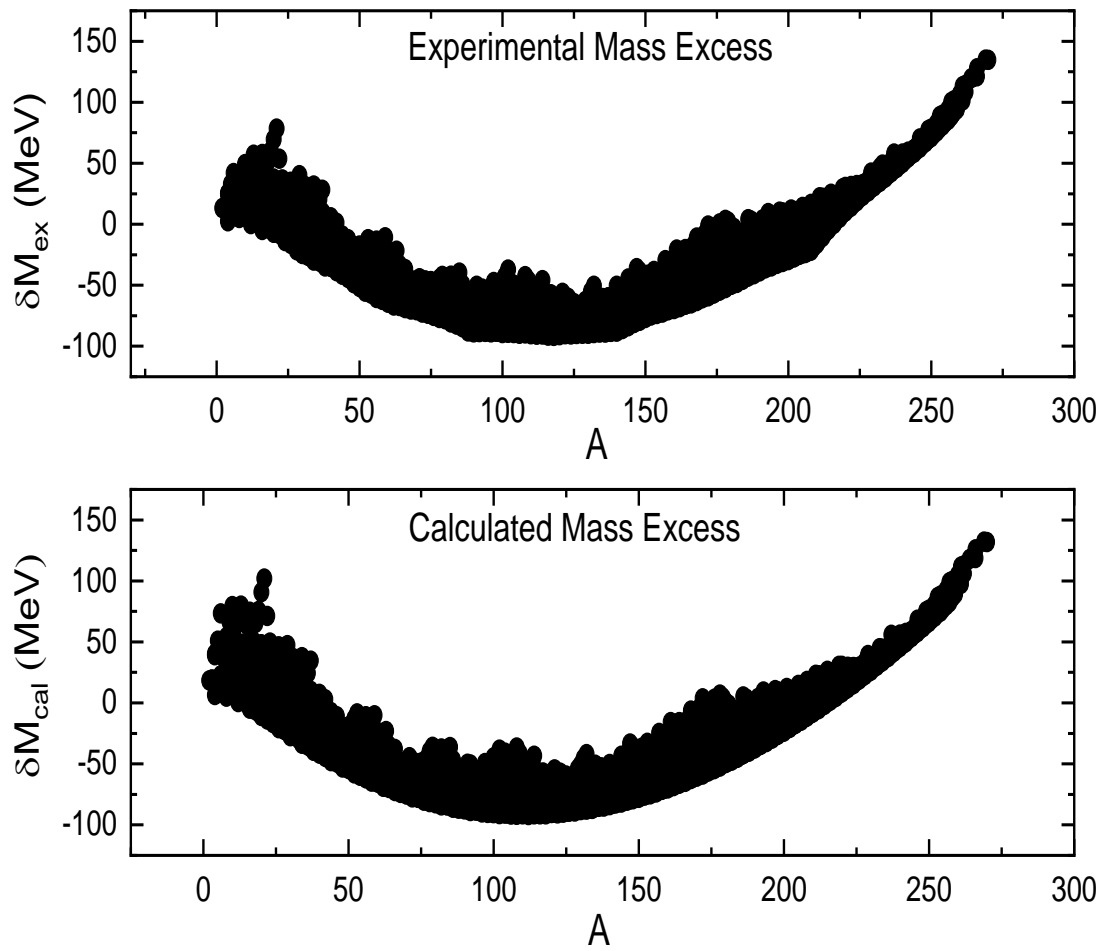
**Table 3.1:** Comparison of our SEMF coefficients values to those of previous works based on AME data.

### 3.2.4.2. Comparison with AME2020

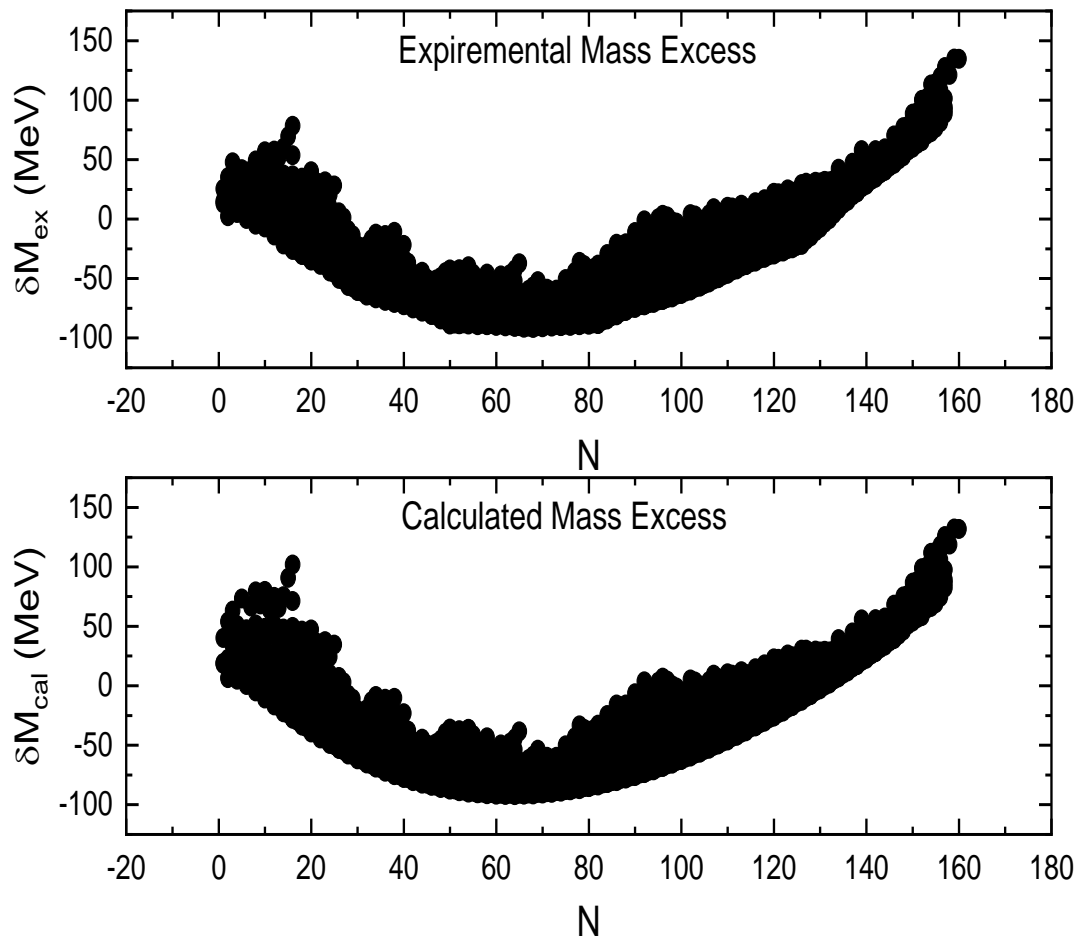
#### a) Mass and binding energy

Using our obtained set of coefficients in the SEMF allows us to reproduce the values of the atomic masses and the binding energies for each nucleus. A comparison of our mass excess results with the experimental ones (AME 2020) is represented as function of  $A$  in figure 3.1 and as function of  $N$  in figure 3.2. A similar comparison between our results and the AME ones of the binding energies per nucleon is represented as function of  $A$  and  $N$  in Figure 3.3.

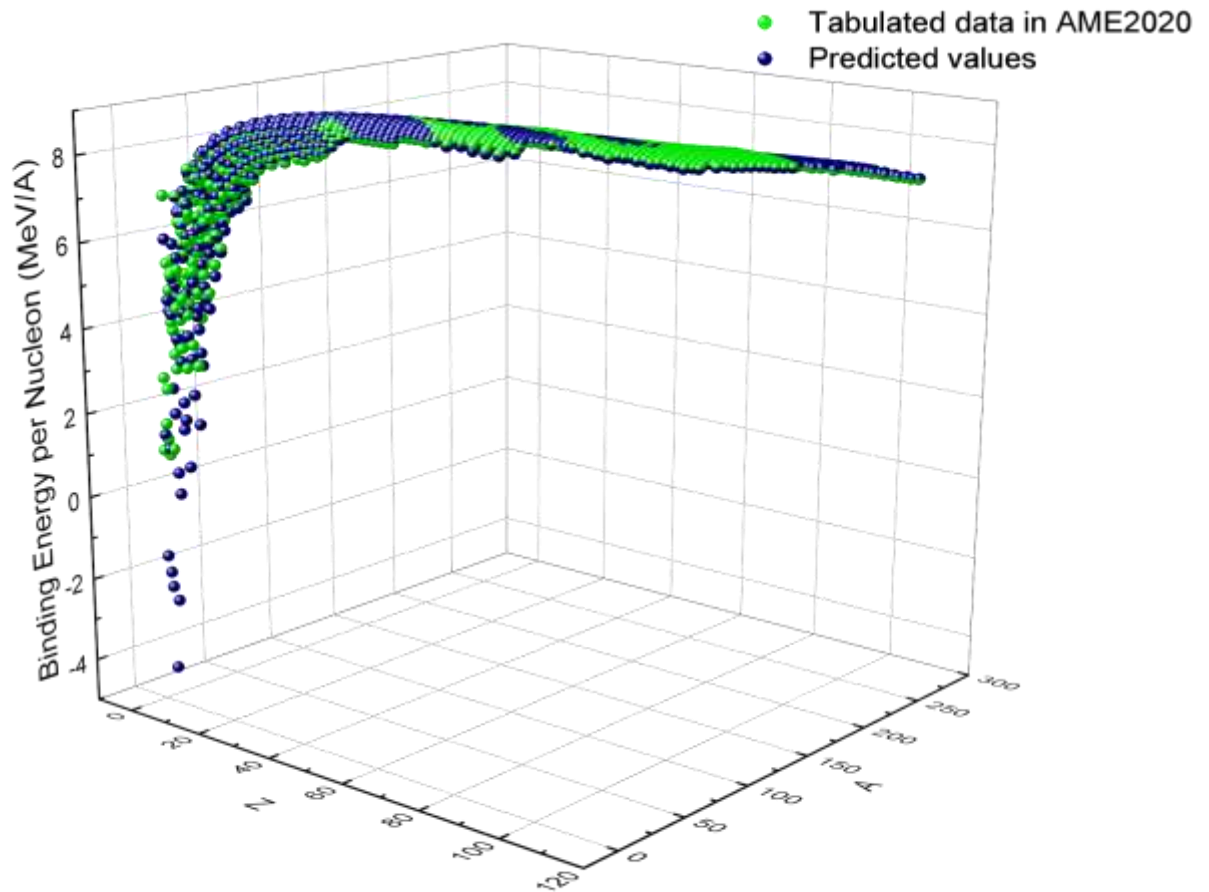
From the figures 3.1 and 3.2, one can notice that the calculated masses have globally the same shape as the experimental ones. The figure 3.3 gives the same observation for the binding energies per nucleon. A good agreement for the mass numbers  $A > 50$  can be observed. However, the figure show discrepancy for light nuclei, particularly in the region of  $A < 20$ . This was predicted because the SEMF is not precise for the light nuclei.



**Fig 3.1:** Variation of experimental [4] and calculated mass excess according to  $A$ .



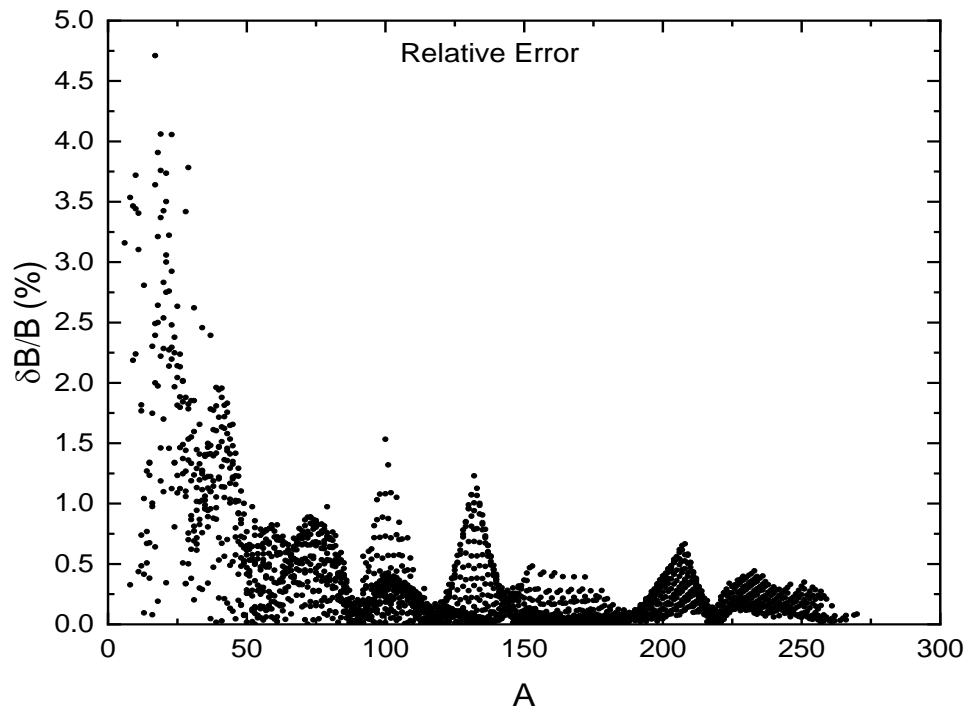
**Fig 3.2:** Variation of experimental [4] and calculated mass excess according to the neutron number  $N$ .



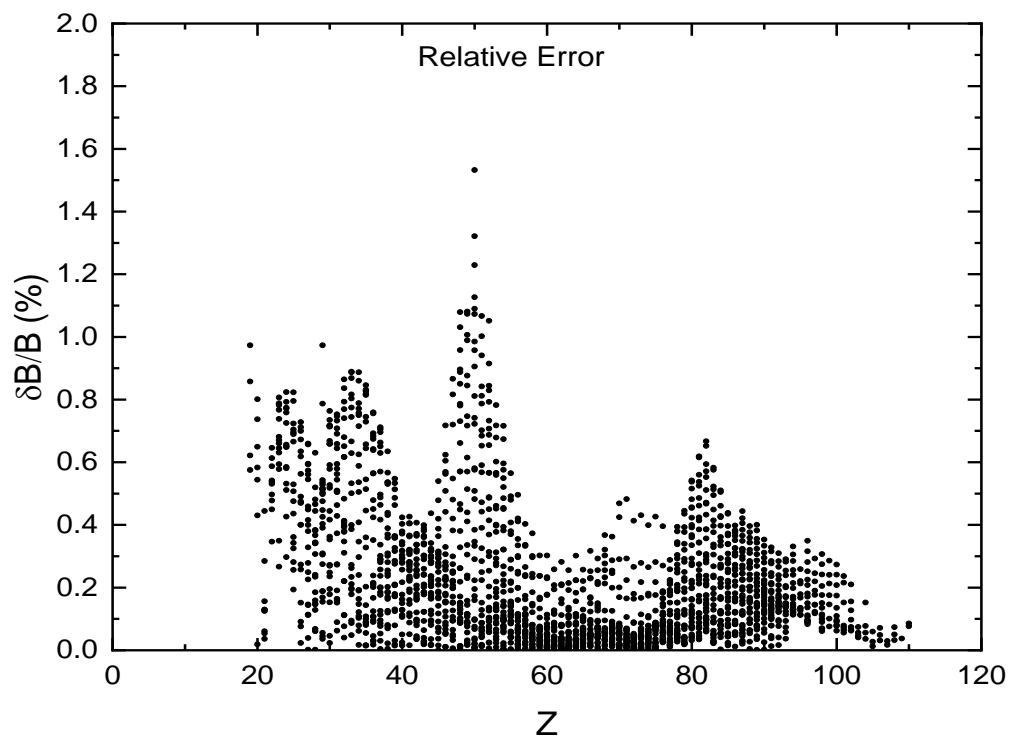
**Fig 3.3:** 3D comparison of tabulated binding energy per nucleon data given by AME2020 [4] versus those predicted according to  $Z$  and  $A$ .

### b) Relative Error

We calculated the relative error  $\varepsilon$  between the predicted and tabulated values, it is presented versus  $A$  and  $Z$  in figs 3.4 and 3.5 respectively. We can show certain values of  $A$  and  $Z$  for which  $\varepsilon$  is minimum. This behavior can be explained by the fact that the nuclei possess a particular stability around the magic numbers. Indeed, the nuclei having  $Z$  or  $N$  around these numbers have a spherical shape and their binding energy can be perfectly described by the liquid drop model. Every time we walk away from these numbers, the error increases during the adjustment of the experimental values of the mass by the present model.



**Fig 3.4:** Variation of relative error according to the mass number  $A$ .



**Fig 3.5:** Variation of relative error according to  $Z$ .

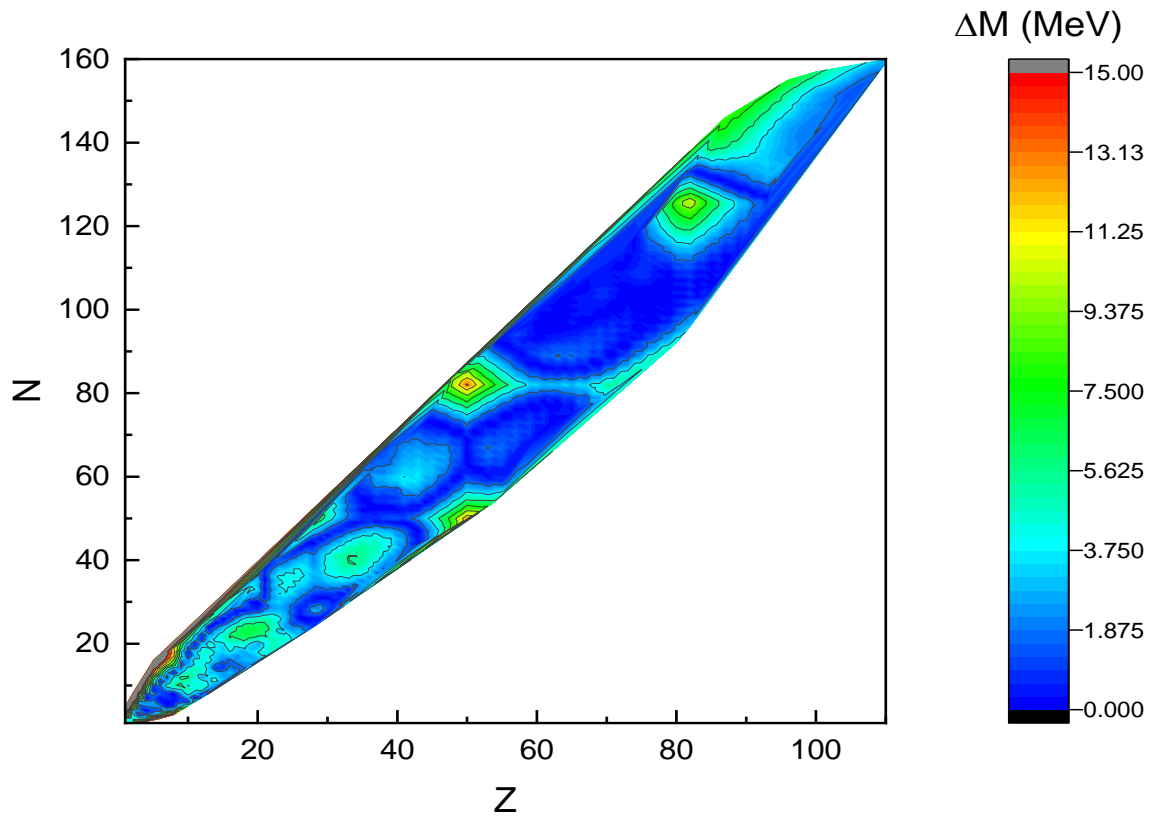
Four different categories of the average percentage errors are presented in table 3.2, according to several mass number intervals. The obtained values of  $\varepsilon$  show that our set of values can be used as coefficients in the SEMF with very excellent precision in the region  $140 < A < 200$ , and with good accuracy in the region  $50 < A < 140$  and  $A > 200$ . For  $A < 50$ , it is not recommended to use the present model to estimate the atomic mass.

$[A_1, A_2]$	$A < 50$	$50 < A < 140$	$140 < A < 200$	$A > 200$
Relative error $\varepsilon$ (%)	9.26173509	0.32157739	0.09942255	0.21141242

**Table 3.2:** Different categories of percentage errors.

To describe in a more precise way the behavior of the error of the adjustment around  $Z$  and  $N$ , the difference between the calculated and the experimental values is presented (in absolute value) in figure 3.6. The propagation of this difference is represented in color on a curve having the number of protons and neutrons as axes. This representation allows us to determine the regions with the maximum or minimum deviation. One can notice that along the whole region the average deviation is about 1 *MeV*. The regions having a relatively larger errors are for  $A < 20$ .





**Fig 3.6:** Variation of  $\Delta M = |M_{exp} - M_{cal}|$  according to  $Z$  and  $N$ .

## Conclusion

In this chapter, an adjustment of the experimental data by the liquid drop model has been made to find the SEMF coefficients. This adjustment is based on the atomic masses of 2550 nuclides of the AME 2020 data. The obtained coefficients exhibited excellent agreement with the atomic masses and the binding energy of nuclei with  $A > 50$ .

## Conclusion

In this work we have calculated the coefficients of the Semi-Empirical Mass formula: volume, surface, coulomb, asymmetry and pairing coefficient. An adjustment by the least square method of 2550 experimental masses extracted from the AME mass evaluation was carried out by minimizing  $\sigma^2$  which is more appropriate since it reduces absolute errors.

The obtained results were used to calculate the atomic masses and the binding energies of the nuclides and then compared with the experimental values. The calculated values were in great accordance with the experimental ones for  $A > 50$  yielding relative errors that oscillate between less than 0.05% and 1.5%. Since Bethe–Weizsäcker mass formula is based on a liquid drop model, it was indeed expected that it reproduces better results for medium and heavy nuclei than for light nuclei. The large discrepancy between the two values observed for light nuclei can be attributed to the deformation effects.

The present work can be improved in the future by taking into account several effects such as the deformation of nuclei, shell correction.

Finally, even though the SEMF is not considered as the complete expression to provide the binding energy for a given nucleus, it is a good indicator for first-level precision of calculations involving binding energy, especially to exclude heavy nuclei stability. In addition, this formula is still a fundamental keystone in nuclear physics with respect to teaching and research.

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