Least-squares fitting applied to nuclear mass formulas. Resolution by the Gauss-Seidel method

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A numerical method optimizing the coefficients of the semi empirical mass formula or those of similar mass formulas is presented. The optimization is based on the least-squares adjustments method and leads to the resolution of a linear system which is solved by iterations according to the Gauss-Seidel scheme. The steps of the algorithm are given in detail. In practice the method is very simple to implement and is able to treat large data in a very fast way. In fact, although this method has been illustrated here by specific examples, it can be applied without difficulty to any experimental or statistical data of the same type, i.e. those leading to linear system characterized by symmetric and positive-definite matrices.

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I. CONSTRUCTION OF THE LINEAR SYSTEM OF EQUATIONS FROM A MINIMIZATION PROCEDURE

A. Principle of the method: Linear combination of independent functions

The least squares method \[1,2\] has historically attributed to Gauss (1795). This method is applied in various scientific fields, such as statistics, geodesy, economy, optimization, etc. ... The present work proposes to apply it to the optimisation of the semi-empirical \[3,4\], mass formula or to formulas of the same type. In this category, we can cite: (a) The FRDM (the best) and FRLDM models with complete calculation of shell and pairing corrections also considering several kinds of nuclear deformations \[5\], (b) The “Pomorski-Dudek model” \[6\] with shell and pairing corrections, (c) The “Royer model” with shell and pairing corrections but without nuclear deformation \[7\], (d) The well-known droplet model of Myers based on the Thomas-Fermi approximation with and without shell correction \[8\]. Nuclear mass formulas are an important tool in the evaluation of some ground-state properties, nuclear reactions and in the prediction of the neutron/proton drip lines. All these formulas can be optimized in the same way by the method described by the following procedure.

At the beginning, suppose that for each pair \((x_i, y_i)\) of independent variables, we have to measure a correlated data \(B_{\text{exp}}(x_i, y_i)\). If we make \(n\) measurements, we will have \(i = 1, 2, ..., n\) and in practice we thus obtain a table with three columns of \(n\) data, i.e. \(x_i, y_i, B_{\text{exp}}(x_i, y_i)\). In the following, for the discrete indices of summation we adopt the general convenient “rule” that any discrete index such as for example \(k\), will vary from \(k = 1\) (first data) to \(k = k_{\text{max}}\) (last data). For example, in the previous cited case the index “\(n\)” (last value of \(i\)) has been replaced by \(i_{\text{max}}\). In the same way, the index \(j\) will vary from 1 to \(j_{\text{max}}\), the index \(k\) will vary from 1 to \(k_{\text{max}}\), etc...

In this work, we are looking for a mathematical expression \(B_{\text{theo}}(x_i, y_i)\) which can approximate “as much as possible” the experimental data \(B_{\text{exp}}(x_i, y_i)\). The theoretical expression \(B_{\text{theo}}(x_i, y_i)\) is defined by a suitable linear combination of independent functions in which some coefficient have to be determined on the basis of the least squares method. This linear combination is of the following form:

\[
B_{\text{theo}}(x_i, y_i) = \sum_{k=1}^{k_{\text{max}}} b_k F_k(x_i, y_i) + \sum_{j=1}^{j_{\text{max}}} c_j G_j(x_i, y_i) \quad i = 1, i_{\text{max}}
\]

(1)

In order to lighten the writing, we set: \(B_{\text{exp}}(x_i, y_i) = B_{\text{exp}}(i)\), \(F_k(x_i, y_i) = F_k(i)\), \(G_j(x_i, y_i) = G_j(i)\), \(B_{\text{theo}}(x_i, y_i) = B_{\text{theo}}(i)\).

As mentioned before we will use the least squares method. Only the coefficients \(b_k\) will be chosen by variation (all other quantities are supposed to be known) so as to minimize the total sum of the squared deviations of the theoretical values with respect to the experimental values.

\[
E(b_1, b_2, ..., b_{k_{\text{max}}}) = \sum_{i=1}^{i_{\text{max}}} (B_{\text{exp}}(i) - B_{\text{theo}}(i))^2
\]

(2)

In Eq. (1), the coefficients \(c_j\) will be maintained constant. Thus, this linear combination contains a “varied part” and a “constant part”. In the sums of Eq. (1) \(k_{\text{max}}\) is the number of “varied” coefficients \(b_k\) and \(j_{\text{max}}\) is the number of “non varied” coefficients \(c_j\). With the “light” representation defined just above, \(B_{\text{theo}}\) which appears in Eq. (2) and which is defined by equation (1), becomes:

\[
B_{\text{theo}}(i) = \sum_{k=1}^{k_{\text{max}}} b_k F_k(i) + \sum_{j=1}^{j_{\text{max}}} c_j G_j(i), \quad i = 1, i_{\text{max}}
\]

(3)

Thus, according to the least squares principle, we must minimize the sum given by Eq. (2) with respect to the quantities \(b_k\). The minimum sought (we will show later that this critical point is indeed a minimum) of this functional corresponds to the system of equations defined by:

\[
\frac{\partial E(b_1, b_2, ..., b_{k_{\text{max}}})}{\partial b_p} = 0 \quad p = 1, 2, ..., k_{\text{max}}
\]

(4)

In this expression, it is worth to repeat that all the quantities are known and fixed, only the coefficients \(b_p\) are unknown and are therefore determined by variations (minimization). This leads to a system of \(k_{\text{max}}\) equations with \(k_{\text{max}}\)
unknown quantities $b_p$ (see Eq. (4)). By definition the function $E(b_1, b_2, ..., b_{k_{\text{max}}})$ in Eq. (2) is a linear combination of $b_p$, therefore it is continuous with respect to these variables. We thus obtain by derivation and permutation of summations, the following set of equations, each equation corresponds to a fixed $p$ value:

$$- \sum_{i=1}^{\text{imax}} B_{\exp}(i) F_p(i) + \sum_{k=1}^{\text{kmax}} b_k \sum_{i=1}^{\text{imax}} F_k(i) F_p(i) + \sum_{j=1}^{\text{jmax}} c_j \sum_{i=1}^{\text{imax}} G_j(i) F_p(i) = 0 \quad (5)$$

It is convenient to set:

$$\sum_{i=1}^{\text{imax}} F_k(i) F_p(i) = \Phi_{kp}, \quad (6)$$

$$\sum_{i=1}^{\text{imax}} G_j(i) F_p(i) = \Gamma_{jp} \quad (7)$$

$$\sum_{i=1}^{\text{imax}} B_{\exp}(i) F_p(i) = \beta_p \quad (8)$$

the previous set of equations become:

$$\sum_{k=1}^{\text{kmax}} b_k \Phi_{kp} = \beta_p - \sum_{j=1}^{\text{jmax}} c_j \Gamma_{jp} \quad (9)$$

or in equivalent way, in matrix representation:

$$\begin{bmatrix} \Phi_{11} & \Phi_{12} & \cdots & \Phi_{1q} \\ \Phi_{21} & \Phi_{22} & \cdots & \Phi_{2q} \\ \vdots & \vdots & \cdots & \vdots \\ \Phi_{q1} & \Phi_{q2} & \cdots & \Phi_{qq} \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_q \end{bmatrix} = \begin{bmatrix} \gamma_1 \\ \gamma_2 \\ \vdots \\ \gamma_q \end{bmatrix} \quad (10)$$

Here, $q = k_{\text{max}}$ and $\gamma_p = \beta_p - \sum_{j=1}^{\text{jmax}} c_j \Gamma_{jp}$.

It is clear from equation (6) that the matrix $\Phi$ is real and symmetric. Let us define the rectangular matrix $F$ by its matrix elements $F(i,k) = F_k(i)$, and let us calculate the product $F^T F$ where $F^T$ is the transpose of the matrix $F$. So

$$(F^T F)_{kp} = \sum_j F^T(k,j) F(j,p) = \sum_j F_k(j) F_p(j) = \Phi_{kp} \quad (11)$$

therefore $F^T F = \Phi$. Thus, the matrix $\Phi$ can be set in the form of a product of a matrix and its transpose. Moreover, $F$ is constituted by $k_{\text{max}}$ linearly independent column-vectors. Consequently the matrix $\Phi$ is real, symmetric and positive definite, it is therefore invertible and the system given by Eq. (9) has always one solution and only one (i.e., the set $(b_1, b_2, ..., b_{k_{\text{max}}})$) which verify Eq. (10).

**B. The system has always a solution**

It is clear from equation (6) that the matrix $\Phi$ is real and symmetric. Let us define the rectangular matrix $F$ by its matrix elements $F(i,k) = F_k(i)$, and let us calculate the product $F^T F$ where $F^T$ is the transpose of the matrix $F$. So

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C. Nature of the critical point

In fact, the condition of Eq. (4) does not give necessarily a minimum but corresponds generally to a critical point (minimum, maximum or saddle point). To show the nature of this critical point, it is necessary to study the Hessian matrix \( H_{pq} \) of the function \( E \) defined above by Eq. (2). The elements of the Hessian matrix of \( E \) are given by:

\[
H_{pq} = \frac{\partial^2 E(b_1, b_2, ..., b_{k_{max}})}{\partial b_p \partial b_q} \tag{12}
\]

The first derivative is that given by the left member of Eq. (5). A second derivative of \( E \) gives:

\[
H_{pq} = \frac{\partial^2 E(b_1, b_2, ..., b_{k_{max}})}{\partial b_p \partial b_q} = \Phi_{pq} \tag{13}
\]

The Hessian matrix \( H \) is no more than the matrix \( \Phi \). So the Hessian matrix is symmetric, real and positive definite, therefore the critical point (extremum) is always a minimum.

II. RESOLUTION BY THE GAUSS-SEIDEL METHOD

A. Gauss-Seidel vs some other methods

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. In practice, the implementation of a numerical method is always a compromise between several advantages and inconveniences. For simplicity of programming, the Jacobi and Gauss-Seidel methods prevail over the conjugate gradient method. Compared to the method of Jacobi, that of Gauss-Seidel is not suitable for parallelization. But this advantage is of little interest here because the iterations are based on a single short formula and also because the Gauss-Seidel method converges faster than that of Jacobi. Finally, Gauss-Seidel method was preferred. Because, the matrix \( \Phi \) of the system (9) is symmetrical and definite-positive, the Gauss-Seidel method always converges whatever the starting point is. The convergence is thus guaranteed.

B. Algorithm of the iterative procedure

In Eq. (9) we can isolate the term \( k = p \) expressing thus the coefficient \( b_p \) as a linear combination of the remaining terms:

\[
b_p = \frac{\beta_p - \sum_{k \neq p} b_k \Phi_{kp} - \sum_{j=1}^{j_{max}} c_j \Gamma_{jp}}{\Phi_{pp}} \quad p = 1, 2, ..., k_{max} \tag{14}
\]

It should be noted that each unknown \( b_p \) appears only in the left-hand side of the equation. It is thus only expressed by the remaining set of unknowns. The denominator is by definition:

\[
\Phi_{pp} = \sum_{i=1}^{i_{max}} (F_p(i))^2 \tag{15}
\]

It is then strictly positive (the only exception would be that for fixed \( p \), the \( F_p(i) \) are all zero, which would be equivalent to taking a null function, such a choice would be absurd). So the denominator does not present a problem. The Gauss-Seidel method consists in successive calculations, \( b_1, b_2, b_3, ... \). In each iteration the new value replaces the old value of the previous according to the following steps:
The first “round” corresponds to the $k_{\text{max}}$ first iterations. The successive iterations (determinations of $b_k$) follow the scheme:

$$(b_0^0, b_1^0, ..., b_{k_{\text{max}}}^0) \rightarrow b_1^1$$

$$(b_1^0, b_1^1, ..., b_{k_{\text{max}}}^0) \rightarrow b_2^1$$

$$(b_1^1, b_2^1, ..., b_{k_{\text{max}}}^0) \rightarrow b_3^1$$

$$...$$

$$(b_1^1, b_2^1, ..., b_{k_{\text{max}}}^1) \rightarrow b_1^2$$

here $b_k^k$ corresponds to the iteration number $k$ of the $p$th coefficient of the unknown set. In fact one round corresponds simply to one iteration for all the unknowns of the set $(b_1, b_2, ..., b_{k_{\text{max}}})$.

The second “round” (which is also a set of $k_{\text{max}}$ iterations) is defined by similar iterations, starting from the last iteration of the first "round".

$$(b_1^1, b_1^2, ..., b_{k_{\text{max}}}^1) \rightarrow b_2^2$$

$$(b_1^1, b_2^1, ..., b_{k_{\text{max}}}^2) \rightarrow b_3^2$$

$$...$$

$$(b_1^1, b_2^1, ..., b_{k_{\text{max}}}^2) \rightarrow b_1^3$$

etc, ..... This process continue until convergence, i.e. until a stable set $(b_1^0, b_2^0, ..., b_{k_{\text{max}}}^n)$ after a sufficient number $n$ of “rounds”.

Thus each round is constituted by $k_{\text{max}}$ iterations, in each iteration one of the coefficient $b_p$ is determined by Eq. \[15\] and the old value is “immediately” replaced by the new one.

Obviously, at the starting of the procedure, an initial set $(b_1^0, b_2^0, ..., b_{k_{\text{max}}}^0)$ must be chosen. Moreover, we know from the beginning of the present section that the iterative procedure always converges, whatever the values of the initial set. However, in order not to slow down the process by an awkward choice at the start of the iterations, it is convenient to start from a “suitable” set chosen for example on the basis of physical considerations.

In practice, the most important point in this method, is to store once and for all the matrices $\Phi_{kp}$, $\Gamma_{jp}$ and the vector $\beta_p$ at the start of the program before the beginning of the iterations. It is also possible to use the symmetry of $\Phi_{kp}$ to reduce greatly the calculations. Moreover it should be noted that the matrix $\Gamma_{jp}$ (see Eq. \[7\]) which corresponds to the coefficients which are not “varied” is in general much smaller than the matrix $\Phi_{kp}$ because in order to obtain an efficient optimization, it is more advantageous to vary the maximum number of parameters. Indeed, due to physical constraints only some parameters are maintained constant. The present considerations leads to simplify greatly the programming and the efficiency of the code.

### III. ILLUSTRATIONS OF THIS METHOD

In fact this algorithm applies to any linear system, but here the main motivation was to implement it to the optimization of the coefficients of mass formulas of nuclear physics.

In this numerical study we will consider two cases: The simple case of the semi empirical mass formula and a more elaborate version of the liquid drop mass model containing a larger number of corrective terms.

#### A. The Bethe-Weizsaker formula

1. Steps of the algorithm for a simple case

The semi empirical mass formula or Bethe-Weizsaker formula \[3, 4\] is well known. It approaches theoretically the binding energy of the atomic nucleus only as a function of the number of $N$ neutrons and $Z$ protons. The theoretical mass of the nuclei can be deduced straightforwardly from this binding energy. The standard Bethe-Weizsaker formula gives the theoretical expression of the binding energy $B_{\text{th eo}}(N, Z)$ of the atomic nucleus as a function of a five contribution:

$$B_{\text{th eo}}(A, Z) \approx a_V A - a_S A^{2/3} - a_C Z^2 / A^{1/3} - a_\alpha (A - 2Z)^2 / A + \delta(A, Z)$$

(16)
With $A = N + Z$. The first four terms are respectively the well known volume, surface, Coulomb and asymmetry energies. The fifth is the pairing energy term:

$$
\delta(A, Z) = \varepsilon 12.0/A^{1/2}
$$

where $\varepsilon = 0$ if $A$ odd, $\varepsilon = +1$ if $N$ and $Z$ even, $\varepsilon = -1$ if $N$ and $Z$ odd.

Here the procedure was done in FORTRAN 90 language but due to the simplicity of the algorithm described here it is obviously possible to use other language codes. The goal of the method is to solve Eq. (14) in order to find the four optimized constants $(a_V, a_S, a_C, a_a)$. In this typical example, the steps of the algorithm are illustrated as follows:

- Reading and storing the values of numbers of neutrons and protons $(N_i, Z_i)$ and their experimental binding energy from an input data file.

- Construction of the four functions $F_k(x_i, y_i)$ of Eq. (18) corresponding to the varied coefficient $(k = 1, 4)$: Remembering that for each nucleus “number $i$” represents a couple $(N_i, Z_i)$ and setting $A_i = N_i + Z_i$, we will have here:

  $$
  \begin{align*}
  F_1(i) &= F_1(N_i, Z_i) = A_i \\
  F_2(i) &= F_2(N_i, Z_i) = -A_i^{2/3} \\
  F_3(i) &= F_3(N_i, Z_i) = -Z_i^2/A_i^{1/3} \\
  F_4(i) &= F_4(N_i, Z_i) = -(A_i - 2Z_i)^2/A_i
  \end{align*}
  $$

- Construction of the function $G_1(i) = G_1(x_i, y_i) = \varepsilon a_p/A_i^{1/2}$ (Eq. (7)), there is here only one function $G$. We set $c_1 = 1$ since this coefficient is not varied.

- Before the iterations, the following matrices must be calculated and stored in the memory of the computer:

  $$
  \begin{align*}
  \Phi_{kp} &= \sum_{i=1}^{imax} F_k(i)F_p(i) \\
  \Gamma_{jp} &= \sum_{i=1}^{imax} F_j(i)G_p(i) \\
  \beta_p &= \sum_{i=1}^{imax} B_{exp}(i)F_p(i)
  \end{align*}
  $$

$B_{exp}(N_i, Z_i) = B_{exp}(i)$ is the experimental binding energy of the “$i$-th” nucleus, the summation is done over $i$ up to the number of nuclei which is equal to $imax$.

- Choosing a starting set $(b_1^0, b_2^0, b_3^0, b_4^0) = (a_V^0, a_S^0, a_C^0, a_a^0)$

- Use Eq. (14) to determine the unknowns by an iterating sequence as follows:

  $$
  \begin{align*}
  (a_V^0, a_S^0, a_C^0, a_a^0) &\rightarrow a_V^1 \\
  (a_V^0, a_S^0, a_C^0, a_a^0) &\rightarrow a_S^1 \\
  (a_V^0, a_S^0, a_C^0, a_a^0) &\rightarrow a_C^1 \\
  (a_V^0, a_S^0, a_C^0, a_a^0) &\rightarrow a_a^1 \\
  \end{align*}
  $$

  etc.... A new set (four iterations in this case) is calculated in one round as explained above.

- Stop the process as soon as successive iterations does not change the results anymore (up to a desired reasonable fixed precision)

- Evaluating root mean square deviation from experimental
The experimental binding energy of each nuclei is extracted from the recent updated Atomic Mass Evaluation, i.e. AME 2020 table, published in [9, 10]. Non-experimental (i.e. estimated) values are not taken into account considering only nuclei with $N \geq 8$ and $Z \geq 8$. In this case the number of nuclei ($i_{\text{max}}$) for the least square fit is equal to 2452. The atomic masses are given with a maximum uncertainty of $\pm 0.0009u$ (unified mass unit).

As usual, the root mean square deviation is defined by:

$$
\sigma = \sqrt{\frac{\sum_{i=1}^{i_{\text{max}}} (B_{\text{exp}}(i) - B_{\text{theo}}(i))^2}{i_{\text{max}}}}^{1/2}
$$

(20)

where $i = (N_i, Z_i)$ and $B_{\text{theo}}$ is given by Eq. (16). The calculations are made on a desktop P.C. computer with Intel i3 4160 processor, and a memory of 16 Gbytes (DDR3 type).

To study convergence, the number of total iterations was set at 80,000,000 (80 million of iterations). However, in spite of the number of iterations, the execution time is only about 21 seconds for this case where only four quantities were varied. The values of the coefficients are recorded for a certain number of iterations (see table I). For this small system, one notes a stability of the results for the four coefficients starting from 100000 iterations. Here, stability is defined arbitrarily by requiring that the 8 digits after the decimal point no longer change. With these stabilized values we obtain a root mean square deviation of 3.06 MeV in the binding energy. The “optimized” formula is thus:

$$
B_{\text{theo}}(A, Z) \approx 15.5461A - 16.9598A^{2/3} - 0.7036Z^2/A^{1/3} - 23.0253(A - 2Z)^2/A + \delta(A, Z)
$$

(21)

It is well known that the basic standard empirical formula with five terms of which four coefficients are optimized does not allow great precision. A refinement is possible with the increase of the number of corrective terms and the introduction of the shell and pairing corrections. This greatly improves the precision (see below the liquid drop formula).

### B. The liquid drop mass model

The liquid drop mass formula gives better results. In this respect it is worth to mention that there are several versions of this model. One of such improved formula is given by the following equation which is very close to the ones [5–7] (and several references quoted therein):
\[ B_{\text{theo}}(A, Z) \approx a_V(1.0 - k_V I^2 - k'_V I^4)A \\
- a_S(1.0 - k_S I^2 - k'_S I^4)A^{2/3} B_S(\beta) \\
- a_{\text{curv}}(1.0 - k_{\text{curv}} I^2 - k'_{\text{curv}} I^4)A^{1/3} B_{\text{curv}}(\beta) \\
- a_C(Z^2/A^{1/3}) B_{\text{coul}}(\beta) + f_p(Z^2/A) B_{\text{coul}}(\beta) \\
+ a_{\text{exch}} Z^2 A^{1/3} + W |I| + a_0 A^{1/2} + \varepsilon_p + E_{\text{cong}} \]

(22)

The different versions of the liquid drop mass models are justified through various theories and approximation (but this is beyond the scope of this paper). The volume energy is given by the term containing the constant \( a_V \) and then we have the surface energy (with constant \( a_S \)). These two contributions contain a part of the asymmetry energy defined in the Bethe-Weizsaker formula seen before. Here, the relative neutron excess is \( I = (N - Z)/A \). The three following contributions correspond to the curvature contribution \( (a_{\text{curv}}, \text{coul}) \), the Coulomb energy \( (a_c) \) and the the diffuseness correction term \( (f_p) \) of the Coulomb energy. The other three following terms, are respectively the exchange Coulomb energy \( (a_{\text{exch}}) \), the Wigner correction \( W \), and the \( A^4 \) correction. At last, the two last contributions are (i) the smooth pairing energy defined as before and (ii) the congruence energy given by \( E_{\text{cong}} = 10 \exp(-4.2I^2) \). The surface, curvature and Coulomb energy are taken deformation dependent through the quantities \( B_S(\beta), B_{\text{curv}}(\beta) \) and \( B_{\text{coul}}(\beta) \) where \( \beta \) is the quadrupole deformation as defined in Ref. [1]. All these quantities can be found in the Ref. [1]. Anyway this version of the liquid drop mass formula contains 16 contributions in which 14 are varied (the \( b_k \)). The “family” of models in which shell and pairing corrections are taken into account belongs to the so-called Microscopic-Macroscopic (MicMac) Model.

Whatever the number of elements involved in this formula, the steps of the algorithm are strictly the same as the one seen above. We will avoid repeating the operations described above. We only will confine ourselves to see the performances in time (speed) and in quality (precision) for this case.

This time, the calculations take approximately 91 seconds which is a good time if we consider that 80 millions of iterations are performed with a set of 14 unknowns. Table 11 shows the convergence of the three quantities \( (a_V, a_S, a_C) \) among the fourteen unknown of Eq. (22). It is to be noted that “8-digit stability after the decimal point” is reached after 20,000,000 (20 million) iterations. The root mean square deviation is then about 1.81 MeV. Compared to the semi empirical, the precision is greatly improved \( (\sigma \approx 1.81 \text{ MeV against } \sigma \approx 3.06 \text{ MeV}) \). The resulting formula is given by Eq. (23).

| Iterations | \( a_V \) | \( a_S \) | \( a_C \) |
|-----------|----------|----------|----------|
| 100       | -80.04729872 | -34.2577039 | -5.1507732 |
| 500       | -16.05087356 | 15.2624854 | -7.8999599 |
| 1000      | -7.37605620 | 16.4220924 | -8.8403629 |
| 5000      | 25.81407742 | 13.71052549 | -11.5082339 |
| 10000     | 46.16667756 | 66.73928076 | -12.1795777 |
| 50000     | 56.60653888 | 80.29100831 | -9.72129294 |
| 100000    | 42.11538222 | 86.75529165 | -7.17358506 |
| 500000    | 11.31733037 | 51.58243500 | -1.01117089 |
| 1000000   | 12.17115008 | 80.04729872 | -0.68255779 |
| 5000000   | 66.73928076 | 15.00144952 | -12.17695777 |

TABLE II. Iterations and convergence of three coefficient of the liquid drop mass formula
\[ B_{\text{theo}}(A, Z) \approx 16.3984(1.0 - 9.65912I^2 - 281.1899I^4)A \\
-24.8568(1.0 + 125.7999I^2 - 2318.6417I^4)A^{2/3}B_S(\beta) \\
+17.8930(1.0 + 358.6967I^2 - 4640.8412I^4)A^{1/3}B_{\text{curve}}(\beta) \\
-0.720708(Z^2/A^{1/3})B_{\text{coul}}(\beta) + 1.54147(Z^2/A) \\
-0.000558043Z^2A^{1/3} - 19.6944|I| - 24.4926A^0 + \varepsilon_p + E_{\text{cong}} \quad (23) \]

If we take into account the shell and pairing corrections (evaluated in a separate theoretical calculations), the root mean square deviation is in a dramatic way reduced to \( \sigma \approx 0.864 \text{ MeV} \). This explains why shell and pairing corrections are absolutely necessary in this kind of formulas.

It is worth to emphasize that direct comparison between various type of mass formulas proposed in the litterature has only a relative meaning because very often the “basis”, i.e. the set and the number of nuclei is not the same. There are other factors involved, such as the fact that the microscopic corrections are model dependent. Moreover, in some serious calculations, the root mean square deviation is weighted by some measurement error, etc...

**IV. CONCLUSION**

The goal of the present work consisted essentially in determining the best linear combination (i.e. the best coefficients,) of suitable functions intended to approximate the experimental binding energy of atomic nuclei. A very simple algorithm based on the Gauss-Seidel method is described in detail. The method is characterized by the maximum of simplicity in the procedure. This simplicity is the guarantee of efficiency and speed on a practical level.

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