Mapping the N-Z plane: residual mass regularities

J.G. Hirsch, A. Frank, and V. Velázquez

Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de México, Apartado Postal 70-543, 04510 México, D.F., México
e-mail: hirsch@nuclecu.unam.mx, frank@nuclecu.unam.mx, vmva@hp.uciencias.unam.mx

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A new development in the study of the deviations between experimental nuclear masses and those calculated in the framework of the Finite Range Droplet Model is introduced. Some frequencies are isolated and used in a simple fit to reduce significantly the error width. The presence of this regular residual correlations suggests that the Strutinsky method of including microscopic fluctuations in nuclear masses could be improved.

Keywords: Nuclear masses; FRDM; fluctuation

Se presenta una formulación novedosa del estudio de las diferencias entre las masas nucleares medidas y las calculadas con el FRDM. Se aislaron algunas frecuencias, que permiten reducir significativamente el error promedio. La existencia de regularidades en los errores sugiere que el método de Strutinsky puede ser mejorado incluyendo fluctuaciones microscópicas.

Descriptors: Masas nucleares; FRDM; fluctuaciones.

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1. Introduction

The prediction of nuclear masses is of fundamental importance for a complete understanding of the nuclear processes that power the Sun, and the synthesis and relative abundances of the elements [1]. Möller et al. [2], Duflo and Zuker [3], Goriely et al. [4], among many others, have developed mass formulae that calculate and predict the masses (and often other properties) of as many as 8979 nucleotides. There is a permanent search for better parameterizations that decrease the difference with the experimental masses and produce reliable predictions for unstable nuclei.

The atomic mass excesses have been tabulated for 8979 nuclei ranging from $^{16}\text{O}$ to $\text{A}=339$ in [2], calculated with a Finite Range Droplet macroscopic Model and a folded-Yukawa single-particle microscopic model, FRDM for short. The microscopic sector includes a Lipkin-Nogami calculation of pairing gaps besides Strutinsky shell-corrections. Ground-state energies are minimized with respect to shape degrees of freedom. Only 9 constants are adjusted to the ground-state masses of 1654 nuclei, with a mass model error of 0.669 MeV in the entire region of nuclei ranging from $^{16}\text{O}$ to $^{263}$.

The main motivation for the present work arose from the detailed study of the nuclear mass error distribution shown in Fig. 1, which displays the number of nuclei with a given interval of FRDM mass errors [2], for the 1654 isotopes with measured masses in 1995. The symmetrical distribution with two peaks around the origin was completely unexpected. In this article we study the regularities in the differences between measured and calculated masses, showing that they are closely related to the presence of this double peak. Figure 1 shows the FRDM distribution of nuclei [2] for different intervals of mass errors. The intermediate curve (diamonds) corresponds to a mass error interval of 0.1 MeV where the double peak is quite evident.

Enlarging the mass error interval to 0.2 MeV (triangles) softens the curvature but the presence of the double peak is still very clear. In the opposite direction, an interval of 0.05 MeV (squares) produces larger fluctuations and some apparent interference, but it is evident that the distribution still displays the peaks. We can thus conclude that the effect is real and not an artifact of a particular distribution interval.

We carried out additional tests to verify the persistence of the double peak, including only nuclei with $\text{A} \geq 40$ and $\text{A} \geq 60$, normalizing the distribution according to the rule $\text{A}^{-1/3}$, and including the experimental errors. In all circumstances the double peak remained.

Figure 2 contains the distribution of FRDM mass differences [2]

$$\Delta M(N, Z) \equiv M_{\text{exp}}(N, Z) - M_{\text{th}}(N, Z),$$

in the proton number (N) - neutron number (Z) space. We can see large domains with a similar error (each tone is associated to the magnitude of the error). It is remarkable that very well defined correlated areas of the same gray tone exist, which is a clear indication of remaining systematics and correlation.

Both the distribution of mass errors in the N-Z plane and the presence of the double peak in the error distribution suggest the presence of important correlations which are not taken into account in the FRDM mass formula. In the next sections these correlations are quantified and parametrized.

2. Regularities in the mass errors

In order to visualize the oscillatory patterns suggested in Fig. 2, different cuts were performed along selected directions on the N-Z plane in [6], then a Fourier analysis was performed, and the frequency dependence of the spectral function was analyzed. In the present study we propose some
alternative sequences to the mentioned cuts. The discrete Fourier transforms $F_k$ are calculated as

$$F_k = \frac{1}{\sqrt{N}} \sum_j \frac{\Delta M(j)}{\gamma} \exp \left( -\frac{2\pi i j k}{N} \right), \quad (2)$$

where $N$ is the number of mass differences $\Delta M$ in a given series. The parameter $\gamma$ makes $F_k$ dimensionless. Given that it only affects the global scale of the Fourier amplitudes, we made the simple selection $\gamma = 1$ MeV. The Fourier amplitudes are plotted as functions of the frequency $f = k/N$. The presence of a few frequencies with notorious large components underlines the existence of an oscillatory behavior of the mass errors.

2.1. Fixed $A$ or $T_z$

In Ref. 6 an analysis for the errors distribution for fixed $N$ or $Z$ was performed, where different chains of isotopes and isotones with 20 or more nuclei exhibited clear regularities. The presence of these regularities implied a periodicity in the error, and a Fourier analysis for this set of chains revealed well defined peak for low frequency $f \approx 1/20 = 0.05$.

To map the mass error data in term of variables with the maximum possible number of nuclei along each chain, the following transformation is employed

$$\tilde{A} = \ln [\sqrt{2} (N \sin \theta + Z \cos \theta)]$$

$$\tilde{T}_z = \ln [\sqrt{2} (N \cos \theta - Z \sin \theta)]. \quad (3)$$

Both $\tilde{A}$ and $\tilde{T}_z$ are, by construction, integer numbers. To avoid introducing artificial noise, the data are softened by the interpolation of mass errors for unphysical values of $\tilde{T}_z, \tilde{A}$, i.e. those with $\tilde{T}_z$ even and $\tilde{A}$ odd, or viceversa. This process is necessary to eliminate the large number of zeros which are induced by the transformation, which create artificial high frequency noise in the data.

Definition (3) has the advantage that, for $\theta = 45^\circ$, $\tilde{A} = A, \tilde{T}_z = 2T_z$. There are seven values of $T_z$ which have more than 40 nuclei with measured masses. They are $2T_z = 5, 6, 7, 8, 16, 17, 18$. Their mass differences $\Delta M$ are plotted as a function of the mass number $A$ in the seven inserts shown in Fig. 3 (left insert). The clustering of negative and positive errors is evident, again exhibiting the presence of residual correlations between the mass errors and the atomic and neutron numbers $(Z, N)$, or, equivalently, with the isospin projection and the mass numbers.

The squared amplitudes of the Fourier transforms of the mass differences are shown in Fig. 3 (right insert). For the first four isotopic chains ($2T_z = 5, 6, 7, 8$) there is a prominent peak at $f \approx 0.033$, i.e. a period $\Delta A \approx 30$, which is about one third the size of each set of nuclei. The remaining three chains exhibit also a peak at low frequencies, but lower and wider.

2.2. Rotated $\tilde{A}$ and $\tilde{T}_z$

We found that the best orientation, in order to have as many isotopes as possible with the same $\tilde{T}_z$, is $\theta = 56^\circ$. With this transformation, there are 174 isotopes with $\tilde{T}_z = 0$.

Figure 4 (left insert) displays the mass errors for 7 values of $\tilde{T}_z$, from $\tilde{T}_z = -4$ to 2. The regularities seen in Fig. 2 as regions with the same gray tone are seen here in the different plots, as groupings of nuclei with similar positive or negative mass differences, for the same $\tilde{A}$ region. Besides the two large groups with positive and negative mass errors below $\tilde{A} = 50$, there are evident regions with negative errors close to $\tilde{A} = 100$, and with positive mass differences for $150 < A < 200$.

A Fourier analysis of the previous results is presented in Fig. 4 (right insert). It is clear that for all the chains a few low frequencies again dominate the spectrum. In some chains there are also some higher frequencies which seem to be relevant, while for $\tilde{T}_z = 0$ their contribution is small. These frequencies, close to $f = 0.5$, are associated to oscillations with period 2, i.e. strong fluctuations between one nucleus and its closest neighbors.

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In Fig. 5 the contribution of very few frequencies to the mass differences, for the chains with $T_z = -2, -1, 0$ and 1 are presented. The upper panels show the full sequences of mass differences, the medium panels the contribution of the four frequencies with the largest amplitudes, and the lower panels the remaining mass errors. In all cases it is apparent...
that the regularities are quite significant, and that the sub-
traction of these systematic errors would lead to important
improvements in mass calculations.

2.3. Bustrofedon: all data aligned

Plotting the mass differences for different Z, Fig. 6 top, and
for different N, Fig. 6 bottom, is very common in mass cal-
culations. Both plots exhibit some degree of structure. In this
way we obtain a plot of mass differences as a function of Z,
with all the isotopes plotted along the same vertical line. The
difficulty in quantifying these regularities lies in the simple
fact that the are many nuclei with a given N or Z. For this
reason in [6] we have analyzed the data using different cuts.

Another way to organize the FRDM mass errors for the
1654 nuclei with measured masses is to order them in a sin-
gle list, numbered in increasing order. To avoid jumps, we
have ordered the isotopes along a βούτροφηδον (bustrofe-
don) line, which literally means “in the way the ox ploughs”.
Nuclei were ordered in increasing mass order. For a given
even A, they were accommodated following the increase in
N-Z, and those nuclei with odd A starting from the largest
value of N-Z, and going on in decreasing order. The middle
panel exhibits the same mass differences plotted against the
order number, from 1 to 1654. It provides a univalued func-
tion, whose Fourier transform can be calculated. The squared
amplitudes are presented in Fig. 7.

As it was the case for the cuts for given N, Z, A or T_z, the
fully ordered data Fourier amplitudes are completely domi-
nated by a few low frequencies. It is also remarkable that
for \( \ln(f) > -3 \) the frequency distribution clearly resembles a
power law.

Removing the five frequencies with the largest Fourier
components (|\( F_k | > 3 \)) generates a noisier pattern. Fig-
ure 8 shows the mass differences plotted as function of the
order index, and the results of leaving only the frequencies
with amplitudes |\( F_k | \) larger (or smaller) than 3. There are
only five frequencies with Fourier amplitudes whose absolute
value is larger than 3. From them the dominant frequency is
the one with period \( \Delta i = 207 \). The regular pattern generated
by these five frequencies in displayed in the middle panel of
Fig. 8. The remnant, shown in the bottom panel, is clearly
closer to white noise, while some bumps remain.

From the analysis presented in this section, we can con-
clude that there are conspicuous correlations in the FRDM
mass differences, whose periodic character is clearly exhib-
3. Removing the regularities

Having established that there are patent regularities in the differences between the masses calculated using the FRDM [2] and the measured ones, we will proceed to eliminate them in a simple way, by removing the two frequencies which contribute the most to the mass errors as functions of N and Z. We introduce an amplitude and a phase for each frequency, having a total of six parameters for protons and six for neutrons. The functions which minimize the errors separately for protons and neutrons are:

\[
\Delta_1(N) = 0.30 \sin(2\pi \times 0.12 N + 0.284) \\
+0.20 \sin(2\pi \times 0.047 N + 1.06) \\
\]

\[
\Delta_1(Z) = 0.23 \sin(2\pi \times 0.020 Z - 0.83) \\
+0.10 \sin(2\pi \times 0.053 Z + 3.74) \\
\]

In a fit including all nuclei, we found

\[
\Delta_2(N) = 0.21 \sin(2\pi \times 0.011 N + 0.86) + 0.34 \sin(2\pi \times 0.049 N + 0.17) \\
\Delta_2(Z) = 0.14 \sin(2\pi \times 0.025 Z - 0.74) - 0.19 \sin(2\pi \times 0.075 Z - 5.53) \\
\]

\[
\Delta_2(N, Z) = \Delta_2(N) + \Delta_2(Z), \\
\]

while including only nuclei with A ≥ 65 the best fit is

\[
\Delta_3(N) = 0.65 \sin(2\pi \times 0.009 N + 2.03) \\
+0.19 \sin(2\pi \times 0.047 N + 1.00) \\
\]

\[
\Delta_3(Z) = 2.90 \sin(2\pi \times 0.018 Z - 3.51) \\
+2.61 \sin(2\pi \times 0.019 Z - 0.74) \\
\]

\[
\Delta_3(N, Z) = \Delta_3(N) + \Delta_3(Z). \\
\]

The $$\Delta_1$$ are functions only of N or Z, and were adjusted using six parameters, optimized for the 1350 nuclei with A ≥ 65. $$\Delta_2$$ and $$\Delta_3$$ are obtained by including at the same time the corrections in Z and N, for all the nuclei in the first case, and for those with A ≥ 65 in the second. The fitted frequencies

\[
\Delta_3(N) = \Delta_3(N) + \Delta_3(Z). \\
\]
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**Figure 9.** Mass differences plotted as function of Z (left) and N (right), for $A \geq 65$. The upper panels exhibit the FRDM results, the intermediate ones the sinusoidal corrections, and the lower panels the corrected mass differences.

are all between 0.01 and 0.05, in agreement with the dominant Fourier frequencies found in the previous section.

The effect of removing these sinusoidal components as functions of N and Z is shown in Fig. 9, for those nuclei with masses larger than 65.

While the regular pattern is more apparent as a function of N, on the right hand side panels, in both cases the ‘corrected’ masses are more compact and compressed at smaller errors.

Obtaining a better fit of the known nuclear masses by the inclusion of six or twelve extra variables is by no means surprising. However, the use of sinusoidal functions of N and Z is strongly motivated by the data themselves. The fit does not only reduce the overall error, but makes the double peak in the error distribution disappear, as shown in Fig. 10.

After removing the oscillatory components, the r.m.s. mass errors is reduced from 0.681 MeV to 0.597 MeV for all nuclei, and from 0.534 MeV to 0.462 MeV for nuclei with $A \geq 65$.

**Figure 10.** Distribution of FRDM mass differences corrected with a sinusoidal function of Z, of N, and of Z and N.

**4. Final remarks**

In the present study we have shown that the differences between the masses calculated using the FRDM of Möller et al. [2] and the measured ones have a well defined oscillatory component as function of N and Z, which can be removed with an appropriate fit, significantly reducing the error width, and concentrating the error distribution on a single peak around zero.

The remaining correlations can only originate in the microscopic terms in the mass formula, which in the FRDM are evaluated using the Strutinsky method [9]. Having shown that these correlations have a simple and clear dependence in the proton and neutron numbers, we are studying the possible removal of these effects by a refinement of the Strutinsky method, whose results will be reported elsewhere [10].

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