Image reconstruction of nuclear masses

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The differences between measured masses and Liquid Drop Model (LDM) predictions have well known regularities, which can be analyzed as a two-dimensional texture on the N-Z plane. The remaining microscopic effects, obtained after removing the smooth LDM mass contributions, have proved difficult to model. They contain all the information related to shell closures, nuclear deformation and the residual nuclear interactions, and display a well defined pattern. In the present work the more than 2000 known nuclear masses are studied as an array in the N-Z plane, viewed through a mask, behind which the approximately 7000 unknown unstable nuclei that can exist between the proton and neutron drip lines are hidden. Employing a Fourier transform deconvolution method these masses can be predicted. The image reconstruction technique allows the precise prediction of nuclear masses in the vicinity of the region of nuclei with measured masses, improving any reference model. Other potential applications of the present approach are outlined.

Keywords: Nuclear physics; data analysis; other topics in nuclear structure; nuclear masses.

Las diferencias entre las masas medidas y las predicciones del Modelo de Gota (LDM, por sus siglas en inglés) tienen regularidades bien conocidas, que se pueden analizar como una textura bi-dimensional en el plano N-Z. Los efectos microscópicos remanentes, obtenidos después de haber sustraido las contribuciones suaves del LDM, resultan ser difícil para el modelo. Contienen toda la información sobre la cerradura de capas, deformaciones nucleares y la interacción residual nuclear, mostrando un patrón bien definido. En el presente trabajo más de 2000 masas nucleares conocidas son estudiadas como un arreglo en el plano N-Z tras una máscara, detrás de la cual son escondidas aproximadamente 7000 núcleos inestables y desconocidos, que pueden existir entre la dropline de los protones y la de los neutrones. Aplicando el método de la transformación de Fourer estas masas se pueden predecir. La técnica de la reconstrucción de imagen permite la predicción precisa de masas nucleares en la vecindad de la región de masas nucleares medidas, mejorando cualquier modelo de referencia. Se exponen otras aplicaciones potenciales del presente procedimiento.

Descritores: Física nuclear; análisis de datos; otros temas en estructura nuclear; masas nucleares.

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Nuclei are particularly complex systems, ranging from a single proton to more than three hundred nucleons, too large for a detailed microscopic treatment but too small for statistical methods. Their interest is not restricted to nuclear physicists since the atomic nuclei that constitute our world are manufactured inside stars, defining their evolution and fate. Nuclei are not easily subject to theoretical scrutiny and display a rich variety of behaviour as a function of $N$ and $Z$, the number of neutrons and protons, respectively. Arguably, the most basic property of a nucleus is its mass. Understanding nuclear masses provides a test of our basic knowledge of nuclear structure and is an essential ingredient of the fundamental astrophysical problem of nucleosynthesis, which often takes place in far-from-stability conditions, on ultra-short time-scales [1]. Though great progress has been made in the challenging task of measuring the mass of short-lived nuclei which are far from the region of stable, naturally occurring isotopes, theory is needed to predict their properties and guide experiments that search, for example, for regions of increased stability [2]. Despite the efforts invested in developing techniques which can accurately describe these masses, the predictions made by different models often turn out to be disconcertingly different, even in regions close to known masses. Reliable theoretical models and methodologies that can predict the mass and other properties of these “exotic” nuclei are still missing [3]. Here we present a new procedure which combines well-known nuclear models with image reconstruction techniques. A colour-coded image is built by taking the differences between measured masses and the predictions given by the different theoretical models. This image is viewed as part of a larger array in the $(N, Z)$ plane, where unknown nuclear masses are hidden, covered by a “mask”. We apply a suitably adapted deconvolution algorithm, used in astronomical observations, to “open the window” and see the rest of the pattern. We show that it is possible to improve significantly mass predictions in regions not too far
from measured nuclear masses. This procedure can be applied to other physical observables and might be extended to regions far away from the valley of stability.

The efforts to calculate nuclear masses have been hampered by the absence of a true effective theory of the nuclear interaction and by the difficulties inherent to quantum many-body calculations. Instead, simplified approaches to model the atomic nucleus have been devised. The cornerstone of nuclear mass models is the semi-empirical mass formula proposed by von Weizsäcker [4], Bethe and Bacher [5] in the 30s, which is based on a picture of the nucleus as a uniform, very dense, charged liquid drop—the so-called liquid-drop model (LDM). Although the LDM gives an accurate overall description of nuclear masses, it lacks quantum-mechanical shell effects and hence large deviations from the measured masses are observed in certain regions of the nuclear chart. The inclusion of shell effects usually requires more sophisticated treatments, like the finite-range droplet model [6], which combines macroscopic effects with microscopic shell and pairing corrections, the approach of Duflo and Zuker (DZ) [7] inspired by the nuclear shell model, and the Hartree-Fock approach [8]. It is in general difficult, however, to match theory and experiment (for all known nuclei) with an average precision better than about 0.5 MeV [3]. More troublesome is the fact that different model predictions tend to diverge from each other when extending them to regions of nuclei with unknown mass.

The starting point in the proposed approach is the striking colour pattern in the \((N, Z)\) plane shown in Fig. 1, which results after taking the difference between measured masses \([9,10]\) and improved LDM predictions (see, e.g., Ref. 11 and references therein). In Fig. 1 we observe a residual pattern, related to shell closures, nuclear deformations and residual interactions, in a compelling graphic form. This suggests an approach to the problem of mass prediction based on image reconstruction techniques. The basic idea is to consider that the more than 2000 known nuclear masses represent a partial view of a larger image array in the \((N, Z)\) plane, and that all other nuclei (perhaps around 7000 in number) which might exist between the neutron and proton drip lines remain hidden, covered by a “mask”. Thus, the question is: Can we “open the window” to unveil the remainder of the pattern or, at least, part of it? We show here that indeed this information can be, at least partially, reliably uncovered with image reconstruction techniques. The success of the approach, however, strongly depends upon whether the remaining physical features in the problem can be coded in terms of (global) regularities in the \((N, Z)\) plane, which can be modeled by a finite number of harmonic components. The reconstruction also depends on how well the original models describe the experimental data, and how systematic the remaining differences are. In this work we remove from consideration the region of light nuclei with \(N, Z < 28\). An important assumption of this approach is that the observed regularity and smoothness of the mass landscape remains throughout \([13]\). Although steep changes in mass may occur in a rather short interval, e.g., due to shell structure or shape transitions, there are no sudden jumps. The landscape varies smoothly as a function of nucleon numbers, as can be observed in Fig. 1. However, since non-periodic patterns, such as shell closures (so-called “magic” numbers), are difficult to extrapolate by harmonic components, we find it necessary to incorporate additional physical information into the procedure (see below).

We display the mass table by a two-dimensional array of pixels, with \(N\) in the horizontal position and \(Z\) in the vertical one. Differences between experimental masses \(m_{\text{expt}}(N,Z)\) and calculated ones \(m_{\text{th}}(N,Z)\) define the colour image function

\[
i(N, Z) \equiv m_{\text{expt}}(N, Z) - m_{\text{th}}(N, Z).
\] (1)

The relation between \(i(N, Z)\) and the full pattern \(m(N, Z)\) is then given by

\[
i(N, Z) = m(N, Z) \cdot w(N, Z),
\] (2)

where \(w(N, Z)\) is a binary mask function, taking the value 1 for positions \((N, Z)\) where nuclear masses are known, and 0 otherwise (although a “weighted” mask may be used instead—see Ref. 12). We thus need to extract \(m(N, Z)\) from Eq. (2). Formally, this is a deconvolution problem. If \(I(k_N, k_Z)\), \(M(k_N, k_Z)\) and \(W(k_N, k_Z)\) are the Fourier transforms of \(i(N, Z)\), \(m(N, Z)\) and \(w(N, Z)\), respectively, then

\[
I(k_N, k_Z) = M(k_N, k_Z) \ast W(k_N, KZ),
\] (3)

where \(M \ast W\) is the convolution of the functions \(M\) and \(W\). Since both \(i(N, Z)\) and \(w(N, Z)\) are known for the whole domain, their Fourier transforms \(I(k_N, k_Z)\) and \(W(k_N, k_Z)\) can be evaluated directly. The problem is narrowed down to obtaining the function \(M(k_N, k_Z)\), from which \(m(N, Z)\) can be recovered by applying an inverse Fourier transform. Deconvolution is non-trivial and may lead to non-unique solutions, but there exist several algorithms, such as the CLEAN method, often used in radioastronomy \([14,15]\), and the maximum entropy method \([16]\) which provide testable methodologies. We have chosen a specially adapted version of the
TABLE I. AME95-03 test: Predictability test for the set of nuclei in AME03 and not in AME95, restricted to $N, Z \geq 28$.

<table>
<thead>
<tr>
<th>Model</th>
<th>RMS</th>
<th>RMS (with CLEAN)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LDM, Eq. (2) in [19]</td>
<td>1.9307 MeV</td>
<td>0.8763 MeV</td>
</tr>
<tr>
<td>LDMM, Eq. (4)</td>
<td>0.9955 MeV</td>
<td>0.3718 MeV</td>
</tr>
<tr>
<td>DZ model [7]</td>
<td>0.3384 MeV</td>
<td>0.2797 MeV</td>
</tr>
</tbody>
</table>

TABLE II. AME03-border test: Predictability test for the set of nuclei in the border of AME03, restricted to $N, Z \geq 28$.

<table>
<thead>
<tr>
<th>Model</th>
<th>RMS</th>
<th>RMS (with CLEAN)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LDM, Eq. (2) in [19]</td>
<td>2.7763 MeV</td>
<td>0.9168 MeV</td>
</tr>
<tr>
<td>LDMM, Eq. (4)</td>
<td>1.9804 MeV</td>
<td>0.9333 MeV</td>
</tr>
<tr>
<td>DZ model [7]</td>
<td>0.4039 MeV</td>
<td>0.3133 MeV</td>
</tr>
</tbody>
</table>

The main objective in this Letter is to provide a measure of predictability in the extrapolated mass differences $\Delta m = m_{\text{expt}} - m_{\text{th}}$ obtained with the CLEAN method. Two tests are applied. The first measures the predictability of the mass differences corresponding to the set of 371 experimental masses in AME03, not present in the previous AME95 compilation. We refer to this test as the “AME95-03 test”. The second test consists of predicting the mass differences of 301 nuclei at the border of the AME03 measured landscape. This “AME03-border test” is designed to measure the smoothness of the extrapolation and the ability of the method to make short-range predictions. We apply both tests to three models with different degrees of accuracy. The first is a macroscopic LDM with 7 parameters (Eq. (2) in [19]), which are determined by fitting (a) the (updated) AME95 data for the AME95-03 test, or (b) the AME03 data without border for the AME03-border test. The second model is an upgrade of this macroscopic LDM by the inclusion of schematic microscopic shell corrections [19]:

$$BE_{\text{LDMM}}(N, Z) = BE_{\text{LDM}}(N, Z) - a_1 F_{\text{max}} + a_2 F F_{\text{max}} + a_{\text{const}} , \quad (4)$$
In Figs. 2 and 3 we plot \( S_{\nu} \) versus \( Z \). The largest improvement (\( \sim 54\% \)) in the LDM (Eq. (2) in [19]) we also find a large rms reduction of \( \sim 52\% \) for the DZ model (see Table I). For the simple test, the improved rms, surprisingly, is comparable with the correction terms in the LDM of Eq. (4). Nevertheless, this rms reduction represents a significant correction.

In all tests the CLEAN method is iterated until a root-mean-square (rms) deviation of 100 keV is achieved for the input data fit. The algorithm, applied subject to a set of appropriate conditions [18], proved to be very robust. Table I shows a comparison of the rms results for the AME95-03 test, and those obtained with the CLEAN method for each model. Table II gives a similar comparison for the AME03-border test.

In the AME95-03 test the largest CLEAN improvement (\( \sim 62\% \) rms reduction) is obtained for the LDMM of Eq. (4). The improved rms, surprisingly, is comparable with the corresponding rms in the DZ model (see Table I). For the simple LDM (Eq. (2) in [19]) we also find a large rms reduction of \( \sim 54\% \) while for the DZ model we find it to be \( \sim 20\% \). The latter smaller improvement is expected, as this model is already in very good agreement with the experimental masses. Nevertheless, this rms reduction represents a significant correction.

A similar situation occurs for the AME03-border test. The largest improvement (\( \sim 66\% \) rms reduction) occurs for the macroscopic LDM, followed by LDMM of Eq. (4) with a \( \sim 52\% \) rms reduction. Again, as in the AME95-03 test, the rms in the DZ model decreases by \( \sim 20\% \). These results suggest that the CLEAN method can efficiently incorporate the residual patterns observed in the experimental masses. The rms, however, being an average measure, is not a sufficiently clear gauge. Therefore, we now turn to an amplified view of our results, using two-neutron separation energies \( S_{2n} \).

Two-neutron separation energies,

\[
S_{2n}(N, Z) = BE(N, Z) - BE(N - 2, Z),
\]

contain detailed information about nuclear structure effects. In Figs. 2 and 3 we plot \( S_{2n} \) for isotope series in the \( N \sim 78-128 \) region for the AME95-03 test using the LDMM of Eq. (4) and the DZ model, respectively.

The predictions of the macroscopic LDM (not shown here for lack of space), are completely flat, without any structure at all. In contrast, the data display strong variations at the magic numbers \( N = 82 \) and 126, and a substructure at \( N \sim 90 \). After reconstruction those structures are well described (with an rms of \( \sim 0.1 \) MeV) in the fitted region (AME95 data). On the other hand, the benchmark AME03 data are also surprisingly well predicted (with an rms of 0.8763 MeV—see Table I). Although the shell structures are thus well described by the CLEAN algorithm, the reconstruction is not sufficiently constrained. This is illustrated by the presence of spurious substructures in the \( N \sim 90 \) to 100 region, which, although small in magnitude, are not seen in the \( S_{2n} \) data. To minimize such spurious effects, it is necessary to impose additional constraints and this can be achieved, e.g., by schematically including shell correction terms as it is done in the LDMM of Eq. (4).

Figure 2 shows the \( S_{2n} \) in the \( N \sim 78-128 \) region of the AME95-03 test, obtained with the LDMM (isotopic lines in Fig. 2a), and the results obtained after applying the reconstruction algorithm (isotopic lines in Fig. 2b). In LDMM the magic numbers \( N = 82 \) and 126 are incorporated into the model from the beginning. The experimental \( S_{2n} \) in those regions display discontinuities which are well described by LDMM. However, the substructure observed in the data at \( N \sim 90 \) is not properly accounted for (see Fig. 2a). After applying the reconstruction to LDMM, the substructure is correctly described (with an rms of \( \sim 0.1 \) MeV) in the fitted region (AME95 data). It is remarkable that the region of the benchmark AME03 data (green bullets in Fig. 2) is also accurately predicted (with an rms of 0.3718 MeV—see Table I). The constraints imposed by the schematic shell correction terms in the LDMM of Eq. (4) are thus sufficient to remove the spurious substructure observed in the LDMM reconstruction.

The results for the \( S_{2n} \) obtained with the DZ model in the \( N \sim 78-128 \) region of the AME95-03 test, and its improvement by the image reconstruction method, are shown in Figs. 3a and 3b, respectively. In this case, the DZ model shows the presence of the substructure at \( N \sim 90 \) but the experimental \( S_{2n} \) are not accurately described. Furthermore, the isotopic lines become flat outside the region where measurements are available. The DZ model has an rms of 0.3384 MeV (see Table I), giving an excellent overall description of the \( S_{2n} \) in the predicted region. Nevertheless, the reconstruction method can be used to improve the description by a significant \( \sim 20\% \).

We have made similar tests in the \( N \sim 110-160 \) region for the AME03-border case, using the \( S_{2n} \) obtained with the LDM, LDMM and DZ models, and the corresponding calculations using the image reconstruction method. The improvements as a result of the CLEAN procedure are of the same quality as for the AME95-03 test. Details will be discussed elsewhere [18].
Summing up, we have shown that the CLEAN reconstruction method is able to encode residual effects on nuclear masses and can be used to improve the predictions of theoretical models in a reliable way, at least for regions not too far from measured cases. The method can be applied to other observables, whenever a sufficient amount of measured data is available.

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