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Perspectives on nuclear mass formulae

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We discuss different nuclear mass tables (experimental and calculated) in the context of the Garvey-Kelson relations and show how these relations can provide a very useful tool to test and improve the consistency of the models.

Keywords: Binding energies and masses.

Se discuten las masas nucleares en el marco de las relaciones Garvey-Kelson y cómo usar esas relaciones para probar y mejorar la consistencia de modelos teóricos.

Descriptores: Energías de amarre y masas nucleares.

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1. Introduction

Nuclear masses [1] have been of great interest to nuclear physics ever since the beginning of the field. They reflect the role of the strong nuclear interaction on nuclear binding energies and their study has led to many important advances, including the existence of magic numbers and the charge independence and short range character of the nuclear force. At present, we know the nuclear masses of approximately 2000 nuclei out of the roughly 7000 expected between the nuclear drip lines. Many important questions remain unanswered, however, including for example the properties of binding energies close to the drip lines and in the predicted islands of superheavy nuclei. In addition, nuclear masses provide crucial input to calculations in nuclear astrophysics [2]. For this reason, we must resort to nuclear mass models, with the hope that they can predict nuclear masses reliably in regions in which they are not measured. Several models have been developed to calculate and predict unknown nuclear masses over the last 70 years. While the accuracy of the present state-of-the-art calculations are impressive, it is still insufficient in some cases, for example in calculations of relevance to the astrophysical neutron-capture (*n*-process). In this kind of processes, a iron nucleus captures rapidly (*r*-process) or slowly (*s*-process) neutrons , where rapidly or slowly means with respect to the β^- decay rate, and then decays transforming a neutron into a proton. This process is thought to be responsible for the existence of heavy nuclei such as gold or uranium [3,4].

The simplest mass model is the Liquid Drop Model [5], which incorporates the essential macroscopic physics. This model assumes that the nucleus resembles a very dense, charged liquid drop. The Finite Range Droplet Model [6] is often considered the standard by which to calculate nuclear masses. It is a very sophisticated liquid drop model, which includes microscopic input in the form of shell and pairing corrections. Another model of special interest is due to Duflo and Zuker [7], which is based on the Nuclear Shell Model and which has had considerable success. There are also completely microscopic approaches, which employ the Hartree-Fock-Bogolyubov mean-field formalism [8] and global effective interactions.

In addition to these global mass models, there are also local methods in which the mass of a given nucleus is related to those of its neighbors. The Garvey-Kelson relations [9] is the most relevant such method and has been used by Jänecke [10] and coworkers to generate nuclear mass tables. In this work we too use the Garvey-Kelson mass relations, but, as we will soon explain, in a very different way.

In this work we study several nuclear mass tables, as derived from the different theoretical approaches described above and fitted to the most recent tabulation of experimental masses (AME03) [11]. We discuss how the Garvey-Kelson (GK) relations, in an optimized version, can be used to assess the various mass tables and in particular how well they extrapolate to unknown regions. In the next section, we introduce the models tested in this work and compare their relative RMS deviations with respect to the experimental data. In Sec. 3, we describe the GK relations and their use in tests of the various mass models. We summarize our main conclusions in the last section.

2. Nuclear mass tables

We can divide the theoretical approaches to calculate nuclear masses into two main groups: local and global methods. Global methods rely on the available experimental information from the entire nuclear landscape to build a mass table. In contrast, local methods focus on the experimental information of the surrounding nuclei to evaluate the mass of a given nucleus. A typical example of a global method is the liquid drop mass (LDM) formula. The parameters of this formula, which enter linearly, are fitted to reproduce the measured binding energies. Other global methods include the Finite Range Droplet Model (FRDM) of Möller and collaborators, models based on the Hartree-Fock-Bogoliubov (HFB) method and the Shell Model inspired formula developed by Duflo and Zuker (DZ). The Garvey-Kelson (GK) relations are an example of a local method. But there are others, such as the short range extrapolations used by Audi, Wapstra and Thibault in atomic mass evaluations or approaches based on neural networks. Finally, we wish to mention a new technique which has been used as a global method and does not make any assumptions about the dependence of the nuclear masses on the number of protons or neutrons. This technique is known as the CLEAN method [12,13] and currently focuses on nuclear masses from a phenomenological point of view. It can, however, also be applied to a restricted set of nuclei and turned into a local method, and furthermore can be applied to other physical quantities, such as nuclear radii, excitation energies or electromagnetic transition rates.

We will not go into details here on the detailed ingredients of the different methods for building mass models, as this information can be found elsewhere [1,5-8]. Rather, we simply use the mass tables as published and compute the root mean square (rms) deviations between the masses in these tables and the measured masses. These deviations are summarized in Table I. The starting point to build this table is the set of 2149 nuclei for which masses were available in AME03. This set has been divided into two subsets with 1760 and 389 nuclei, respectively. The first involves those nuclei whose masses were available in the earlier atomic mass evaluation AME95 [14]. We refer to this as the *Fit* set, since this is the input data set that was employed by the different models to fit their relevant parameters. The second column in Table I shows the rms deviations between the experimental and calculated masses for the nuclei present in the *Fit* set. The second subset consists of the rest of the nuclei in the AME03 table, namely those that were not included in AME95. We denote this as the *Prediction* set. The third column in Table I shows the rms deviations between the experimental and calculated masses for the nuclei present in the *Prediction* set. These numbers give an idea on how each model extrapolates to unknown nuclei. We have included in the last row the rms deviations corresponding to the short range extrapolations made to AME95 from systematics. We see that none of the models can obtain an rms value as low as exhibited by the short-range extrapolation of the AME95 masses. We also note that the results obtained from the CLEAN fits, whose

TABLE I. Comparison between the *Fit* and *Prediction* root mean square (rms) deviations (in keV) among different models (see text for details).

Model	Fit rms	Prediction rms
HFB	651	693
FRDM	679	533
DZ	343	422
CLEAN I	199	859
CLEAN II	199	679
CLEAN III	199	373
AME95	–	295

details can be found in Ref. 13, become better as the input data contains more physical information. The input data in CLEAN I consists of the differences between the experimental and the calculated masses from the simple liquid drop formula. In CLEAN II a more sophisticated liquid drop formula [15], which includes shell corrections associated with valence nucleons, has been used to evaluate the differences that define the input data. Finally the differences between the experimental and the calculated masses with the Duflo-Zuker formula were used as the input data in CLEAN III. This calculation shows the best results of all the mass models analyzed in this work.

3. The Garvey-Kelson relations

The previous section measured the success of a mass model through its rms deviation from the experimental data. This is only a reflection of the mean behavior of the calculated data, however. In this section we show how we can use the Garvey-Kelson (GK) relations, appropriately combined [16,17], to provide a more subtle test of a nuclear mass model.

The most commonly used GK mass relations can be obtained by cancelling to first order the different interactions between nucleons in a extreme single-particle picture of the nucleus. Alternatively they can be inferred [18] by imposing the following equalities:

$$\epsilon_{2n-1p}(N+2,\, Z+1) = \epsilon_{1n-2p}(N+1,\, Z+2), \quad (1)$$

$$\epsilon_{2n-2p}(N+1,\, Z+2) = \epsilon_{1n-2p}(N+1,\, Z+2) + \epsilon_{2n-1p}(N+2,\, Z+1), \quad (2)$$

where $\epsilon_{jn-ip}(N,\, Z)$ represents the interaction energy between the last j neutrons and the last i protons and is defined by

$$B(N+j,\, Z+i) = B(N,\, Z) + S_{jn}(N+j,\, Z) + S_{ip}(N,\, Z+i) + \epsilon_{jn-ip}(N+j,\, Z+i). \quad (3)$$

Here $B(N,\, Z)$, $S_{jn}(N,\, Z)$ and $S_{ip}(N,\, Z)$ are the binding energy and the separation energies of j neutrons and i protons in a nucleus with N neutrons and Z protons, respectively.

The relations (1) and (2), expressed in terms of binding energies, give rise to the following GK relations:

$$B(N+2,\, Z-2) - B(N,\, Z) + B(N,\, Z-1) - B(N+1,\, Z-2) + B(N+1,\, Z) - B(N+2,\, Z-1) = 0, \quad (4)$$

and

$$B(N+2,\, Z) - B(N,\, Z-2) + B(N+1,\, Z-2) - B(N+2,\, Z-1) + B(N,\, Z-1) - B(N+1,\, Z) = 0. \quad (5)$$

If instead of N and Z, the mass number $A = N + Z$ and the isospin $T_Z = (N-Z)/2$ are used, we obtain

$$B(A,\, T_Z+2) - B(A,\, T_Z) + B\left(A-1,\, T_Z+\frac{1}{2}\right) - B\left(A-1,\, T_Z+\frac{3}{2}\right) + B\left(A+1,\, T_Z+\frac{1}{2}\right) - B\left(A+1,\, T_Z+\frac{3}{2}\right) = 0, \quad (6)$$

and

$$B\left(A+2,\, T_Z+1\right) - B\left(A-2,\, T_Z+1\right) + B\left(A-1,\, T_Z+\frac{3}{2}\right) - B\left(A+1,\, T_Z+\frac{3}{2}\right) + B\left(A-1,\, T_Z+\frac{1}{2}\right) - B\left(A+1,\, T_Z+\frac{1}{2}\right) = 0, \quad (7)$$

in which it is now clear that they represent differences between three pairs of nuclei with A or T_Z fixed. Thus, they can be considered as relations between discrete derivatives.

Following the procedure described in Ref. 17, we have applied systematically these relations to the experimental binding energies reported in AME03. As was explained in that reference, it is possible to apply up to 12 different GK relations to each nucleus. If we denote by n the number of different GK relations applied to a given nucleus, then we can calculate the rms deviation from zero for those nuclei in

TABLE II. The rms deviations for masses (in keV) calculated with the GK relations for different n.

	$n \geq 1$	$n \geq 4$	$n \geq 7$	$n = 12$
$A \geq 16$	182	152	123	87
$A \geq 60$	115	98	86	76

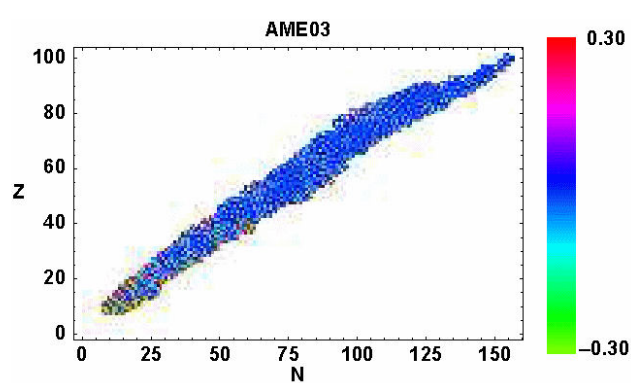

FIGURE 1.Mean deviations (color coded) from zero when the GK relations are applied over AME03 data. Red refers to nuclei with deviations or 0.3 MeV or greater, green to nuclei for which they are -0.3 MeV or less.

TABLE III. The rms deviations for masses (in keV) calculated with the GK relations for $n = 12$ and the different parities of N and Z.

	o-o	e-o	e-o	e-e
rms	106	85	88	67
%	35.0	23.7	25.6	15.7

TABLE IV. The rms deviations (in keV) from the GK relations with $n = 12$ for the FRDM, DZ, and HFB mass models. The results are shown both for nuclei in the AME03 tabulation and for the full set of particle-stable nuclei (including the predicted masses). Below the columns marked with # the number of nuclei is quoted.

Model	All nuclei		AME03	
	#	rms	#	rms
DZ	7431	44	1007	36
FRDM	7223	280	1007	103
HFB	7296	343	1007	138
CLEAN I	7718	47	1007	36
CLEAN II	7723	46	1007	33
CLEAN III	7431	45	1007	37

which the same number n are used. Table II shows these rms deviations for $A \geq 16$ and $A \geq 60$. We can see that as n increases the deviation from zero diminishes, *i.e.* the accuracy of the GK relations improves. Furthermore, the GK relations are more reliable for medium and heavy nuclei, since the rms deviations increase for $A < 60$. This can be seen clearly in Fig. 1, where the mean deviations from zero for each nucleus are plotted in the $N - Z$ plane according to a color scale. Points marked in red or green correspond to nuclei with deviations whose absolute values are above 0.3 MeV. These points are concentrated at low values of N, Z. Apart from this, the rest of the figure presents a rather homogeneous background, with no discernible correlations in N and Z. We conclude that for light nuclei the GK relations are less well satisfied and that the extreme single-particle picture with interactions cancelling to first order on which they are based are not well justified. In contrast, for medium and heavy nuclei, the results suggest that the GK relations can be applied reliably and as such can be used to perform interpolations between known masses, producing in this way accurate predictions for unmeasured masses of nuclei that are close to known regions.

Despite the success of the GK relations for medium and heavy nuclei noted above, there are still some nuclei that stand out in Fig. 1 as having somewhat larger than usual deviations. Most of these are odd-odd nuclei. To confirm whether this is a systematic feature, we restrict to those nuclei for which $n = 12$ relations can be applied and calculate separately the rms deviations between the GK prediction and the measured mass for even-even, odd-even, even-odd and odd-odd nuclei. Table III summarizes the results of these calculations. We see that the contribution of odd-odd nuclei to the total rms deviation is a factor of two larger than the contribution of even-even nuclei. A possible way to qualitatively understand this was pointed out in Ref. 17. It is based on the idea that there may be an effective enhancement of the neutron-proton interaction energy for odd-odd nuclei, which is not contained in the GK mass prescription and which should not be present to the same extent in odd-mass or even-even nuclei.

We also carried out a similar analysis for the various mass models described in the previous section. Namely for each mass model we determined the GK predicted masses and then compared the results with those of the model. We carried out the analysis for all nuclei in AME03, but restricted to those for which $n = 12$ GK estimates are possible. As noted earlier, these are the nuclei for which the GK relations work best. The rms deviations from zero are shown in column 3 of Table IV. We observe that the rms deviations from the DZ and CLEAN fits (about 45 keV) underestimate the experimental result (87 keV) by a factor of two, indicating that these approaches produce nuclear mass surfaces in the N-Z plane that are smoother than the experimental mass surface. In contrast, the results from FRDM and HFB show a large discrepancy compared to the experimental value. Here we want to emphasize that these results are obtained when the GK relations are applied over the whole nuclear mass tables, including both fitted and extrapolated binding energies. We also checked the corresponding behavior of these models when restricted to the input data set, namely to the fitted binding energies only, and show the corresponding results in column 5. We see that the results from CLEAN and DZ are consistent with the corresponding results in column 3, whereas the FRDM and HFB deviations are much larger when using the full data set than when using the fit data set only. Note that when only the fit data sets were used these two models were consistent with the GK relations at a level roughly comparable to the experimental data, but that the level of agreement becomes much worse for both of them when the new data was added. This suggests that these two models do not extrapolate well to unknown masses.

In Figs. 2 to 7, we plot the mean deviations from zero of the GK relations in the N-Z plane for each model. We see that each mass model, when studied in this way, exhibits correlations in N and Z. This is in contrast to Fig. 1, where

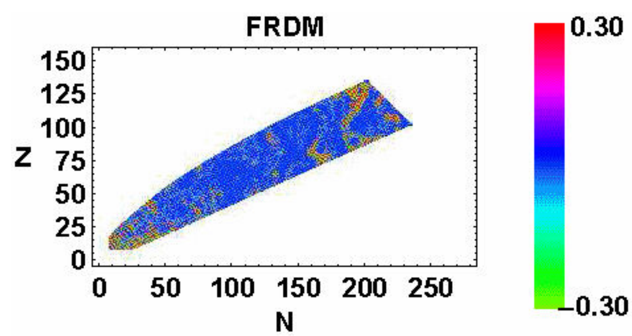

FIGURE 2. As in Fig. 1, for the FRDM nuclear mass table.

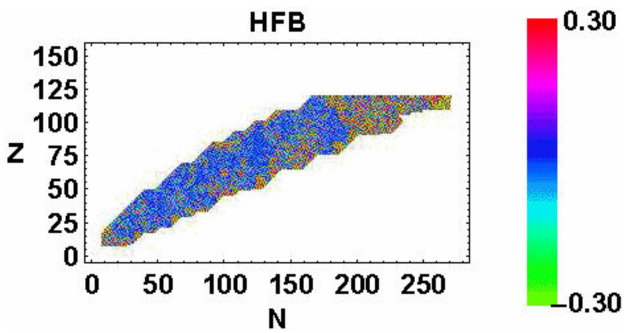

FIGURE 3. As in Fig. 1, for the HFB nuclear mass table.

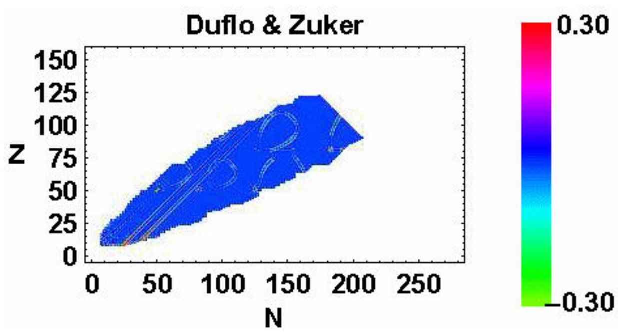

FIGURE 4. As in Fig. 1, for the Duflo-Zuker nuclear mass table.

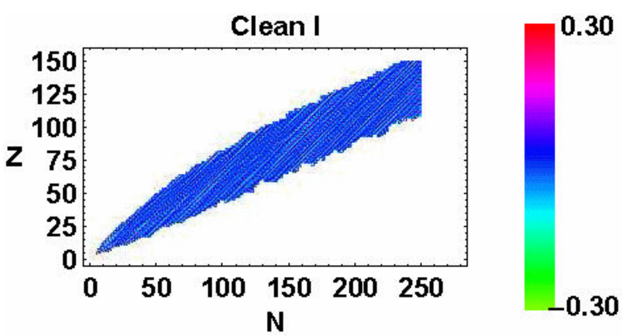

FIGURE 5. As in Fig. 1, for the CLEAN I nuclear mass table.

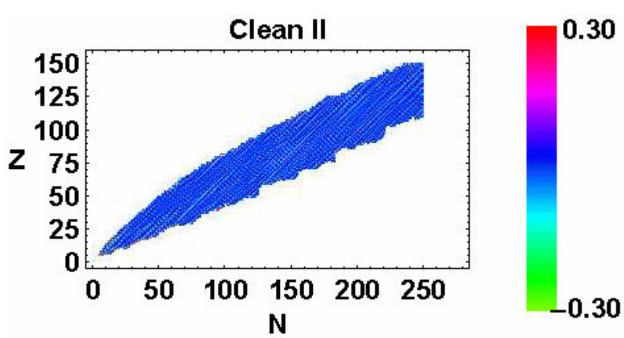

FIGURE 6. As in Fig. 1, for the CLEAN II nuclear mass table.

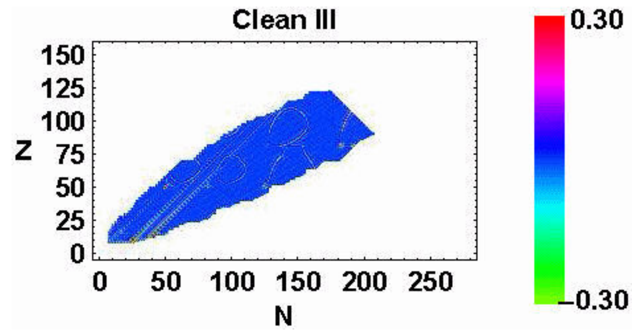

FIGURE 7. As in Fig. 1, for the CLEAN III nuclear mass table.

the GK predictions were compared to the associated experimental masses, and where no such correlations appeared. This suggests that the different mass models incorporate, albeit perhaps in different ways, some spurious correlations not present in the experimental data.

4. Conclusions

We have analyzed several nuclear mass models and compared them with the experimental data. We first performed the classical analysis based on rms deviations, both with the data that was included in their fits and with the newer data that has since appeared. We also tested how these models compare with predictions based on the Garvey-Kelson mass relations, so as to gauge the smoothness of the mass surface generated by that mass formula. Our results show that the GK relations are violated slightly when applied to the experimental data, with an rms deviation of about 100 keV. Of the various mass models we have considered, we find that the one obtained by applying the CLEAN method to the Duflo-Zuker mass formula produces the best mass table. A careful analysis of the GK relations applied to odd-odd nuclei, which could help elucidate the role of neutron-proton correlations on nuclear masses, is currently in progress.

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