

## Nuclear Masses Set Bounds on Quantum Chaos

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It has been suggested that chaotic motion inside the nucleus may significantly limit the accuracy with which nuclear masses can be calculated. Using a power spectrum analysis we show that the inclusion of additional physical contributions in mass calculations, through many-body interactions or local information, removes the chaotic signal in the discrepancies between calculated and measured masses. Furthermore, a systematic application of global mass formulas and of a set of relationships among neighboring nuclei to more than 2000 nuclear masses allows one to set an unambiguous upper bound for the average errors in calculated masses, which turn out to be almost an order of magnitude smaller than estimated chaotic components.

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The importance of an accurate knowledge of nuclear masses to understand the processes occurring in astrophysical phenomena has been abundantly stressed [1]. Though great progress has been made in the challenging task of measuring the mass of exotic nuclei, theoretical models are still necessary to *predict* their mass in regions far from stability [2]. Advances in the calculation of atomic masses have been hampered by the absence of an exact theory of the nuclear interaction and by the difficulties inherent to quantum many-body calculations, so diverse models which attempt to bring forth the fundamental physics of the atomic nucleus have been devised. The simplest approach is that of the liquid-drop model (LDM) [3]. It incorporates the essential macroscopic terms, which means that the nucleus is pictured as a very dense, charged liquid drop. Including the discrete character of the nucleons and their basic interactions requires more sophisticated treatments. The finite-range droplet model (FRDM) [4], which combines the macroscopic effects with microscopic shell and pairing corrections, has become the *de facto* standard for mass formulas. A microscopically inspired model has been introduced by Duflo and Zuker (DZ) [5–7] with positive results. Finally, among the mean-field methods it is also worth mentioning the Skyrme-Hartree-Fock approach [8,9]. These mass formulas can calculate and predict the masses (and often other properties) of as many as 8979 nuclides [2], but it is in general difficult to match theory and experiment (for all known nuclei) to an average precision better than about 0.5 MeV [2]. This minute quantity, corresponding to less than a part in  $10^5$  of the mass of a typical nucleus, still represents a significant fraction of the energy released in nuclear decays, strongly affecting the extrapolations of proton and neutron separation energies required in astrophysical processes [1,2].

Can these deficiencies of the mass formulas have a chaotic origin? It was recently suggested that there might be an inherent limit to the accuracy with which nuclear

masses can be calculated [10], due to the presence of chaotic motion inside the atomic nucleus [11]. The nature of quantum chaos is still an open question and diverse points of view coexist in the literature [12,13]. Classical chaotic behavior has been understood in terms of deterministic equations whose time evolution, however, has a sensitive dependence on their initial conditions. A different kind of unpredictability arises from the quantum nature of atoms, a behavior codified in Heisenberg's uncertainty principle. Yet, when these two sources of unpredictable features combine, the result is very difficult to fathom. It would appear that quantum uncertainty can smooth the characteristic signals of chaos, but experiments with Rydberg atoms in strong magnetic fields [14] and quantum dots [15] clearly display its footprints.

The presence of chaotic motion in highly excited nuclear systems can be gauged through the statistics of the high-lying energy levels or resonances [16–18] and their comparison with random matrix theory [19]. It has been convincingly shown that the power spectrum (Fourier transform squared) of the fluctuations of a chaotic quantum energy spectra is characterized by  $1/f$  noise [20]. The basic corollary of random matrix theory [18] is that near or around the neutron absorption threshold, predictability is hopeless and only a statistical analysis makes sense. The possible existence of a remnant of chaos at the level of the ground state [10] was addressed by Bohigas and Leboeuf [11] from a novel perspective. The errors among experimental and calculated masses in [4] are interpreted in terms of two types of contributions. The first one is associated with a regular part, related to the underlying collective dynamics (LDM), plus a shell-energy correction, while the other is assumed to arise from some inherent dynamics, possibly higher-order interactions among nucleons [11], that lead to chaotic behavior.

In this context it is worth analyzing the differences between measured and calculated masses using well-

known mass models, looking for signals of quantum chaos, and, if these are found, figuring out if such chaos is inherent to nuclear masses or an artifact of the approximations in the many-body theories. It is our purpose to also test the assertion that a lower limit on how accurately nuclear masses can be calculated may have already been reached [10]. To estimate the best available accuracy, we use a different approach to calculate known nuclear masses. Besides the “global” formulas of which FRDM has become the standard, there are a number of “local” mass formulas. These local methods are usually effective when we require the calculation of the masses of a set of nuclei, which are fairly close to other nuclei of known mass, exploiting the relative smoothness of the masses  $M(N, Z)$  as a function of neutron ( $N$ ) and proton ( $Z$ ) numbers to deduce systematic trends. Among these methods there are the equations connecting the masses of particular neighboring nuclei known as the Garvey-Kelson (GK) relations [21,22]. These relations do not involve free parameters and can be *derived* from a simple nuclear-model picture. Strictly speaking, they do *not* yield an independent calculational tool, but they do provide strong indications that a large fraction of the mass values have a smooth and regular behavior. In this interpretation, the GK relations can be viewed as a simple methodology to estimate nuclear masses from those of its neighbors.

In this Letter we carry out a systematic analysis of mass errors using different global mass formulas, supplemented with a study of the estimates arising from the GK relations, which we use to set an upper limit on the intrinsic precision with which masses can be estimated when enough local information is available.

There are different types of GK relations [23], and the two best known are [21–23]

$$\begin{aligned} & -M(N+1, Z-2) + M(N+1, Z) \\ & -M(N+2, Z-1) + M(N+2, Z-2) \\ & \quad -M(N, Z) + M(N, Z-1) = 0, \quad (1) \end{aligned}$$

$$\begin{aligned} & M(N+2, Z) - M(N, Z-2) \\ & + M(N+1, Z-2) - M(N+2, Z-1) \\ & \quad + M(N, Z-1) - M(N+1, Z) = 0. \quad (2) \end{aligned}$$

These simple equations are based on the independent-particle shell model and, furthermore, constructed such that neutron-neutron, neutron-proton, and proton-proton interactions cancel. Both GK relations provide an estimate for the mass of a given nucleus in terms of five of its neighbors. This calculation can be done in six different forms, as we can choose any of the six terms in the formula to be evaluated from the others. Using both formulas, we can have a maximum of 12 estimates for the mass of a given nucleus, if the masses of all the required neighboring nuclei are known. Of course, there are cases where only 11 evaluations are possible, and so on. About half of all nuclei

with measured masses [24] can be estimated in 12 different ways and, in all cases, our estimate corresponds to the average value. To our knowledge, the systematic application of GK relations in this extended fashion is new.

Since from this simple method we obtain a specific mass value entirely determined by the behavior of the neighboring nuclei, we may conclude that these values represent a uniform and smooth component of the nuclear masses. In this sense they provide an upper estimate of the intrinsic precision limit with which they can be calculated, when enough local information is available. Fluctuations on top of the regular behavior predicted by different mass formulas and the GK relations are analyzed in the second part of this paper.

In what follows we compare the mass deviations found in three of the global methods (LDM, FRDM, DZ) and those in the GK estimates made above. The corresponding root-mean-square (rms) deviations for  $N$  nuclei

$$\sigma_{\text{rms}} = \left[ \frac{1}{N} \sum_{j=1}^N (M_j^{\text{exp}} - M_j^{\text{th}})^2 \right]^{1/2}, \quad (3)$$

are displayed in Table I, which also shows deviations for the smaller samples GK- $n$  which involve the application of at least  $n$  GK relations. Note the decrease in the errors from LDM to DZ, as a consequence of the inclusion of shell corrections (FRDM) and terms that mimic two-body interactions (DZ). A similar effect is also seen in the GK estimates with an increase in precision proportional to the number of GK relations applied. We conclude from this analysis that, if an intrinsic precision limit exists at all in the calculation of nuclear masses, it is smaller than 100 keV. We remark that the uncertainty range implied by these calculations is consistent with recent estimates of the effect of statistical fluctuations of high-lying configurations near the neutron threshold on the ground-state energy [25]. We also stress that experimental errors are lower than the estimates shown in Table I. For example, the average experimental error is  $\sigma_{\text{expt}} \approx 20$  keV for the nuclei in GK-12.

Another relevant question is whether nuclear masses far from stability can be predicted with a similar accuracy. In this respect, the GK relations cannot by themselves offer a simple answer, but large-scale shell model calculations shed some light on this important issue [26]. Sophisticated new calculations indicate that predictive power seems robust against long-distance extrapolations. Masses of 67 light nuclei in the  $fp$  shell, many of them unstable, were calculated with an average error of 215 keV [27]. Errors

TABLE I. The mass rms deviations  $\sigma_{\text{rms}}$ , in keV, for LDM, FRDM, DZ, and different GK calculations.

	LDM	FRDM	DZ	GK-1	GK-4	GK-7	GK-12
$A \geq 16$	3211	653	362	171	131	112	86
$A \geq 60$	3177	529	320	115	100	88	80

come mostly from isospin violation, and do not increase far from stability. Large-scale shell model calculations for the  $N = 126$  Po-Pu isotones [28] find errors in the binding energies smaller than 50 keV along the whole chain, with no increase for unstable nuclei, and “imply a high predictive power for ground-state binding energies beyond the experimentally known nuclei.” [28]

We now proceed to consider the presence of quantum chaos and analyze to this end the statistical characteristics of the mass fluctuations present in the different models. A direct 2D study in the  $N$ - $Z$  plane exhibits clear evidence of the correlations between mass errors in neighboring nuclei [29] which, proceeding through the four models (LDM, FRDM, DZ, and GK), decrease in size. It is, however, difficult to perform a systematic analysis of them because of the irregular form of the nuclear-data chart, and because cuts along fixed  $N$ ,  $Z$ , or  $A$  lines have a small number of nuclei, making it difficult to extract unequivocal conclusions [29,30]. To overcome these difficulties, we organize all nuclei with measured masses by ordering them in a *boustrophedon* single, 1D list [31], numbered as follows. Even- $A$  nuclei are ordered by increasing  $N - Z$ , while odd- $A$  ones follow a decreasing value of  $N - Z$ . Figure 1 displays the mass differences plotted against the order

number, for the four sets of calculations. The LDM errors are conspicuously large around shell closures, as expected. The presence of strong residual correlations in these deviations is also apparent from Fig. 1. Regions with large positive or negative errors can be clearly seen in FRDM. The distribution of the DZ errors is closer to the horizontal axis, and the correlations are less pronounced, although not completely absent. Finally, the remaining GK discrepancies are small and highly fluctuating, without any remarkable feature except for larger errors for  $A < 60$ .

Since the ordering provides single-valued functions, the discrete Fourier transforms

$$F_k = \frac{1}{\sqrt{N}} \sum_j \frac{M_j^{\text{exp}} - M_j^{\text{th}}}{\sigma_{\text{rms}}} \exp\left(\frac{-2\pi i j k}{N}\right) \quad (4)$$

can be evaluated. The corresponding spectral distributions can then be fitted to a power law of the form  $|F(\omega)|^2 \sim \omega^m$  with  $\omega = k/N$ . The squared amplitudes  $|F_k|^2$  are shown in Fig. 2 where the straight lines are fitted to obtain the slopes, which in a log-log plot correspond to the value of  $m$  in the corresponding power law. While fluctuations are large, the results are remarkable. The gradual vanishing of the slope in the different calculations from top to bottom is evident from the figure.

The fluctuation study allows the application of results well-known from noise analysis. Signals with strong correlations over a long range tend to have a Brownian motion behavior, where their power spectrum approaches the power law  $|F(\omega)|^2 \sim \omega^m$ , with  $m = -2$ . At the other end of the correlation spectrum is white noise, where there is no remaining coherence, which implies a flat frequency dependence  $m = 0$ ; that is, all frequencies have equal weight. Intermediate values of the slope  $m$  correspond to transitional regimes. The first three sets of mass deviations in Fig. 2 give rise to power laws with  $m$  ranging from  $-1.8$  to  $-0.5$ , consistent with a slow transition from substantial correlations to smaller (but still significant) ones for the associated mass fluctuations. The chaoticity discussed in Ref. [11], according to the  $m = -1$  criteria put forward in Ref. [20], seems indeed to be present in the FRDM deviations, while it tends to diminish in the microscopic DZ calculations. In contrast, we find that the GK analysis is essentially consistent with white noise.

In summary, a careful use of several global mass formulas and a systematic application of the Garvey-Kelson relations imply that there is no evidence that nuclear masses cannot be calculated with an average accuracy of better than 100 keV. While mass errors in mean-field calculations like the FRDM behave like quantum chaos, with a slope in their power spectrum close to  $-1$ , microscopic models' results correspond to smaller slopes. Finally, for the local GK relations the remaining mass deviations behave very much like white noise. These results seem to confirm that the chaotic behavior in the fluctuations arises from neglected many-body effects. The more physical information is included in the model,

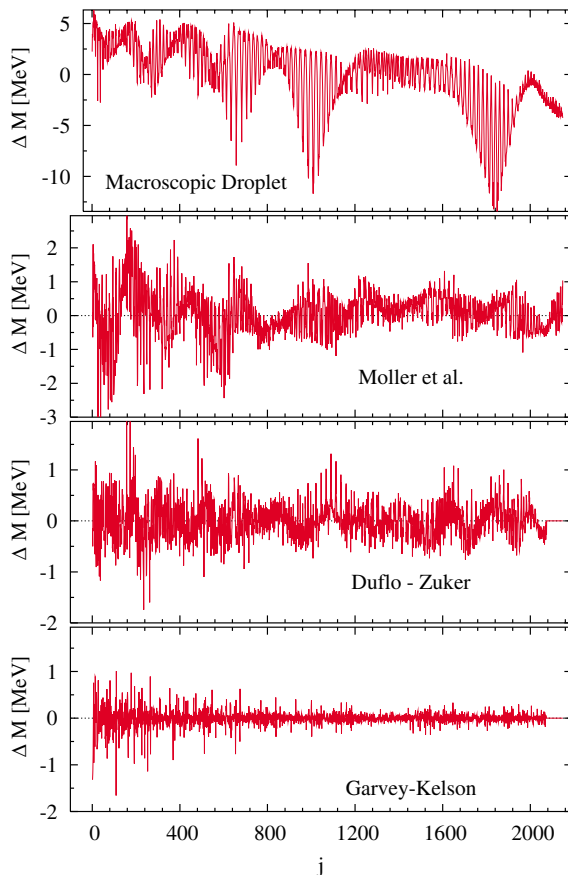


FIG. 1 (color online). Differences, in MeV, between the measured masses [24] and those obtained in LDM, FRDM, DZ, and GK, plotted against the order number  $j$ .

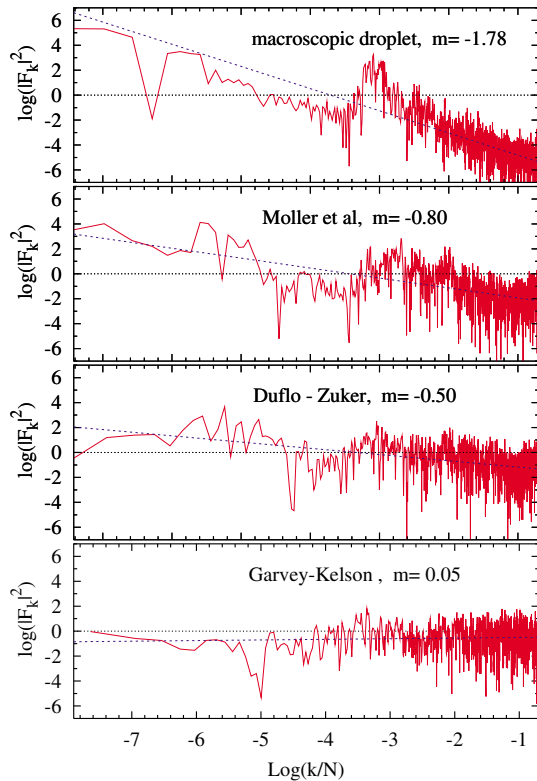


FIG. 2 (color online). Squared amplitudes of the Fourier transforms of the mass differences obtained in LDM, FRDM, DZ, and GK, plotted against the frequency  $\omega = k/N$ .

through many-body terms or by means of local information which measure the regular and smooth components in the mass systematics, the less presence of chaos is observed. The local calculations could in principle be reproducing the chaotic dynamics, which would imply that no *a priori* limit exists on predictability. A different interpretation is that the errors (that simulate chaotic behavior) are simply removed by the many-body effects. In any case, our results strongly suggest an upper bound of approximately 100 keV as a precision limit for the calculation of nuclear masses. Although the presence of (chaos-related) unpredictability at such small scales cannot be ruled out by our study, we believe this is encouraging news in the quest for reliable predictions of nuclear masses.

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