Correlations in Nuclear Masses

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It was recently suggested that the error with respect to experimental data in nuclear mass calculations is due to the presence of chaotic motion. The theory was tested by analyzing the typical error size. A more sensitive quantity, the correlations of the mass error between neighboring nuclei, is studied here. The results provide further support to this physical interpretation.

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The precision of nuclear mass spectrometry has dramatically improved in recent years. Thanks to the Penning trap technique, mass measurements with relative precision as high as 10^{-8}, or even 10^{-10} for stable nuclei, may be achieved [1]. This unprecedented accuracy has important consequences in different areas, like the determination of fundamental constants, symmetry violations, metrology, stellar evolution, and nucleosynthesis.

An additional motivation for such precise measurements is to establish accurate and predictive mass formulas. Global nuclear mass calculations have been pursued over the years with increasing accuracy [2–4] [see Ref. [5] for a review on recent experimental and theoretical developments]. Despite the numerous parameters contained in the different models and the variety of the approaches adopted, two peculiar features emerge from these calculations. On the one hand, different models yield similar results for the known masses. A typical accuracy is 5×10^{-4} for a medium-heavy nucleus whose total (binding) energy is of the order of 1000 MeV. On the other hand, the predictions of different mass models strongly diverge when applied to unknown regions (they may differ by several MeV, i.e., relative variations of order 5×10^{-3}).

These two features point towards the possibility of a basic underlying physical mechanism not appropriately incorporated into the present models. This mechanism should explain, in particular, the observed differences between measured and calculated masses. In Ref. [6] it was shown that the presence of chaotic layers in the nucleonic motion, whatever its physical origin may be, leads to a contribution to the nuclear mass whose typical size σ_{ch} is given by

$$\sigma_{\mathrm{ch}} = \frac{2.8}{A^{1/3}}\ \mathrm{MeV}, \qquad (1)$$

where A is the mass number. Equation (1), obtained through a mean-field theory, follows from very general arguments, and is independent of any detailed information concerning the system. It provides an order-of-magnitude estimate of the chaotic contribution, and determines the onset of a new regime. Figure 1 shows, as a function of A, the comparison between this prediction and the typical size of the error of several nuclear mass formulas using the most recent experimental compilation [7]. Three different global mass models are compared. Two of them are based on mean-field theory. The first one is a non-self-consistent macroscopic-microscopic model [2], the second one is a self-consistent calculation based on Hartree-Fock-BCS [3], while the third one [4] is a shell-model based calculation with parametrized monopole and multipole terms. The agreement with Eq. (1) for the two mean-field models is remarkable. The mass number dependence of the error is also well described for the third model with, however, a factor of order two between their amplitudes, a tendency that one might expect for a model that includes substantial residual interaction effects.

When the difference between calculated and measured masses is plotted as a function of the neutron number (or of any other relevant parameter), an oscillatory curve, whose typical amplitude is shown in Fig. 1, is observed. This curve does not look as a random white noise signal but shows structures. This qualitative remark is consistent with theoretical expectations. Indeed, it is known from semi-

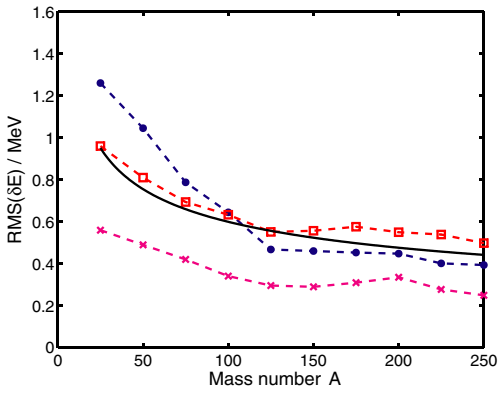

FIG. 1 (color online). Root mean square of the difference between experimentally measured and calculated masses. Dots, squares, and crosses from the calculations of Refs. [2–4], respectively. The solid line shows the chaotic contribution, Eq. (1).

classical mean-field theories [6,8] that the fluctuations of the mass produced by chaotic layers are dominated by the short classical orbits. The statistical properties of these orbits show system-dependent features. As a consequence, definite nonrandom fluctuations for the chaotic component of the mass are expected. Some of the predictions, like the asymmetry and non-Gaussian nature of the probability distribution of the oscillations [8], have been tested recently [9]. Thus, in the present context chaos should not be assimilated to a random unpredictable process. Though it may be a difficult task to explicitly compute its contribution for each nucleus [10] because, generically, the detailed oscillatory structure of this contribution is very sensitive to details of the Hamiltonian, it does not set an *a priori* bound to the accuracy of the theoretical mass calculations [11]. This view differs from that expressed in Ref. [12], where it is stated that the (partially) chaotic nuclear motion imposes limits *in principle* on the accuracy of the calculations of binding energies [cf Ref. [10]]. Moreover, and in contrast to global microscopic mass models, seemingly random deviations of typical size $\lesssim 100$ keV are observed in algebraic mass relations designed to locally cancel the interactions between nucleons [13].

Our aim here is to further develop the analysis of the mass errors in terms of chaotic motion by computing the autocorrelation function at different neutron numbers. Compared to the estimate of the typical error size, this is a finer analysis of the fluctuations that tests more subtle dynamical information. As discussed below, by assuming the errors are due to the contribution of chaotic motion, it is possible to obtain definite predictions which, in particular, fix a typical scale of the correlations.

Fluctuations of the nuclear masses may be written, in a semiclassical mean-field expansion, as [6]

$$\tilde{U}(x) = 2\hbar^2 \sum_p \sum_{r=1}^{\infty} \frac{A_{p,r}}{r^2 \tau_p^2} \cos(rS_p/\hbar + \nu_{p,r}). \qquad (2)$$

The sum is over all the primitive periodic orbits p (and their repetitions r) of a classical underlying effective single-particle Hamiltonian. Each orbit is characterized by its action S_p, stability amplitude $A_{p,r}$, period $\tau_p = \partial S_p/\partial E$, and Maslov index $\nu_{p,r}$. x is a parameter on which the effective potential depends. Though we let it for the moment unspecified, it will be chosen below to be the number of neutrons. The orbits entering this expression are all evaluated at the Fermi energy E_F. The latter is related to the mass number through the condition $\int_0^{E_F} \bar{\rho}(E, x) dE = A$, where $\bar{\rho}$ is the average single-particle density of states.

When the parameter x is varied, the correlation function of the energy fluctuations $\tilde{U}$ is defined as,

$$C(x) = \langle \tilde{U}(x_0 - x/2)\tilde{U}(x_0 + x/2)\rangle_{x_0}, \qquad (3)$$

where the brackets denote an average over a suitable parameter window, which is large compared to the typical scales of oscillation of $\tilde{U}$ and small on a classical scale. The correlation is evaluated using Eq. (2). When the parameter x varies, and for a large number of particles where $S_p \gg \hbar$, the main contributions to the variations of $\tilde{U}$ come from the variations of the action. In a linear approximation, valid when the variations are large compared to $\hbar$ but small compared to S_p, the action varies as $S(x_0 \pm x/2) = S(x_0) \pm Q_p x/2$, where $Q_p = \partial S_p/\partial x|_{x_0}$. Then, from (3) and (2), dropping terms whose average is zero, we obtain

$$C(x) = 2\hbar^4 \Big\langle \sum_{p,p'} \sum_{r,r'} \frac{A_{p,r}}{r^2 \tau_p^2} \frac{A_{p',r'}}{r'^2 \tau_{p'}^2} \cos\Big(\frac{rS_p - r'S_{p'}}{\hbar}\Big) \times \cos\Big(\frac{rQ_p + r'Q_{p'}}{2\hbar} x\Big)\Big\rangle_{x_0}. \qquad (4)$$

The double sum contains interfering terms between different orbits. However, as shown in Ref. [8], it is not necessary to consider them. The main contributing orbits are in fact the shortest ones (i.e., those having the shortest period). Their contribution is well approximated by taking into account only the diagonal terms $p = p'$, $r = r'$,

$$C(x) = 2\hbar^4 \sum_{p,r} \frac{A_{p,r}^2}{r^4 \tau_p^4} \cos\Big(\frac{rQ_p}{\hbar} x\Big) \qquad (5)$$

$$= \frac{\hbar^2}{2\pi^2} \int_0^{\infty} \frac{d\tau}{\tau^4} \Big\langle \cos\Big(\frac{Qx}{\hbar}\Big)\Big\rangle_{\tau} K_D(\tau). \qquad (6)$$

In Eq. (6) we have used the semiclassical expression of the spectral form factor, Eq. (8) below, to express the autocorrelation in terms of an integral over time. The average over the cosine function is computed over the whole set of periodic orbits of period between τ and $\tau + d\tau$. Denoting $P_\tau(Q)$ the distribution of the values of Q of all these orbits, then

$$\langle \cos(Qx/\hbar)\rangle_\tau = \int_{-\infty}^{\infty} \cos(Qx/\hbar) P_\tau(Q) dQ. \qquad (7)$$

Equations (5) and (6) are valid for both regular and chaotic motion. To proceed further, we must specify the type of dynamics we are considering. As in [6], we identify the error between experimental ($U_{\rm exp}$) and calculated mass ($U_{\rm calc}$) as originating from the chaotic contribution ($\tilde{U}$) of the nuclear motion, $U_{\rm exp} = U_{\rm calc} + \tilde{U}$. When the motion is chaotic, the number of periodic orbits having period between τ and $\tau + d\tau$ grows exponentially with τ. There are numerical as well as theoretical evidences indicating that the distribution function $P_\tau(Q)$ is in this case Gaussian, of average $\langle Q\rangle_\tau = \eta\tau$ and width $\langle Q^2\rangle_\tau = \alpha\tau$ [14]. Nontrivial dynamical information is contained in α. When x represents variations of the neutron number, the parameter η takes into account the effect of the increase of the volume of the nucleus as a neutron is added, implying an increase

of the average action (or length) of the orbits. Finally, an explicit expression for $K_D(\tau)$ is also needed. The semiclassical expression for $K_D(\tau)$ contains detailed information about the discrete spectrum of periods τ_p of the periodic orbits,

$$K_D(\tau) = h^2 \sum_{p,r} A_{p,r}^2 \delta(\tau - r\tau_p). \tag{8}$$

Here, we will not take into account this detailed information, but instead use, as in [6], a continuous approximation [8]

$$K_D(\tau) \approx \begin{cases} K_D(\tau) = 0 & \tau < \tau_{\min} \\ K_D(\tau) = 2\tau & \tau \geq \tau_{\min}, \end{cases} \tag{9}$$

where $\tau_{\min}$ is the period of the shortest periodic orbit of the system. This schematic approximation incorporates two important features. On the one hand, it contains a system-dependent information, namely, the truncation for times smaller than $\tau_{\min}$. On the other hand, it displays the universality observed in chaotic systems with time reversal invariance for times $\tau_{\min} \ll \tau \ll h\bar{\rho}$, namely, the linear growth characteristic of random matrix theory.

Using the Gaussian form of $P_\tau(Q)$ in Eq. (7) as well as the approximation (9) of $K_D(\tau)$, the correlation function Eq. (6), normalized to one at the origin, takes the form

$$C(\zeta) = \frac{\zeta^4}{2} \int_{\zeta^2/2}^{\infty} \frac{dy}{y^3} \cos\left(\frac{ay}{\zeta}\right) e^{-y/2}, \tag{10}$$

where the dimensionless parameters ζ and a are given by

$$\zeta = \frac{\sqrt{2\alpha\tau_{\min}}}{\hbar} x \quad \text{and} \quad a = \sqrt{\frac{2\tau_{\min}}{\alpha}} \eta. \tag{11}$$

Following the lines developed in Ref. [14], a computation of the average increase of the orbit's action when the volume V of the nucleus changes by δV gives $\eta = E_F \delta V / V$. Computing δV when a neutron is added, and using the expression $\tau_{\min}/\alpha = (\pi\sigma_x)^{-2}$ [8], where $\sigma_x = \langle(\partial\tilde{U}/\partial x)^2\rangle_x^{1/2}$, we obtain $a = (\sqrt{2}/\pi A) E_F/\sigma_x$. A reasonable estimate for σ_x, that has been tested numerically, is $\sim 3/A^{1/3}$ MeV. Then $a \sim 37/(2\pi A^{2/3})$, which is of order 0.5 for $A \approx 50$ and 0.2 for $A \approx 200$. We have verified that, for these values of a, the error introduced by setting $a = 0$ in Eq. (10) is less than 7×10^{-2} for any ζ. Setting a to zero, the final result can be expressed as

$$C(\zeta) = \left(1 - \frac{\zeta^2}{4}\right) e^{-\zeta^2/4} + \frac{\zeta^4}{16} \Gamma(0, \zeta^2/4), \tag{12}$$

where $\Gamma(s, z) = \int_z^\infty t^{s-1} e^{-t} dt$. Through the reparametrization (11), all the system specific features have been incorporated in ζ. This leads to a "universal" function, Eq. (12). Why it is so, as well as the validity of this result, is discussed below [15].

The parameter α contains detailed physical information related to the single-particle spectrum [14]. However, it is difficult to extract the relevant information from experimental data. To circumvent this difficulty, the alternative expression [8]

$$\zeta = \sqrt{\langle(\partial_{x_0}\tilde{U})^2\rangle / \langle\tilde{U}^2\rangle}\, x, \tag{13}$$

where $\partial_{x_0}\tilde{U} = \partial\tilde{U}(x_0)/\partial x_0$, is more convenient for our purpose because it only involves properties of $\tilde{U}$. Though the structure of Eq. (13) is reminiscent of the reparametrization introduced in the context of random matrices and universal parametric correlations [14,17], there are, however, important differences: in the latter case single-particle energies are considered and universalities are exhibited, whereas here parametric correlations of thermodynamic properties of a Fermi gas are considered, and important system specific features are shown to emerge (see below).

From data, we have analyzed the following correlation function

$$C_Z(dN) = \frac{\langle\tilde{U}(Z, N)\tilde{U}(Z, N + dN)\rangle_N}{\langle\tilde{U}^2\rangle_N}, \tag{14}$$

where $\tilde{U}(Z, N)$ is the difference between calculated and measured masses for a nucleus having Z protons and N neutrons, and dN is the difference in neutron number along an isotopic chain (a similar analysis for isotonic chains can also be performed). For a specific dN and Z every available $f(N) = \tilde{U}(Z, N)\tilde{U}(Z, N + dN)$ is calculated. To compute the mean value with respect to N one has to sum all the $f(N)$'s and divide by the total number of nuclei in the isotope chain. This normalization ensures the nonnegativity of the Fourier transform of the correlation function. The average $\langle\tilde{U}^2\rangle_N$ is obtained by setting $dN = 0$. In order to improve the statistics, that are severely limited by the length of the isotopic chains, a further average is computed over neighboring chains,

$$C(dN) = \langle C_Z(dN)\rangle_Z. \tag{15}$$

Finally, to compare with Eq. (12), the correlation $C(dN)$ should be expressed in terms of the parameter ζ. For each dN, (locally) the value of ζ is computed from Eq. (13), where $\partial_{x_0}\tilde{U} = \tilde{U}(Z, N + 1) - \tilde{U}(Z, N)$, and averages over N and Z are as before.

Figure 2 shows the normalized experimental correlation function of the nuclear mass errors, Eq. (15), plotted as a function of ζ, compared to the prediction (12). The three different models studied give very similar results, in good agreement with theory. The overall quality of the prediction is comparable to Fig. 1. The independence of the result with respect to the model used is a strong support for our interpretation, though the influence of effects beyond mean-field theory still need to be clarified.

Though Eq. (12) is a continuous function of ζ [in particular, it behaves as $C(\zeta) \approx 1 - \zeta^2/2$ close to the origin], we have chosen to plot it at discrete values of ζ,

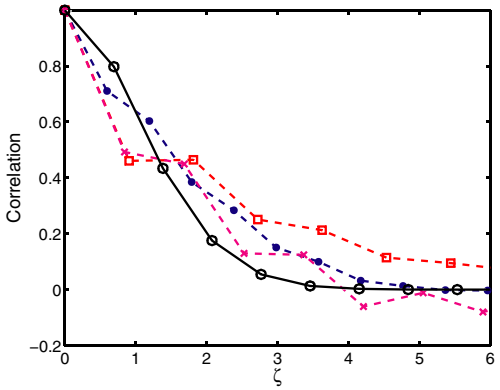

FIG. 2 (color online). Correlation of the mass errors between neighboring isotopes as a function of the dimensionless parameter ζ. Circles, squares, and crosses correspond to the same models as in Fig. 1. The solid line is the theoretical result Eq. (12).

with a step similar to the experimental one. The half-width of the correlation function $C(\zeta)$ is of order 1.5, which corresponds to neutron differences $dN \approx 2$, giving the parameter range over which the chaotic contributions of different isotopes are correlated. The existence of correlations extending over a few nucleons seems to be consistent with the high accuracy with which Garvey-Kelson-type mass relations are fulfilled [13], as mentioned before.

The main approximation in Eq. (12) is the replacement of the diagonal form factor, Eq. (8), by the function (9). By this, the system specific spectrum of periodic orbits is replaced by a function that keeps only one relevant scale, the period $\tau_{\min}$ of the shortest one. It is this simplification that, through the reparametrization (11), allows to obtain a universal correlation function $C(\zeta)$. Although this leads to a reasonable approximation, at least for the available neutron differences, the exact form of the correlation function of the chaotic contribution to the mass would be better described by the discrete sum (5). This sum depends on the precise properties of the periodic orbits, and is therefore system and model dependent. Because of its discrete nature, generically oscillations of the correlation as a function of x are expected. This contrasts with the uniform universal nonoscillatory decay given by Eq. (12), which is clearly an artifact of the approximation (9). Some tendency towards negative values, and therefore of oscillatory behavior, seems to be present in the autocorrelation of the errors shown in Fig. 2 at large values of ζ. However, to be conclusive, larger values of ζ, which are not experimentally available, are needed [this problem might be overcome by considering different nuclear chains [9]].

To conclude, let us recall that shell effects described by periodic orbit theory related to regular motion are very familiar in nuclear physics, particularly since the work of Strutinsky [see Ref. [16] for a recent discussion]. What about the contribution of unstable chaotic orbits? It has been recently suggested that the size of the differences between measured and computed binding energies can be attributed to the presence of nuclear chaotic motion. The work presented here goes one step further in this direction by studying the autocorrelation function of the chaotic contribution to nuclear masses. The result, that depends on some well-identified physical parameters, is in good agreement with the autocorrelation computed from several existing models along isotopic chains. This gives further support to the view that chaotic dynamics effects are present in the ground state of atomic nuclei.

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