Nuclear masses: evidence of order–chaos coexistence

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Abstract

Shell corrections are important in the determination of nuclear ground–state masses and shapes. Although general arguments favor a regular single–particle dynamics, symmetry–breaking and the presence of chaotic layers cannot be excluded. The latter provide a natural framework that explains the observed differences between experimental and computed masses.

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Different approaches have been developed to reproduce the systematics of the observed nuclear masses. Some of them are of microscopic origin, while others, more phenomenological, are inspired from liquid drop models or Thomas–Fermi approximations. Often, the total energy is expressed as the sum of two terms

$$U(Z,N,x) = \overline{U}(Z,N,x) + \widetilde{U}(Z,N,x) \ , \tag{1}$$

where Z and N are the proton and neutron numbers, respectively, and x represents a set of parameters that define the shape of the atomic nucleus. The first term $\overline{U}$ describes the bulk (macroscopic) properties of the nucleus, and contains all the contributions that vary smoothly with proton and neutron numbers. Its typical value is close to 8 MeV/A throughout the periodic table, where $A = N + Z$ is the mass number. The second term $\widetilde{U}$ describes shell effects, related to the shape–dependent microscopic fluctuations of the nuclear wavefunctions [1]. A method to incorporate these effects in a consistent manner was originally proposed by Strutinsky [2].

Global nuclear mass calculations have been pursued over the years with increasing precision [3,4]. Despite the numerous parameters contained in the models, the accuracy of the results obtained and the quality of the predictions are impressive. Different models and potentials yield similar results, and give an accuracy of 5×10^{-4} for a medium–heavy nucleus whose total (binding) energy is of the order of 1000 MeV.

One may ask whether the difference between measured and computed masses has a particular significance, since it seems to be quite model independent. Among other possibilities, a natural explanation would come from many-body effects not included in the mean–field scheme. Our purpose here is to show that there is a very natural and appealing dynamical explanation. We will argue that $\widetilde{U}$ may be splitted into two parts, $\widetilde{U} = \widetilde{U}_{reg} + \widetilde{U}_{ch}$, and that the present calculated masses are able to correctly reproduce only $\widetilde{U}_{reg}$. The two contributions $\widetilde{U}_{reg}$ and $\widetilde{U}_{ch}$ originate in regular and chaotic components of the motion of the nucleons, respectively. Although our calculations are done within a mean–field approximation, the final result for the fluctuations produced by the chaotic part of the motion are in fact of a much more general validity, and may be interpreted as arising from the residual interactions.

With essentially no free parameters, this dynamical symmetry–breaking mechanism provides a quantitative description of the basic observations on nuclear masses. First, the amplitude of $\widetilde{U}_{ch}$ is much smaller than that of $\widetilde{U}_{reg}$. Second, the typical size of the fluctuations $\widetilde{U}_{reg}$ have a constant amplitude as a function of the number of nucleons. The RMS of $\widetilde{U}_{reg}$ is found to be of about 3 MeV, which is in good agreement with the typical size of the difference $\delta U = U_{exp} - \overline{U}$ between the experimental and the computed bulk properties of the nuclei [3]. Third, the RMS of $\widetilde{U}_{ch}$ is of order 0.5 MeV, in good agreement with the typical size of the difference $\delta U = U_{exp} - U_{calc}$ between the experimental and the calculated masses including shell effects [3,4]. The mass-number dependence of this difference is also well reproduced.

From a semiclassical point of view, shell effects are interpreted as modulations in the single–particle spectrum produced by the periodic orbits of the corresponding classical dynamics [5,6]. Given the single–particle energy levels $E_j(x)$ computed from some Hamiltonian $H(x)$, the level density $\rho(E,x) = \sum_j \delta\left[E - E_j(x)\right]$ is approximated by

$$\rho(E,x) = \overline{\rho}(E,x) + \widetilde{\rho}(E,x) \ . \tag{2}$$

The quantity $\overline{\rho}$ is the average density of states, whereas the oscillating part is expressed as

$$\widetilde{\rho} = 2 \sum_p \sum_{r=1}^{\infty} A_{p,r}(E,x) \cos\left[r S_p(E,x)/\hbar + \nu_{p,r} \right] \ . \tag{3}$$

The sum is over all the primitive periodic orbits p (and their repetitions r) of the single–particle Hamiltonian. Each orbit is characterized by its action S_p, stability amplitude $A_{p,r}$, and Maslov index $\nu_{p,r}$.

The shell correction to the nuclear mass is computed by inserting the oscillatory part of the density of states into the expression of the energy, $\widetilde{U}(x,A,T) = \int dE \ E \ \widetilde{\rho}(E,x) \ f(E,\mu,T)$, with f the Fermi function. In a semiclassical expansion, the leading order of the integral comes from the energy dependence of the action, and the dependence of the prefactors can be ignored. Setting moreover the temperature T to zero, one obtains

$$\widetilde{U}(x,A) = 2\hbar^2 \sum_p \sum_{r=1}^{\infty} \frac{A_{p,r}}{r^2 \ \tau_p^2} \cos(r S_p/\hbar + \nu_{p,r}) \ , \tag{4}$$

where $\tau_p = \partial S_p/\partial E$ are the periods of the periodic orbits. The classical functions entering this expression *are evaluated at the Fermi energy* E_F, related to the mass number and shape parameters through the condition $\int_0^{E_F} \overline{\rho}(E,x) \ dE = A$. According to Eq. (4), each periodic orbit produces a modulation or bunching of the single–particle states on an energy scale h/τ_p. The presence of fluctuations in the total energy is therefore a very general phenomenon that occurs for an arbitrary Hamiltonian, irrespective of the nature of the corresponding classical dynamics. However, their importance (i.e., their amplitude) depends strongly on the properties of the dynamics, and in particular on its chaotic or regular character [6,7]. In order to see this explicitly, we compute the variance of the fluctuations of the energy. The average is performed over a mass number window around a given nucleid, as when analyzing experimental data. The size of the window is taken to be small with respect to macroscopic quantities like the Fermi energy, but large compared to the typical oscillatory scale of $\widetilde{U}$. This average is denoted by brackets. From Eq. (4) we obtain for the variance a double sum over periodic orbits labeled by the indices p and p'. By considering the dependence of the density of periodic orbits with their period, it has been shown [7,8] that the dominant contribution to the double sum is given by the diagonal terms $p = p'$, $r = r'$. The resulting sum is convergent. Using moreover the semiclassical definition of the form factor,

$$K(\tau) = 2h \int_0^{\infty} d\epsilon \cos(\epsilon\tau/\hbar) \langle \widetilde{\rho}(E-\epsilon/2) \widetilde{\rho}(E+\epsilon/2) \rangle$$

whose diagonal part is

$$K_D(\tau) = h^2 \sum_{p,r} A_{p,r}^2 \ \delta\left(\tau - r\tau_p\right) \ , \tag{5}$$

the energy variance may be written as

$$\langle \widetilde{U}^2 \rangle \approx \frac{\hbar^2}{2\pi^2} \int_0^{\infty} \frac{d\tau}{\tau^4} \ K_D(\tau) \ . \tag{6}$$

This is the basic equation that provides the starting point for our analysis. An accurate evaluation of $\langle \widetilde{U}^2 \rangle$ requires the knowledge of the periodic orbits, and therefore of the Hamiltonian. However, we do not want to make a calculation for a specific system. Instead we are interested in making general statements based on the statistical behavior of the single–particle orbits. That behavior depends on the regular or chaotic nature of the dynamics.

General considerations suggest that the single–particle motion in the nucleus should be dominated by regular orbits. This is based on the following arguments. There are several factors that are important when considering the amplitude of the shell effects as given by Eq. (4). The first one is the prefactor $A_{p,r}/\tau_p^2$. It implies that the more stable and short the periodic orbit is, the larger its contribution. The second is associated with the interference properties. Shells are wave effects: they are determined by a superposition of oscillatory contributions from different periodic orbits. The third factor, closely related to the previous one, is the phase space structure of the periodic orbits, i.e., their degeneracy. It depends on the existence of conserved quantities. In fully chaotic dynamics (where only the energy is conserved), the periodic orbits are isolated and unstable. In contrast, if there are as many conserved quantities as degrees of freedom, the motion is regular (or integrable) and periodic orbits come in degenerate families, all orbits having the same properties (action, stability, etc) within a family. Since many orbits contribute coherently, this degeneracy leads to an enhancement of the size of the shell corrections. In its equilibrium state, and for a given number of nucleons, the nucleus will adapt its shape in order to minimize its energy. This minimization procedure, that takes also into account the contributions from $\overline{U}$, favors regular single–particle dynamics that produce strong effects.

Equation (6) allows to estimate the typical fluctuations arising from a regular dynamics. In the range $\tau_{min} \ll \tau \ll \tau_{_H}$, where τ_{min} is the *period of the shortest periodic orbit* in the semiclassical sum (4) and $\tau_{_H} = h\overline{\rho}$ is the *Heisenberg time*, the form factor of the regular single–particle levels is given by $K_D(\tau) = \tau_{_H}$ [9]. This approximation is not valid for short times, of the order of τ_{min}. The reason is that for $\tau \approx \tau_{min}$, Eq. (5) produces system specific delta function peaks. If for simplicity we ignore this and extrapolate the statistical behavior down to $\tau \approx \tau_{min}$, and moreover use $K_D(\tau) = 0$ for $\tau < \tau_{min}$ (cf. Eq. (5)), then Eq. (6) leads to

$$\langle \widetilde{U}_{reg}^2 \rangle = \frac{1}{24\pi^4}\; g\; E_c^2 \; . \tag{7}$$

The quantity E_c is the *energy associated with the shortest periodic orbit*,

$$E_c = h/\tau_{min} \; , \tag{8}$$

whereas the parameter g measures this energy in units of the *single–particle mean level spacing* $\delta = 1/\overline{\rho}$

$$g = E_c/\delta = \tau_{_H}/\tau_{min} \; ; \tag{9}$$

g counts the number of single–particle states on the scale E_c. To compute E_c we need the period of the shortest orbit. Its length will typically be two or three characteristic nuclear dimensions. For simplicity we assume it to be two. Then, for a flat mean–field, like the Woods–Saxon potential, we have $E_c = \pi E_{_F}/k_{_F} r$, where r is the nuclear radius and $k_{_F}$ is the Fermi wave vector. Since $r \approx 1.1 A^{1/3}$ fm, we arrive at

$$E_c = \frac{77.5}{A^{1/3}} \text{ MeV}. \tag{10}$$

E_c is the largest oscillatory energy scale where coherent bunching effects occur in any thermodynamic quantity. This result should be contrasted to the traditional shell–effect estimate based on the harmonic oscillator potential, $E_c = \hbar w_0 \approx 40/A^{1/3}$ MeV [1].

Since $\delta \approx 2E_F/3A = 25/A$ MeV, Eq. (9) leads to

$$g = \pi A^{2/3}. \tag{11}$$

From these results we obtain for the typical fluctuations $\sigma_{reg} = \sqrt{\langle \widetilde{U}_{reg}^2 \rangle}$ of a nucleus with a regular single–particle dynamics the value

$$\sigma_{reg} = 2.84 \text{ MeV} , \tag{12}$$

an expression independent of the number of nucleons. This estimate is in good agreement with the ~ 3 MeV observed when $\overline{U}$ is subtracted out from the experimental or calculated values. The use of the real nuclear mean level spacing δ to compute (11) (i.e., including spin and isospin degrees of freedom) amounts to treating the different contributions as uncorrelated, and therefore provides a lower bound.

In deriving Eq. (12) a regular single–particle motion of the nucleons has been assumed. Even though we have stressed that a regular motion favors the minimization of the total energy, in the full many–body problem nothing guarantees the perfect integrability of the semiclassical dynamics. If some dynamical symmetries are broken, chaotic components will coexist with regular single–particle motion. The consequences of their presence on the behavior of the nuclear masses will now be discussed.

From a semiclassical point of view, the most simple approximation that can be made in the generic case of a mixed dynamics, when regular orbits coexist with chaotic layers, is to split the sum over periodic orbits in Eq. (4) into two terms, one from the regular part, another from the chaotic part. The shell energy is now written as

$$\widetilde{U} = \widetilde{U}_{reg} + \widetilde{U}_{ch}. \tag{13}$$

The two terms are, from a statistical point of view, independent, $\langle \widetilde{U}_{reg} \widetilde{U}_{ch} \rangle = 0$. This happens because, as already pointed out, the dominant contribution to the energy comes from the short orbits, with $\tau_p \ll \tau_H$. Since the orbits contributing to each term are different, the cross products vanish by the averaging procedure (assuming that the actions of the orbits are incommensurable). The decomposition (13) identifies the difference between measured and computed masses, that have a typical size of ~ 0.5 MeV, with the oscillatory contribution of the periodic orbits lying in the chaotic components.

We are therefore led to evaluate the variance of the shell corrections that originate in the chaotic layers. This can be done from the general Eq. (6). Again, our purpose is to make a statistical estimate valid for a generic chaotic component, with no reference to a particular system. In the range $\tau_{min} \ll \tau \ll \tau_H$ the form factor of chaotic single–particle levels is given by $K_D(\tau) = 2\tau$ [9]. It coincides with the random matrix prediction [10]. This result is not valid for times of the order of τ_{min}. Extending nevertheless this behavior down to $\tau \approx \tau_{min}$, and imposing again $K_D(\tau) = 0$ for $\tau < \tau_{min}$, we now arrive at

$$\langle \widetilde{U}_{ch}^2 \rangle = \frac{1}{8\pi^4} \; E_c^2 \; . \tag{14}$$

Using Eq. (10), the typical size of the fluctuations $\sigma_{ch} = \sqrt{\langle \widetilde{U}_{ch}^2 \rangle}$ of a chaotic component in the single–particle dynamics is given by

$$\sigma_{ch} = \frac{2.78}{A^{1/3}} \; \mathrm{MeV}. \tag{15}$$

This expression has to be compared with the RMS of the difference δU between the experimental and the computed masses, given in Ref. [3]. The comparison is shown in Fig. 1.

The agreement is extremely good. The amplitude in Eq. (15) is uncertain up to an overall factor of say, 2. It can be varied by increasing slightly the period of the shortest orbit (we have chosen the shortest possible one; any modification will diminish σ_{ch}) and by the inclusion of spin and isospin (this increases σ_{ch} by a factor 2 if these components are treated as uncorrelated). The A dependence is very well fitted in the region $A \gtrsim 75$, with deviations observed for lower mass numbers. This is in agreement with the limited accuracy of the Strutinsky corrections and in general of semiclassical theories for light nuclei.

There are several features of the present theory that make its predictions reliable. First of all, Eq.(14) contains only *one physical parameter*, the period of the shortest chaotic periodic orbit, which is a function of A because the size of the nucleus increases with the mass number. But it has no dependence on the relative size of the chaotic region, i.e., on the fraction of phase space occupied by chaotic motion. Without this quite remarkable and important fact we would have been forced to estimate that fraction, something that is hardly possible with present knowledge despite the efforts in this direction since the pioneering work of Ref. [11]. This is in contrast to what happens for the regular regions. The enhancement factor g present in Eq. (7) – but not in Eq. (14) – depends on the corresponding *regular* average level density $\overline{\rho}_{reg}$. The evaluation of g in Eq. (11) assumes that the nuclear single–particle levels are regular, and the good qualitative agreement with the experimental results of $\widetilde{U}_{reg}^2$ suggests that indeed most of the phase space is occupied by regular trajectories. Mixed systems present therefore a peculiar structure of shell effects. The amplitude of the fluctuations of the regular phase space regions is proportional, through the factor g, to the square root of the regular average level density, $\sigma_{reg} \propto \sqrt{\overline{\rho}_{reg}}$. In contrast, the amplitude of the fluctuations associated with the chaotic motion is constant, independent of their phase space volume (aside from the transient nearly–integrable regime, not considered here, where the chaotic layers are formed). In the extreme case of a fully chaotic dynamics, $\overline{\rho}_{reg} = 0$ and $\widetilde{U} = \widetilde{U}_{ch}$.

Equation (14) is in fact quite robust. It is not only independent of the chaotic phase–space volume, but is also valid for arbitrary dimensions. This fact suggests a very natural origin of these fluctuations, that we haven't discussed yet. Although our analysis is based on a single–particle picture, it can be extended to the full many–body phase space. In that space, and in a semiclassical picture, to first approximation the point representing the system follows a very simple trajectory driven by the regular mean–field that dominates the motion. On top of that, it is likely that the residual interactions, not taken into account in that approximation, induce chaotic motion. The presence of chaotic orbits would then introduce additional long–range modulations in the regular single–particle density of states. Eq. (14) would then still be valid to evaluate the amplitude of those modulations, with

τ_{min} the period of the shortest chaotic orbit in the multidimensional space. Rough estimates indicate that τ_{min} is comparable to the three–dimensional non–interacting period. Therefore Eq. (15) presumably gives an estimate of the mass fluctuations arising from neglected many–body effects.

To summarize, we have investigated shell effects of nuclear ground states within a unified framework, namely periodic orbit theory. We show that a dynamical symmetry–breaking mechanism that introduces chaotic layers in the motion of the nucleons produces additional shell corrections to the total energy. The intensity of the effect is, to first approximation, independent of the size or the topology of the layers. It is governed by a single parameter, E_c, which is proportional to the inverse time of flight of a nucleon across the nucleus at Fermi energy. The comparison of the typical size of the chaotic fluctuations is in very good agreement with the deviations between computed and experimental values, for the amplitude as well as for their dependence with the mass number. In contrast, the fluctuations produced by the regular components are independent of the mass number, and are proportional to the regular phase–space volume. The picture we are suggesting is coexistence of order and chaos as produced, for instance, by residual interactions. It manifests in nuclear low–energy properties. Further evidence should be given. In particular, our theory predicts autocorrelations in the total energies [7], as well as the effect of the presence of chaotic layers on the total level density. This deserves further investigation.

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FIGURES

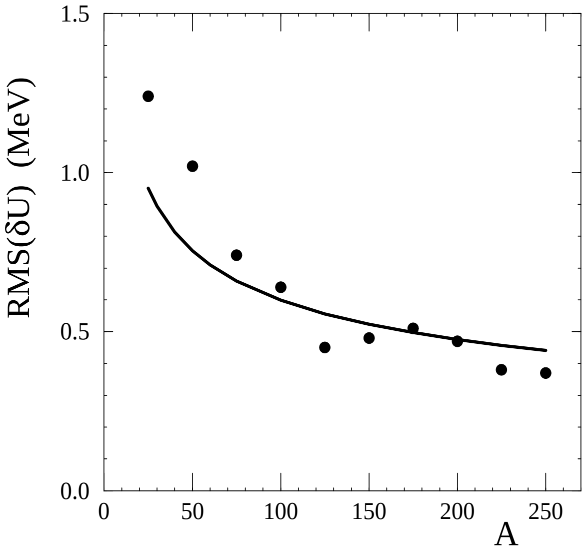

FIG. 1. RMS of the difference δU between computed and observed masses as a function of mass number A. Dots taken from Fig. 7 of Ref. [3]. Solid curve from Eq. (17).