Garvey-Kelson Relations for Nuclear Charge Radii

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The Garvey-Kelson relations (GKRs) are algebraic expressions originally developed to predict nuclear masses. In this letter we show that the GKRs provide a fruitful framework for the prediction of other physical observables that also display a *slowly-varying* dynamics. Based on this concept, we extend the GKRs to the study of *nuclear charge radii*. The GKRs are tested on 455 out of the approximately 800 nuclei whose charge radius is experimentally known. We find a rms deviation between the GK predictions and the experimental values of only 0.01 fm. This should be contrasted against some of the most successful microscopic models that yield rms deviations almost three times as large. Predictions—with reliable uncertainties—are provided for 116 nuclei whose charge radius is presently unknown.

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Theoretical calculations of nuclear ground-state properties may be classified according to two primary trends. One of them is the so-called *macroscopic-microscopic* approach that is naturally rooted in the Strutinsky energy theorem [1]. According to this theorem [2], the nuclear binding energy may be separated into two components—one large and smooth and the other one small and fluctuating. The largest contribution varies smoothly with both mass (A) and atomic (Z) numbers and describes the average trend of the nuclear masses, as in the liquid drop model and its various refinements [3, 4]. In contrast, the small contribution fluctuates due to quantal effects (*e.g., shell corrections*) that are often incorporated through an independent particle model with a realistic potential that also varies smoothly with A and Z. The macroscopic-microscopic approach has enjoyed its greatest success in the work of Möller *et al.* [5] and Duflo and Zuker [6]. The "competing" approach, falling under the general rubric of *mean-field* models, consists of a microscopic description in which the average nuclear potential and the single-particle orbits are determined self-consistently. Although mean-field models vary widely in sophistication, their tenet is an *effective interaction* or *energy density functional* that incorporates as much as possible of the known nuclear dynamics. The effective interaction is parametrized in terms of several empirical constants (e.g., coupling constants and range parameters) that are then fitted to a variety of ground-state observables.

A lesser known approach—in spite of its 40 year existence—is the one by Garvey and Kelson [7, 8]. Rather than attempting a global description of nuclear masses, the formalism is based on *local mass relations*. The Garvey-Kelson relations (GKRs) have been recently revitalized both because of an interest in understanding any inherent limitation in the nuclear-mass models as well as due to their possible applications in stellar nucleosynthesis [9, 10, 11]. In doing so, it was discovered that the GKRs—which are essentially parameter free—rival in accuracy the most successful mass formulae available in the literature [10, 11].

The Garvey-Kelson relations are derived from a few simple physical principles (such as isospin symmetry) and a central assumption of a nuclear mean field and residual interaction that vary slowly with atomic number [7, 8]. Within this picture, Garvey and Kelson introduced the following two local relations—each among the masses of six neighboring nuclei—that allowed them to estimate an unknown nuclear mass from those of its neighbors:

$$\begin{aligned}\Delta M_6^{(1)}(N,Z) \equiv\ & M(N+2,Z-2) - M(N,Z) \\ & + M(N,Z-1) - M(N+1,Z-2) \\ & + M(N+1,Z) - M(N+2,Z-1) = 0\,, \end{aligned} \tag{1a}$$

$$\begin{aligned}\Delta M_6^{(2)}(N,Z) \equiv\ & M(N+2,Z) - M(N,Z-2) \\ & + M(N+1,Z-2) - M(N+2,Z-1) \\ & + M(N,Z-1) - M(N+1,Z) = 0\,. \end{aligned} \tag{1b}$$

It is the aim of this letter to show that this method may be successfully extended to *nuclear charge radii*—a fundamental property of atomic nuclei that is both slowly varying and has a large experimental database [12, 13].

Valuable insights into the success of the GKRs [10, 11] may be gained by recalling that according to Strutinsky's energy theorem [1, 2], the nuclear mass function $M(N,Z)$ may be written as $M = \widetilde{M} + \delta M$, where $\widetilde{M}$ and δM denote the smooth and fluctuating parts of the mass function, respectively. Viewing Eqs. (1) in this light, they can be cast as $\Delta M_6 = \Delta\widetilde{M}_6 + \Delta(\delta M)_6$. Now, a Taylor series expansion of the smoothly-varying (and largest) contribution $\widetilde{M}$ may be performed around the reference point

(N, Z) [14] that yields

$$\Delta\widetilde{M}_6^{(1)}(N,Z) = \frac{\partial^3\widetilde{M}}{\partial Z^2\partial N} - \frac{\partial^3\widetilde{M}}{\partial Z\partial N^2} + \mathcal{O}(\partial^4\widetilde{M})\,, \quad (2a)$$

$$\Delta\widetilde{M}_6^{(2)}(N,Z) = \frac{\partial^3\widetilde{M}}{\partial Z^2\partial N} + \frac{\partial^3\widetilde{M}}{\partial Z\partial N^2} + \mathcal{O}(\partial^4\widetilde{M})\,. \quad (2b)$$

The above result indicates that the particular linear combinations of masses involved in the GKRs induce strong cancellations in the Taylor expansions—making the relations insensitive to the underlying (liquid drop) function as well as to its first and second derivatives. Hence, as long as successive derivatives of the underlying function become progressively smaller (indeed, as in the liquid-drop formula [14]), the GKRs should be satisfied to a very good approximation. Ultimately then, the level of accuracy of the GKRs will depend on the extent to which the fluctuating contributions δM get cancelled out in Eqs. (1). This we expect to be specific to the system under consideration. In the case of atomic nuclei, the rather smooth local behavior with N and Z of the mean-field potentials used to calculate the quantum contributions—plus the fact that in Eqs. (1) the interactions between nucleons cancel to first order in an independent-particle picture [7, 8]—ensures a strong cancellation of the quantum fluctuations among neighboring nuclei.

The above discussion suggests that the success of the GKRs for nuclear masses may be extended to other observables that are driven by a similar underlying physics. In this letter we focus on the nuclear charge radius. The charge radius is a nuclear structure observable that is known with exquisite accuracy for a few nuclei in the periodic table [12, 13]. The systematic measurement of the charge distribution of nuclei started with the pioneering work of Hofstadter in the late 1950's [15] and continues to this day with the advent of powerful continuous electron beam facilities [16]. Although the experimental situation for charge radii lags behind that of nuclear masses, an extensive database of almost 800 charge radii already exists [13]. Moreover, the advent of novel technologies and facilities to perform electron scattering off short-lived isotopes, such as ELISe [17] and SCRIT [18], may extend the data well beyond current limits in the coming years.

From the theoretical side, the most sophisticated approaches to charge radii are based on either macroscopic-microscopic models [19, 20, 21, 22, 23] or microscopic mean-field formulations using effective interactions [24, 25, 26, 27, 28, 29, 30]. When some of these models are used to compare against experimental data, the rms deviations lie in the 0.03 to 0.06 fm range [23]. In this letter we will show that an approach based on local relations of the Garvey-Kelson type represents a very attractive and robust alternative.

Nuclear charge radii display, as in the case of masses, small fluctuations on top of a fairly smooth average behavior [13, 14]. This may be illustrated by employing the liquid-drop inspired formula proposed in Ref. [20]. When such a formula is fitted to the charge radii of the close to 800 nuclei included in the recent 2004 compilation by Angeli [13] we obtain,

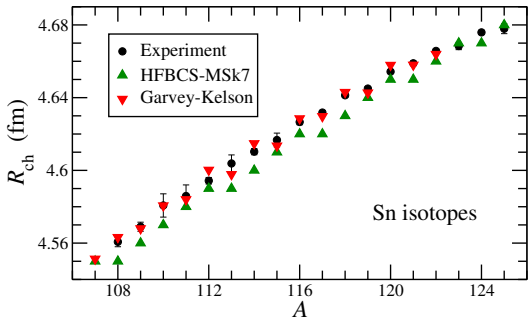

FIG. 1: (Color online) Comparison between theoretical predictions and experimental values [13] for the charge radius of the Sn-isotopes.

$$\begin{aligned} R_{ch}(N,Z) &= 0.4980 + 0.8754\,A^{1/3} \\ &- 0.9845\,\alpha + 0.2703\,A^{1/3}\alpha^2 \text{ fm}\,. \end{aligned} \quad (3)$$

Here $\alpha \equiv (N-Z)/A$ is the neutron-proton asymmetry of the nucleus and the fit produces the moderate rms deviation of 0.041 fm. This liquid-drop inspired formula is particularly useful to estimate the derivatives of the charge radius, as in Eqs. (2). Using a representative set of nuclei—ranging from ^{16}O to ^{208}Pb—we found the third-order derivatives of (3) to be suppressed by 4 to 6 orders of magnitude relative to $R_{ch}(N,Z)$ itself. Moreover, given that mean-field formulations provide quantitatively accurate predictions of ground-state properties, we expect—as in the case of masses—strong cancellations of the fluctuating contributions to the GKRs for nuclear charge radii. These facts open the possibility of applying the GKRs to the study of nuclear charge radii.

The implementation of the GK procedure for charge radii follows closely the approach outlined by Barea and collaborators for the case of nuclear masses [10]. For a given nucleus, there are (depending on the availability of experimental information) at most 12 possible estimates of its charge radius [see Eqs. (1)]. All the available estimates are then averaged to produce a GK prediction for the charge radius of the given nucleus. The result is then compared (when available) to the experimental value [13]. In the event that the experimental value is unavailable, a GK prediction is made for the charge radius of such a nucleus that awaits experimental confirmation. The isotopic chain in Tin with 18 experimentally measured charge radii provides an illustrative example of this scheme. Fig. 1 shows the predictions for the Tin charge radii—including the as yet unmeasured value for ^{107}Sn—using the GK relations and the Hartree-Fock-BCS model with the MSk7 interaction [25]. The HFBCS model of Ref. [25] generates a rms deviation of only 0.0082 fm for

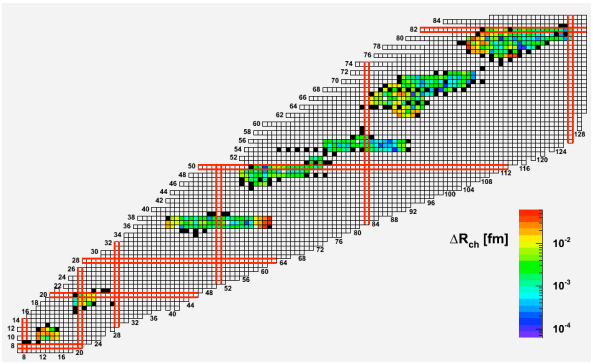

FIG. 2: (Color online) Absolute value of the difference between the GK estimate and the experimental value for the charge radius of 455 nuclei as indicated by the color-coded scale. Black squares denote GK predictions for 116 nuclei whose charge radius has not yet been measured. These predictions are provided in tabular form in Ref. [31].

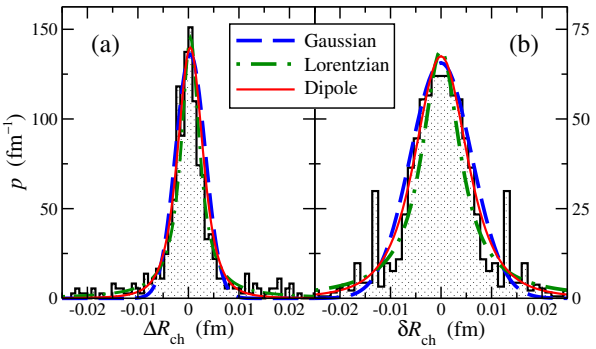

FIG. 3: (Color online) (a) Distribution of the differences between theory and experiment (ΔR_{ch}) for the charge radii of 455 nuclei (see text). Gaussian, Lorentzian, and Dipole probability density functions have been fitted to the histogram. (b) Statistical distribution of the experimental errors (δR_{ch}) for the 796 nuclei included in Angeli's compilation [13].

these isotopes. The authors of [25] have stressed that such a good agreement is essentially parameter free, as all their model parameters were fitted exclusively to nuclear masses. It is rewarding to see that the GKRs—with a rms deviation of 0.0031 fm—work as good, if not better, than the most sophisticated microscopic models available to date. In what follows, we show that this success extends throughout the periodic table.

By proceeding as in the case of the Tin isotopes, GK predictions were made for the charge radius of a total of 571 nuclei. From these, 455 can be compared against experiment while 116 await experimental confirmation (our GK predictions for the 116 nuclei whose charge radius is yet unmeasured may be found in Ref. [31]). This information has been graphically encoded in Fig. 2. The largest deviation between the GK prediction and experiment is about 0.06 fm and this happens for only a handful of nuclei at the edges of two of the populated regions. Most of the predictions are well below this largest value and 331 of them fall within experimental error. Indeed, the rms deviation obtained for the 455 charge radii is of only 0.0097 fm. This may be compared against the rms deviation of 0.0275 fm predicted by the microscopic Hartree-Fock-Bogoliubov model HFB-8 [23] (albeit this comparison includes the 782 experimentally measured charge radii with $Z \geq 8$ and $N \geq 8$ [13]). Note that using the same experimental data set, the new state-of-the-art HFB mass formulas BSk17 [29] and D1M [30] yield similar rms deviations (0.030 and 0.031 fm, respectively).

We next discuss our theoretical errors to better assess the reliability and predictive power of the GKRs. In answering the question of how the errors of the measured charge radii affect the GK predictions, we avoid attaching a theoretical error by simply adding (*e.g.*, in quadratures) the experimental errors associated to the 5 nuclei required to make a single GK estimate. This method of propagating errors is uncontrolled and misleading when applied locally, as the GKRs are satisfied with varying degrees of accuracy throughout the nuclear chart. Rather, we adopt a global approach that provides statistically reliable confidence levels. The histogram in Fig. 3(a) displays the differences ΔR_{ch} between the GK estimate and the central experimental value for the charge radii of the 455 nuclei for which the comparison was possible. Clearly, the probability distribution is very narrow. To extract faithful confidence levels we have fitted ΔR_{ch} to three different probability density functions (PDF): the Gaussian, the Lorentzian, and the Dipole. The plot indicates that the Gaussian PDF falls too fast. From the remaining two, the Dipole gives a slightly better fit than the Lorentzian so we adopt it henceforth. The Dipole PDF is defined as

$$p(x;\mu,\sigma) = (2\sigma^3/\pi)\,\left[(x-\mu)^2+\sigma^2\right]^{-2}\ , \qquad (4)$$

where in the present analysis the optimal values of the mean and the standard deviation for ΔR_{ch} are $\mu = 3.633\times10^{-3}$ fm and $\sigma = 4.554\times10^{-3}$ fm, respectively.

A particularly useful concept is that of *confidence interval* of size n defined as

$$\mathrm{CI}(n) = \int_{\mu-n\sigma}^{\mu+n\sigma} p(x;\mu,\sigma)dx\ . \qquad (5)$$

It represents the probability that a given ΔR_{ch} will fall within $\pm n$ standard deviations of the mean. For the dipole PDF, CI(1) = 0.818 and CI(2) = 0.960. This indicates that the difference between the GK prediction for a nucleus (*e.g.*, any of the 116 given in [31]) and the central experimental value falls in the range $\Delta R_{ch} = (3.633 \pm 4.554)\times10^{-3}$ fm with an 82% confidence level. We have repeated the statistical analysis for the distribution of experimental errors. The various PDFs are plotted in Fig. 3(b) using the same horizontal scale as in 3(a). Evidently, the experimental distribution of errors is significantly wider. Indeed, in fitting a dipole

form to it we obtain a mean of zero (the errors are symmetric) and a standard deviation that is more than twice as large: $\sigma_{\rm exp} = 9.427 \times 10^{-3}$ fm. These results suggest that the GKRs provide a useful and reliable benchmark for the calculation of nuclear charge radii. We trust that our results may motivate the experimental community to perform new measurements and to refine some of the existing ones.

In summary, taking into account that the linear combinations of masses that enter into the Garvey-Kelson relations are proportional to the third derivatives of the slowly-varying part of the nuclear mass function plus a remainder that comes from quantum fluctuations and is locally small, we concluded that the GKRs could be suitably extended to other observables obeying a similar underlying physics. In this letter we showed that this is indeed the case for the nuclear charge radius. Indeed, we made a systematic implementation of the GKRs using the existing experimental database of charge radii [13]. Of the 455 GK predictions that could be compared against experiment, an overall rms deviation of only 0.0097 fm was obtained. Moreover, of these 455 predictions 331 fell within experimental error. For comparison, one of the best microscopic models available in the literature (the HFB-8 model of [23]) yields a rms value of 0.0275 fm. In addition, we were able to make predictions for 116 nuclei [31] whose charge radius is presently unknown. Finally, by performing a global statistical analysis, we attached meaningful theoretical errors to our predictions. A similar analysis of the experimental errors revealed a standard deviation more than twice as large.

In the future, we want to examine to which extent the GK relations may be of use in other finite quantum systems, such as helium and metal clusters where the energy systematics is amenable to be described by a semiclassical mass formula plus quantum corrections on top of it [1]. We also intend to extend the GK predictions to uncharted areas of the table of nuclides with the help of methods from the field of image reconstruction—note that important first steps in this direction have already been taken [32, 33]. This would be particularly attractive for nuclear masses in regions of astrophysical interest and for charge radii of short-lived radioactive nuclei.

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