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Predictions of nuclear charge radii

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The nuclear charge radius is a fundamental property of an atomic nucleus. In this article we study the predictive power of empirical relations for experimental nuclear charge radii of neighboring nuclei and predict the unknown charge radii of 1085 nuclei based on the experimental CR2013 database within an uncertainty of 0.03 fm.

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Nuclear charge radius is a property as fundamental as mass, spin, and parity for an atomic nucleus. It also reflects the evolution of nuclear structure such as neutron skin, shape transition or coexistence, halo, and so on [1–5]. Experimental techniques such as high-energy electron scattering and spectra of μ atoms have been applied to perform measurements of nuclear charge radii (CR). Theoretically mean-field approaches, such as the Hatree-Fock-Bogolyubov (HFB) method, the nuclear shell model, and various approximations of the shell model, have been developed to describe and to predict the CR. There have been a number of updates of experimental CR databases since the early 1970s, and the latest database is the CR2013 [6,7], in which about 1000 experimental data have been evaluated and compiled.

Concerning theoretical studies of the CR, the HFB calculations typically yield a root-mean-squared deviation (RMSD) around 0.027 fm [8], and phenomenological formulas [9–11] present RMSD's around 0.022 fm. Numerical experiments of the Garvey-Kelson relations [12], simulations of the Garvey-Kelson relations of the neighboring nuclear masses [13], present an accuracy of about 0.01 fm. Very recently, simple relations of the CR for four neighboring nuclei, as shown in Ref. [14], give an accuracy of 0.0078 fm.

Because the simple relations of the CR between neighboring nuclei are very accurate, it is interesting and practical to study their predictive power. This is carried out in this article by two numerical experiments: extrapolations of the CR1999 (with a total of 285 data) [15] and CR2004 (with 799 data) [16] databases to the CR2013 database (with 944 data) [7]. We also present our predicted results by extrapolation of the CR2013 database.

Let us begin our discussion with a brief summary of the relations suggested in Ref. [14]. These relations consist of four charge radii of neighboring nuclei, called $1n$-$1p$, $1n$-$2p$, $2n$-$1p$, and $2n$-$2p$ CR relations, respectively, viz.,

$$\begin{aligned} \delta R_{in-jp} &= 0,\ i,j = 1,2; \\ \delta R_{in-jp} &= R(N,Z) + R(N-i,Z-j) \\ &\quad - R(N-i,Z) - R(N,Z-j). \end{aligned} \tag{1}$$

Here $R(N,Z)$ denotes the charge radius of the nucleus with the neutron number N and the proton number Z. In Fig. 1, we present schematic diagrams of four relations given by Eq. (1). Similar to the situation of predicting nuclear masses by using the Garvey-Kelson relations [17], depending on the relative position of a given nucleus for which the charge radius is predicted with respect to other known charge radii, there are maximally four approaches for each relation. We label them by using (1) ∼ (4), with the convention that the signs of charge radii for nuclei at (1) and (2) are positive, and the signs of those at (3) and (4) negative. We take the average of all possible approaches of a given formula(s) as our predicted CR value.

We first report an interesting phenomenon concerning the experimental uncertainty ($\sigma_{\rm exp}$) of the CR2013 database and the description RMSD value ($\sigma_{\rm des}$) of theoretical results obtained by the $\delta R_{1n-1p} = 0$ relation. We define two theoretical RMSD values: one corresponds to predicted results with averaging all possible predicted values, denoted by σ_0, and the other corresponds to those without such an averaging procedure, denoted by σ_0'. In Fig. 2(a) we present a histogram plot of the RMSD values of the CR2013 database; one can see that the uncertainty ($\sigma_{\rm exp}$) of most experimental data is below 0.01 fm. If we concentrate our predicted results for nuclei with $\sigma_{\rm exp}$ below 0.007 fm, as shown in Fig. 2(b), the values of $\sigma_{\rm des}$, including both σ_0 and σ_0', are seen to well correlate with $\sigma_{\rm exp}$; they are reasonably described by $\sigma_{\rm des} = \sigma_{\rm exp}$. This suggests that the uncertainty of predicted CR values would have been considerably smaller than those obtained in Ref. [14], if there had been further refinements of the experimental uncertainty; the theoretical RMSD is in general competitive with experimental uncertainty. It is therefore not surprising to see that for nuclei with $\sigma_{\rm exp} \leqslant 0.036$ fm, σ_0' (0.0072 fm) and σ_0 (0.006 fm) are almost 1 order smaller than $\sigma_{\rm exp}$. For the same reason, $\sigma_0 \simeq \sigma_0'$ for cases with $\sigma_{\rm exp} \leqslant 0.007$ fm, as shown in Fig. 2(b). The difference of σ_0 and σ_0' is 0.001 fm or becomes slightly larger for cases with $\sigma_{\rm exp} > 0.01$ fm, as shown in Fig. 2(a).

Although the three $\delta R_{in-jp} = 0\,[(i,j) = (1,2), (2,1), (2,2)]$ relations in Fig. 1 do not work as accurately as the $\delta R_{1n-1p} = 0$ relation, they are very useful to predict more results within reasonable accuracy. According to Table I, for example, one predicts the CR of 650 nuclei by using the relation $\delta R_{1n-1p} = 0$ with an accuracy $\sigma_0 = 0.0072$ fm and predicts the CR of 855 nuclei by using the four relations given in Fig. 1, with an accuracy of $\sigma_0 = 0.0076$ fm. Similar situations occur in extrapolations when predicting unknown CR values, as we see below.

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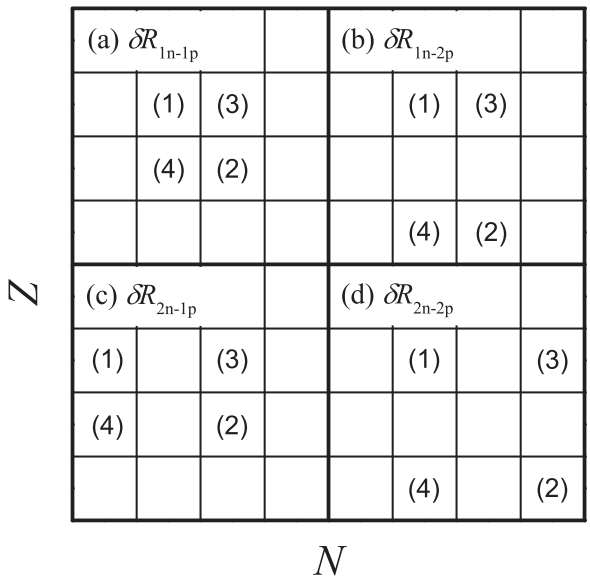

FIG. 1. Schematic diagrams of the so-called $in - jp$ $(i,j = 1,2)$ CR relations, $\delta R_{in-jp} = R(1) + R(2) - R(3) - R(4) = 0$. Similar to the situation in Ref. [17], depending on the relative position of a given nucleus for which the charge radius is predicted with respect to other known charge radii, there are maximally four approaches for each relation. We label them by using (1) ∼ (4), with the convention that the signs of the charge radii for nuclei at (1) and (2) are positive and the signs of those at (3) and (4) are negative.

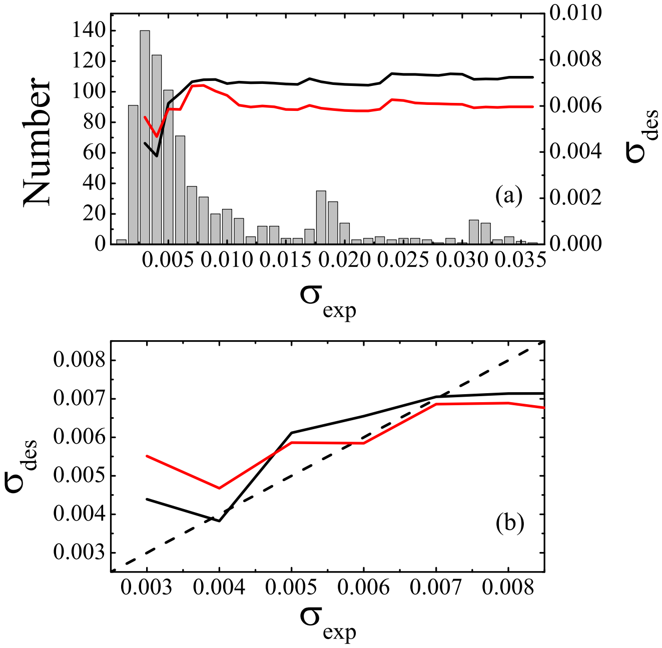

FIG. 2. Experimental uncertainty and theoretical description RMSD (σ_{exp} and σ_{des}) (in fm) of charge radii obtained by the $\delta R_{1n-1p} = 0$ relation based on the CR2013 database. (a) Histogram plot of the number of nuclei versus the given experimental uncertainty σ_{exp}, and a bird's-eye view of theoretical RMSD σ_{des} for nuclei with experimental uncertainty values below a given σ_{exp}. (b) Theoretical RMSD σ_{des} of nuclei with experimental CR uncertainties below a given value of σ_{exp}, for σ_{exp} between 0.002 and 0.0105 fm. The dashed line is plotted by $\sigma_{des} = \sigma_{exp}$. The solid line in black corresponds to σ_0', and the one in red corresponds to σ_0. See the text for details.

TABLE I. σ_0, $\mathcal{N}_0$, σ_1, $\mathcal{N}_1$, σ_2, and $\mathcal{N}_2$ by using only one relation, $\delta R_{in-jp} = 0$ $(i,j = 1,2)$, and those by joint applications of all these relations (denoted by "Total") shown in Fig. 1.

	σ_0	$\mathcal{N}_0$	σ_1	$\mathcal{N}_1$	σ_2	$\mathcal{N}_2$
δR_{1n-1p}	0.0072	650	0.0132	302	0.0174	122
δR_{1n-2p}	0.0116	551	0.0199	189	0.0261	110
δR_{2n-1p}	0.0078	725	0.0221	218	0.0173	85
δR_{2n-2p}	0.0088	682	0.0220	163	0.0246	87
Total	0.0076	855	0.0225	520	0.0147	134

In Fig. 3 we present the deviations of predicted values by extrapolations in comparison with experimental data. Figure 3(a) corresponds to the case of extrapolation from the CR1999 database to the CR2013 database, and Fig. 3(b) corresponds to the case from the CR2004 database to the CR2013 database. In both these two extrapolations, the evaluated data in the CR1999 and CR2004 databases are replaced by those in the CR2013 database. One can see that the accuracy of extrapolation is remarkable, in particular, the extrapolation shown in Fig. 3(a) is based on the CR values of only 285 nuclei. In Table I we list the RMSD values of these two extrapolations, where we present the numbers of the CR predicted, denoted by $\mathcal{N}_1$ and $\mathcal{N}_2$, and the corresponding RMSD values, denoted by σ_1 and σ_2, respectively, for individual $\delta R_{in-jp} = 0$ relations and for the joint application (i.e., the average procedure of Ref. [17]) of all four relations shown in Fig. 1. Clearly, more CR values are accessible in extrapolations within reasonable accuracy, if one resorts to the joint application of more relations. Without details, we note that in the extrapolation of Fig. 3(a), σ_1 equals 0.0136 fm for the same 302 nuclei as those predicted in the extrapolation by using the relation $\delta R_{1n-1p} = 0$, for which σ_1 is 0.0132 fm (see Table I). They are very close to each other.

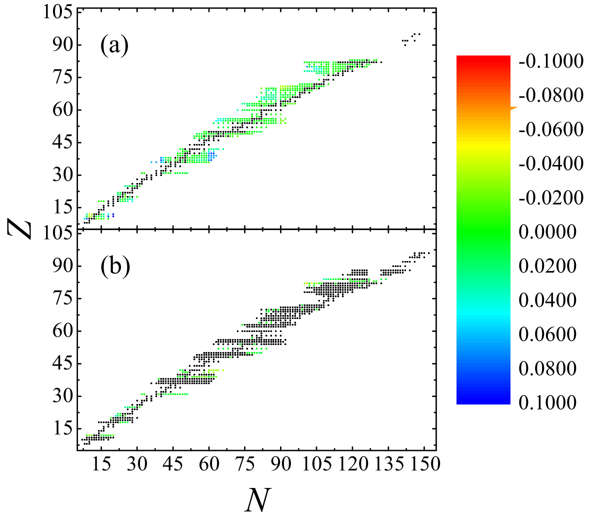

FIG. 3. Deviations (in fm) between experimental charge radii and theoretically extrapolated results obtained by "Total" (see Table I). Panel (a) corresponds to our extrapolation from the CR1999 database to the CR2013 database, and panel (b) corresponds to our extrapolation from the CR2004 database to the CR2013 database. Black dots represent nuclei with experimental data.

It is now interesting to note the exception of CR values for nuclei with proton halos. In this case the CR values are expected to be considerably larger than those without the halo structure. We find that this is indeed the case for $^{17}_{10}\mathrm{Ne}_7$, which was suggested to exhibit a proton halo [18,19]: Our predicted CR of this nucleus is 2.9842 ± 0.0125 fm, which is 0.0572 ± 0.0153 fm smaller than the experimental value (3.0413 ± 0.0088 fm). In the future it will be desirable to measure the CR of $^{25,26}_{15}\mathrm{P}$ [20], the ground states of which have a proton-halo structure, and to investigate whether or not the experimental CR are considerably larger than our predicted values (see Supplemental Material [21]).

Because the empirical formulas are very accurate, it is tempting to predict unknown CR values based on the current database [7]. Towards this, let us first discuss our theoretical uncertainty σ in our extrapolation. In this article the uncertainty (σ) of predicted CR values is evaluated by using the same method used in Refs. [22,23]. For convenience we briefly explain this procedure as follows. Let us denote k as the number of nuclei to be predicted, and $R^i_{\rm exp}$ and $R^i_{\rm th}$ denote the experimental and theoretical CR of the ith nucleus, respectively, where $i = 1,2,\ldots,k$ is an abbreviation of (N,Z). We assume the deviations of predicted results follow Gaussian distribution with the width $\sigma_{\rm th}$, assign a given value of $\sigma^*_{\rm th}$ (e.g., 0.1 fm), and calculate the weight factor ω^*_i for the ith nucleus, namely,

$$\omega^*_i = \frac{1}{\alpha_i^2 + (\sigma^*_{\rm th})^2}, i = 1,2,\ldots,k. \tag{2}$$

Here superscript "$*$" of ω_i and $\sigma_{\rm th}$ in Eq. (2) means that such values are temporary quantities that are to be replaced by new values in iterations. α_i^2 is the sum of squared $\sigma_{\rm exp}$ (experimental error bar) for all CRs adopted in the formula. The calculation $\sigma^*_{\rm th}$ is repeated by using the above ω^*_i, i.e.,

$$(\sigma^*_{\rm th})^2 = \frac{\sum_{i=1}^k \omega_i^{*2}\left[\left(R^i_{\rm th} - R^i_{\rm exp}\right)^2 - \left(\sigma^i_{\rm exp}\right)^2\right]}{\sum_{i=1}^k \omega_i^{*2}}. \tag{3}$$

Iteration of Eqs. (2) and (3) yields a series of $\sigma^*_{\rm th}$ that converges and is the theoretical uncertainty of our formulas. The final uncertainty σ for the ith nucleus in consideration in our tabulated predicted results is taken to be the squared root of the sum over all squared $\sigma_{\rm exp}$ of nuclei involved in the prediction and squared $\sigma_{\rm th}$.

Based on the CR2013 database [7], we predict 1085 CR values, which are not experimentally accessible, by using the four relations $\delta R_{in-jp} = 0$ in Fig. 1, with $\sigma \leqslant 0.03$ fm. We present the distribution of σ in Fig. 4, and we note that actually σ is smaller than 0.02 fm for most predictions. These predicted values are tabulated as Supplemental Material to this article [21].

In summary, in this article we study empirical relations of nuclear charge radii. We have reported an interesting correlation of $\sigma_{\rm des}$ of the simple relation $\delta R_{1n-1p} = 0$ with $\sigma_{\rm exp}$. It is found that the accuracy of this simple relation is competitive with experimental uncertainty. For the CR results with $\sigma_{\rm exp}$ below 0.007 fm, the theoretical description RMSD $\sigma_{\rm des}$ of this empirical formula is statistically equal to $\sigma_{\rm exp}$. This demonstrates that $\delta R_{1n-1p} = 0$ is *actually much more accurate* than previously reported in Ref. [14] (0.0078 fm). For cases with $\sigma_{\rm exp}$ below 0.004 fm (358 nuclei), the value of σ_0' is slightly below 0.004 fm.

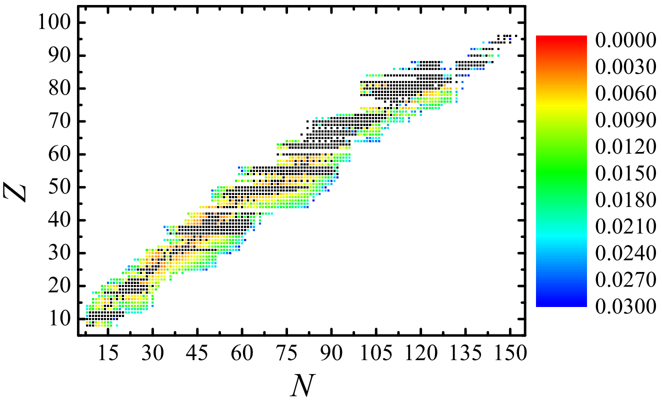

FIG. 4. Theoretical uncertainties (in fm) of our predicted charge radii of 1085 nuclei with $\sigma \leqslant 0.03$ fm, based on the 944 charge radii compiled in the CR2013 database [7]. Black dots correspond to nuclei with experimental data.

We have carried out two numerical experiments of extrapolations, one is from the CR1999 database to the CR2013 database and the other is from the CR2004 database to the CR2013 database. One can see the empirical formulas assumed in this article have strong predictive power. For example, most of the absolute deviations for 520 predicted CR values in the former extrapolation (i.e., based on only 258 experimental CR values) are below 0.03 fm.

Finally, based on the empirical formulas and the CR2013 database, we tabulate our predicted values of unknown charge radii of ground states for 1085 nuclei within theoretical accuracy of 0.03 fm and include them as Supplemental Material to this article [21]. These results are appropriate benchmark values of future experimental measurements. If experimentally observed radii deviate sizably from our predicted values, one might conjecture that sudden variances of charge density distributions will arise; in other words, our predicted data provide us with a convenient tool to study shape variance in unstable nuclei.

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