Nuclear binding energies and empirical proton-neutron interactions

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By using an exponential function to simulate the residual proton-neutron interaction between valence nucleons, we derive a new set of local mass formulas that are competitive with the Garvey-Kelson mass relations for relating neighboring nuclear masses.

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At present there are experimental data on more than 2000 nuclear masses across the periodic table. A model that can accurately describe these data and reliably predict unknown masses is a key goal of nuclear structure theory. Some of the most popular models currently in use are the finite-range droplet model (FRDM) [1], the Duflo-Zuker (D-Z) model [2], and models based on Skyrme-Hartree-Fock-Bogoliubov (SHFB) theory [3]. These models have been used to describe masses for roughly 9000 nuclei, including those for which masses are known and those for which they are not yet known. When applied to nuclei for which experimental masses are known, they reproduce the masses quite well, with rms deviations from the experimental data on ∼670 keV for the FRDM and the SHFB model and ∼380 keV for the D-Z model.

In addition to these global models of nuclear masses, there are also local mass formulas that relate the masses of neighboring nuclei. Particularly well known are the Garvey-Kelson (G-K) mass relations [4]. Recently, Barea *et al*. carried out a systematic analysis of G-K mass relations [5] and have shown that when studying nuclei with masses $A \geqslant 60$ and for which 12 G-K relations can be applied, deviations between masses predicted by the G-K relations and masses predicted by the experimental data are ∼76 keV [6].

In this paper, we show how it is possible to use features of the residual proton-neutron interaction to develop another set of local mass relations that have an accuracy comparable to the G-K relations but require a smaller number of masses to be known to achieve this same level of accuracy.

The residual proton-neutron interaction is well known to be an important fingerprint of the evolution of single-particle structure and the development of nuclear collectivity and nuclear deformation [7]. In 1989, Zhang *et al*. suggested a simple approach to extract the residual proton-neutron interaction ($\delta V_{\rm pn}$) between the last valence neutron and the last valence proton by using the nuclear masses of a few neighboring nuclei [8]. In subsequent works, it was noted that the residual proton-neutron interaction might also prove useful for predicting nuclear masses [9].

Following Zhang *et al.* [8], the residual proton-neutron interaction $\delta V_{\rm pn}(Z,N)$ can be obtained from the relation

$$\begin{aligned} 4\times\delta V_{\rm pn}(Z,N) = {} & [B(Z+1,N+1)-B(Z+1,N-1)] \\ & -[B(Z-1,N+1)-B(Z-1,N-1)], \end{aligned} \tag{1}$$

where $B(Z,N)$ is the negative of the nuclear binding energy for a nucleus with proton number Z and neutron number N. The usefulness of this formula for $\delta V_{\rm pn}$ has been studied extensively in many recent papers [9–17].

In Fig. 1, we present the evolution of $4\delta V_{\rm pn}(Z,N)$ versus proton number Z, for nuclei with $A \geqslant 60$, excluding those for which either the proton number or the neutron number is magic. The binding energies are obtained from the experimental masses given in the 2003 mass table (AME2003) [18].

It is possible to obtain an accurate functional approximation of these results by using an exponential function $f(Z)$ of the proton number Z and a second term, $\delta(Z,N)$, that simulates shell effects. The relevant formula is given by

$$\begin{aligned} 4\times\delta V_{\rm pn}^{\rm fit}(Z,N) &= f(Z)+\delta(Z,N), \\ f(Z) &= \alpha+\beta\times e^{Z/\gamma}, \\ \delta(Z,N) &= a+b\times|(Z-Z_0)\times\Omega_N \\ &\quad -(N-N_0)\Omega_Z, \end{aligned} \tag{2}$$

where

$$\alpha=-906.4,\quad \beta=-6564.4,\quad \gamma=-20.028,$$
$$a=-166.5,\quad b=0.8620.$$

Here α, β, a, and b are in units of kiloelectronvolts and γ is a constant. Also, Z_0 (N_0) is the largest magic number with respect to Z (N), and $\Omega_Z(N)=\sum_j(j+1/2)$ for the valence proton(neutron) shells.

The rms deviation between $4\delta V_{\rm pn}$ obtained using Eq. (1) and those obtained using Eq. (2) is 226 keV. If one sets $\delta(Z,N)=0$, the rms deviation goes up slightly, to 255 keV.

In what follows we in fact use the simpler functional form obtained by ignoring the shell correction term. With this simplifying assumption the functional form for the residual p-n interaction depends solely on Z, and not on N. As we

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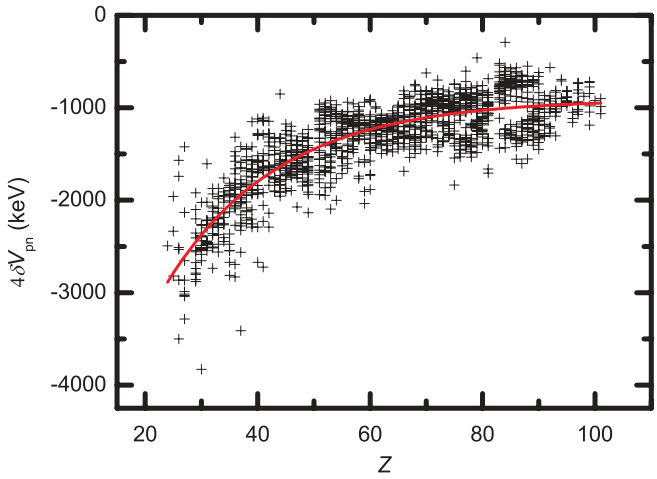

FIG. 1. (Color online) $4\delta V_{\rm pn}$ versus Z for $A \geqslant 60$ using the AME2003 data. The solid (red) curve was plotted using $f(Z)$ in Eq. (2).

see shortly this leads to further useful simplifications in the development of the formalism we present.

The basic idea of the new local mass model we present here is to assume the simplified exponential functional form $f(Z)$ for $4\delta V_{p,n}(Z,N)$ and then to use it in Eq. (1) to *predict* the binding energy of a nucleus from the other three binding energies in that formula. The solid (red) curve in Fig. 1 shows the approximation provided by this to the residual proton-neutron interaction data.

There are four possible equations we can obtain, depending on which of the four masses in Eq. (1) is to be predicted:

$$\begin{aligned} B^{\rm pred}(Z,N) &= B(Z,N-2)+B(Z-2N) \\ &\quad -B(Z-2,N-2)+f(Z-1), \\ B^{\rm pred}(Z,N) &= B(Z,N+2)-B(Z-2,N+2) \\ &\quad +B(Z-2,N)-f(Z-1), \\ B^{\rm pred}(Z,N) &= B(Z,N+2)+B(Z+2,N) \\ &\quad -B(Z+2,N+2)+f(Z+1), \\ B^{\rm pred}(Z,N) &= B(Z,N-2)+B(Z+2,N) \\ &\quad -B(Z+2,N-2)-f(Z+1). \end{aligned} \tag{3}$$

If all of the neighboring masses are available, we can average these four results and obtain

$$\begin{aligned} B^{\rm pred}_{n=4}(Z,N) &= \tfrac{1}{4}[2B(Z+2,N)+2B(Z,N+2) \\ &\quad +2B(Z-2,N)+2B(Z,N-2) \\ &\quad -B(Z+2,N+2)-B(Z+2,N-2) \\ &\quad -B(Z-2,N+2)-B(Z-2,N-2)]. \end{aligned} \tag{4}$$

The subscript $n=4$ is included to indicate that all four approximations of the predicted mass (binding energy) are possible. Note that in the $n=4$ approximation the functional for the residual proton-neutron interaction cancels out. This is true, however, only when we ignore the shell correction contribution to the residual proton-neutron interaction and assume an exponential approximation with its sole dependence on Z.

TABLE I. rms deviations (keV) between the AME2003 data and the binding energies calculated using Eq. (3), Eq. (6), and the G-K relations with $A \geqslant 60$ as a function of the number of predictions n.

Relation	$n \geqslant 1$	$n \geqslant 2$	$n \geqslant 3$	$n \geqslant 4$	$n \geqslant 12$
Eq. (3)	183	137	110	97	–
Eq. (6)	110	93	80	78	–
G-K	115	–	–	98	76

We apply Eq. (3) to the AME2003 database. The rms deviation from experimental data for nuclei with $A \geqslant 60$ is summarized in Table I, where we compare it with the corresponding results obtained using the G-K mass relations.

In the case of the G-K mass relations, however, more nearby masses are involved and thus more mass predictions can be made. Indeed, with the G-K relations it is, in principle, possible to obtain up to 12 predictions, when all neighboring masses are available.

The rms deviation using Eq. (3) is 183 keV for $n \geqslant 1$, in comparison to 115 keV based on the G-K relations. For $n \geqslant 4$, the rms deviation by Eq. (3) is close to that from the G-K relations. However, as already noted it is possible to make more predictions using the G-K relations, and when this is possible the resulting discrepancies are reduced to just 76 keV.

The rms deviation from the AME2003 database is shown in Fig. 2. One sees that large deviations occur when A is relatively small, or along the border of experimentally known nuclei, for which $n=1$.

At this point, we refine Eq. (3) by assuming that the residual proton-neutron interaction $\delta V_{\rm pn}$ for a given nucleus is obtained by averaging the results of the four neighboring nuclei, that is,

$$\begin{aligned} \delta V_{\rm pn}(Z,N) &= \tfrac{1}{4}[\delta V_{\rm pn}(Z+1,N)+\delta V_{\rm pn}(Z-1,N) \\ &\quad +\delta V_{\rm pn}(Z,N+1)+\delta V_{\rm pn}(Z,N-1)]. \end{aligned} \tag{5}$$

Substituting Eq. (1) into this equation, we obtain the mass relation,

$$\begin{aligned} &4B(Z-1,N+1)+4B(Z+1,N-1)-4B(Z-1,N-1) \\ &\quad -4B(Z+1,N+1)+B(Z+2,N+1) \\ &\quad +B(Z+1,N+2)+B(Z-2,N-1) \end{aligned}$$

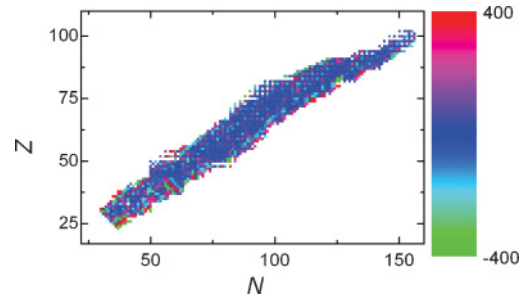

FIG. 2. (Color online) Nuclide charts colored according to the deviations (keV) of binding energies between the measured masses in the AME2003 table and the masses calculated using Eq. (3) for all nuclei.

$$+ B(Z-1, N-2) - B(Z-2, N+1)$$
$$- B(Z-1, N+2) - B(Z+2, N-1)$$
$$- B(Z+1, N-2) = 0. \quad (6)$$

This is a relation involving the masses of 12 neighboring nuclei. From this relation, we can make a variety of mass predictions from those of its neighbors. Here we use it to make predictions for up to $n = 4$ masses, by focusing on the binding energies $B(Z-1, N+1)$, $B(Z+1, N-1)$, $B(Z-1, N-1)$, and $B(Z+1, N+1)$ in the equation. When we apply such a prescription to the AME2003 mass database, we obtain the results given in the second row in Table I. When all four mass predictions are made (i.e., $n = 4$), the rms deviation obtained is 78 keV, close to that obtained using $n = 12$ G-K relations. Of course, there are more than four predictions that can be made with Eq. (3). Nevertheless, we find it intriguing and thus worthy to note that in certain circumstances this new mass relation is able to achieve such a high level of accuracy with just the use of four predictions.

To summarize, we have shown in this paper that, by using an exponential function to simulate the residual proton-neutron interactions, we have been able to obtain a local mass relation that predicts nuclear binding energies from those of neighboring nuclei with the same level of accuracy as the well-known G-K mass relations. More specifically, the rms deviation from experimental data is 97 keV, if the binding energies of all neighboring nuclei are known. With a further refinement of the approach we are able to achieve the even smaller rms deviation of 78 keV, when an appropriate set of mass relations is used.

Finally, it is worth noting here that it is because of the extensive recent works [9–17] aimed at trying to understand the properties of residual proton-neutron interactions that we have been able to arrive at this new approach to predicting the nuclear masses of unknown nuclei.

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