The empirical p-n interactions and atomic masses

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Abstract. The systematics of the empirical proton-neutron (p-n) interactions are studied for better understanding of atomic masses. The odd-even staggering of the interaction between the last proton and the last neutron is partly explained by the pairing interaction, further studies on this phenomenon are needed. Two sets of simple and accurate mass formulas are suggested by using the systematics of the empirical p-n interactions.

1. Introduction
I (A. Arima) would like to thank the organizers for inviting me to this Conference in honor of Jerry P. Draayer's 70th birthday. First of all, I wish to congratulate Jerry P. Draayer on his 70\(^{th}\) birthday.

K. T. Hecht and A. Adler [1] in Michigan, and K. Shimizu, A. Arima in Tokyo and M. Harvey in Chalk River [2] discovered an interesting degeneracy in nuclear single particle energies in 1969 very independently from each other. This dynamical symmetry is called the pseudo spin symmetry. Furthermore in some areas we found that the pseudo SU(3) symmetry works well. I was very impressed by Jerry Draayer and Ted Hecht, who cooperated to study and develop these two dynamical symmetries [3-5]. Since then, I always have been interested in Jerry’s activities.

I would like to talk on the empirical p-n interactions and atomic masses.

There have been great developments theoretically in global mass calculations, for example, the Duflo-Zuker model [6] in 1995, the modified Weizsäcker formula [7] in 2011, etc. [8,9].

These global mass calculations have been applied to 8000\textasciitilde9000 nuclei, and the RMS deviations from experimentally known masses are only 340 keV\textasciitilde580 keV.

Local mass relations, also, have been studied and recognized as very useful to predict nuclear masses. The Garvey-Kelson mass relations [10] are particularly powerful for this purpose. In the study of the local mass relations, it is very essential to study proton-neutron interactions empirically. See the comprehensive reviews Refs. [11,12]. The RMS error (\(\sigma\)) and mean error (\(\varepsilon\)) of fits given by various mass formulas are shown in table 1.

The empirical p-n interactions \(\delta V_{pn}(Z,N)\) are obtained by using the observed masses as follows:

\[
\delta V_{pn}(Z,N) = \frac{1}{4}\left[ B(Z+1,N+1) - B(Z+1,N-1) - B(Z-1,N+1) + B(Z-1,N-1) \right]
\]

Figure 1 shows the empirical p-n interactions taken from Brenner et al [13].
2. Mass predictions by using the empirical p-n interactions

We first generalize the empirical p-n interactions to include the last $i$ protons and $j$ neutrons:

$$
\delta V_{ip,n}(Z,N) = B(Z,N) - B(Z,N-j) - B(Z-i,N) + B(Z-i,N-j)
$$
For $i=1$ and $j=1$, we obtained very similar results to those reported by Basu et al. [14] in 1971, as is shown in figure 2.

![Figure 2. Dependence of $-\delta V_{1p-1n}$ on nuclear mass number $A$. Black circles are for even-$A$, and blue circles for odd-$A$.](image)

In order to estimate orders of magnitude of several typical energies, for example the surface energy and the pairing energy, we use the modified Weizsäcker mass formula as follows.

$$E_{LD}(A,Z) = a_c A + a_s A^{2/3} + E_c + a_{sym} I^2 A + a_{pair} A^{-1/3} \delta_{np} + \Delta_w$$

$$\delta_{np} = \begin{cases} 
2 - I & \text{for even } Z \text{ and even } N \\
I & \text{for odd } Z \text{ and odd } N \\
1 - I & \text{for odd } Z \text{ and even } N \text{ with } Z < N \\
1 & \text{for odd } Z \text{ and even } N \text{ with } Z > N \\
1 - I & \text{for even } Z \text{ and odd } N \text{ with } Z > N \\
1 & \text{for even } Z \text{ and odd } N \text{ with } Z < N 
\end{cases}$$

$$E_c = a_c \frac{Z^2}{A^{1/3}} \left(1 - 0.76Z^{-2/3}\right)$$

where $a_{pair} = 5442.3$ keV and $I = \frac{|N - Z|}{A}$.

The results for $A$(nuclear mass number) $> 100$ are as follows:

- Surface energy $\sim$ 5 keV.
- Coulomb energy $\sim$ 26 keV.
- Symmetry energy $\sim$ 269 keV.
- Pairing energy $\sim$ ±166 keV.

We can confirm that the Garvey-Kelson relations work very well. This means that

$$\delta V_{1p-1n}(Z,N) \approx \delta V_{1p-1n}(Z-1,N+1)$$
$$\delta V_{1p-1n}(Z,N) \approx \delta V_{1p-1n}(Z+1,N+1)$$
We found the following formulae for averaged $\overline{\delta V_{1p-1n}}(A)$ (see figure 2):

$$\overline{\delta V_{1p-1n}}(A) = \begin{cases} 
-(74 + \frac{69861}{A}) \text{ keV for even } A \\
-74 \text{ keV for odd } A 
\end{cases}$$

These formulae indicate that there is an energy difference between even-$A$ and odd-$A$ nuclei which amounts about 440 keV for $A > 100$.

It is reasonable to try to explain this difference by using the pairing interaction. However, as mentioned above, the pairing energy estimated by the modified Weizsäcker mass formula is about $\pm 166$ keV. This means that we can expect about 330 keV as the even-odd energy difference. This difference is smaller than 440 keV found in our present study. We do not know how to explain this remaining difference between even-$A$ and odd-$A$ nuclei.

Casten and his collaborators [15] pointed out that the contribution from the shell effect to $\delta V_{pn}$ is important. We then assume the following formulae for $\delta V_{1p-1n}^{\text{cal}}$, $\delta V_{1p-2n}^{\text{cal}}$ and $\delta V_{2p-1n}^{\text{cal}}$:

$$-\delta V_{1p-1n}^{\text{cal}}(Z, N) = -\overline{\delta V_{1p-1n}}(A) + \Delta_{\text{sh}}(Z, N) + \Delta_{\text{c}}(Z, N) + \Delta_{\text{sym}}(Z, N)$$

$$-\delta V_{1p-2n}^{\text{cal}}(Z, N) = -\overline{\delta V_{1p-2n}}(A) + \Delta_{\text{sh}}(Z, N) + \Delta_{\text{c}}(Z, N) + \Delta_{\text{sym}}(Z, N)$$

$$+ \Delta_{\text{sh}}(Z, N - 1) + \Delta_{\text{c}}(Z, N - 1) + \Delta_{\text{sym}}(Z, N - 1)$$

$$-\delta V_{2p-1n}^{\text{cal}}(Z, N) = -\overline{\delta V_{2p-1n}}(A) + \Delta_{\text{sh}}(Z, N) + \Delta_{\text{c}}(Z, N) + \Delta_{\text{sym}}(Z, N)$$

$$+ \Delta_{\text{sh}}(Z - 1, N) + \Delta_{\text{c}}(Z - 1, N) + \Delta_{\text{sym}}(Z - 1, N)$$

In these formulae,

$$\Delta_{\text{sh}}(Z, N) = a_{\text{sh}} + 2b_{\text{sh}} \left[ \delta_p \Omega_N(N_p - \Omega_z) - \delta_n \Omega_Z(N_n - \Omega_y) \right]$$

where $\delta_p$ ($\delta_n$) equals +1 if the valence protons (neutrons) are particle-like, and -1 if they are hole-like,

$$\Omega_Z = \sum_{j_z} \left( j_z + \frac{1}{2} \right)$$

with $j_z$ representing angular momenta of single-particle levels for valence protons,

and $\Omega_N = \sum_{j_n} \left( j_n + \frac{1}{2} \right)$ with $j_n$ representing angular momenta of single-particle levels for valence neutrons. Furthermore, we used

$$\Delta_{\text{sym}}(Z, N) = a_{\text{sym}} \frac{1}{A(2 + |Ld|)^3} + b_{\text{sym}} A^{-1/3}$$

$$\Delta_{\text{c}}(Z, N) \approx a_{\text{c}} \left( -\frac{4}{9} Z^{4/3} A^{-7/3} - \frac{2}{3} Z A^{-4/3} + \frac{4}{9} Z^2 A^{-7/3} + \frac{4}{9} Z^{1/3} A^{-4/3} \right)$$

We fixed the parameters in those expressions by using the $\chi^2$-fitting procedure. Results thus obtained are shown in table 2.
Table 2. Parameters obtained by the $\chi^2$-fitting procedure. Taken from Ref. [20].

| Parameter | For Even-A | For Odd-A |
|-----------|------------|-----------|
| $a_{th}$  | 58.95      | 15.40     |
| $b_{th}$  | −0.1444    | −0.03157  |
| $a_c$     | −34.80     | 12.00     |
| $a_{sym}$ | 12007      | 22211     |
| $b_{sym}$ | −179.7     | −70.42    |

Looking at the empirical values of those parameters, we are puzzled by large differences between the cases of even-$A$ and odd-$A$. This may reflect the fact that the pairing interaction is not enough to explain the difference between $\delta V_{1p-1n}$ for even-$A$ and $\delta V_{1p-1n}$ for odd-$A$.

Our empirical formula works well to predict nuclear binding energies and other nuclear properties such as separation energies and $\alpha$-decay energies.

We wish to show our results here. But frankly speaking, we are not yet satisfied by our results. We wish to understand for example why the shell effects are different for the cases of even-$A$ and odd-$A$.

Our formulas to predict $B(Z, N)$ by using $\delta V_{1p-2n}^{cal}$ and those obtained by using $\delta V_{1p-2n}^{cal}$ and $\delta V_{2p-1n}^{cal}$ are presented as follows.

\[
\begin{align*}
B_{pred}^{1p-1n} (Z, N) &= B(Z, N - 1) + B(Z - 1, N) - B(Z - 1, N - 1) + \delta V_{1p-1n}^{cal} (Z, N) \\
B_{pred}^{1p-1n} (Z, N) &= B(Z, N - 1) + B(Z + 1, N) - B(Z + 1, N - 1) - \delta V_{1p-1n}^{cal} (Z + 1, N) \\
B_{pred}^{1p-1n} (Z, N) &= B(Z, N + 1) + B(Z + 1, N) - B(Z + 1, N + 1) + \delta V_{1p-1n}^{cal} (Z + 1, N + 1) \\
B_{pred}^{1p-1n} (Z, N) &= B(Z, N + 1) + B(Z - 1, N) - B(Z - 1, N + 1) - \delta V_{1p-1n}^{cal} (Z, N + 1) \\
B_{pred}^{1p-2n} (Z, N) &= B(Z, N - 2) + B(Z - 1, N) - B(Z - 1, N - 2) + \delta V_{1p-2n}^{cal} (Z, N) \\
B_{pred}^{1p-2n} (Z, N) &= B(Z, N - 2) + B(Z + 1, N) - B(Z + 1, N - 2) - \delta V_{1p-2n}^{cal} (Z + 1, N) \\
B_{pred}^{1p-2n} (Z, N) &= B(Z, N + 2) + B(Z + 1, N) - B(Z + 1, N + 2) + \delta V_{1p-2n}^{cal} (Z + 1, N + 2) \\
B_{pred}^{1p-2n} (Z, N) &= B(Z, N + 2) + B(Z - 1, N) - B(Z - 1, N + 2) - \delta V_{1p-2n}^{cal} (Z, N + 2) \\
B_{pred}^{2p-1n} (Z, N) &= B(Z, N - 1) + B(Z - 2, N) - B(Z - 2, N - 1) + \delta V_{2p-1n}^{cal} (Z, N) \\
B_{pred}^{2p-1n} (Z, N) &= B(Z, N - 1) + B(Z + 2, N) - B(Z + 2, N - 1) - \delta V_{2p-1n}^{cal} (Z + 2, N) \\
B_{pred}^{2p-1n} (Z, N) &= B(Z, N + 1) + B(Z + 2, N) - B(Z + 2, N + 1) + \delta V_{2p-1n}^{cal} (Z + 2, N + 1) \\
B_{pred}^{2p-1n} (Z, N) &= B(Z, N + 1) + B(Z - 2, N) - B(Z - 2, N + 1) - \delta V_{2p-1n}^{cal} (Z, N + 1)
\end{align*}
\]

Results thus obtained by the present study are shown in tables 3 and 4. Nuclear masses predicted by the present study are compared with new measurements, together with other predictions in figure 3. Alpha-decay energies are also calculated and are shown in table 5.
Table 3. Pred(1) corresponds to predicted results by using $\delta V_{1p-1n}^\text{cal} (Z,N)$ and experimental database of AME2003, pred(2) are those by using $\delta V_{1p-2n}^\text{cal}$ and $\delta V_{1p-2n}^\text{cal}$. M03 are taken from predicted results in the AME2003 table, and $M_{\text{exp}}$ corresponds to new experimental data after 2003. # denotes the number of available paths to predict the masses from the experimental database.

| Nucleus | $M_{\text{pred(1)}}$ | #(1) | $M_{\text{pred(2)}}$ | #(2) | $M_{03}$ | $\sigma_{03}$ | $M_{\text{exp}}$ | $\sigma_{\text{exp}}$ |
|---------|---------------------|------|---------------------|------|---------|------------|----------------|----------------|
| $^{81}$Ge | -60974.79 | 2 | -60972.83 | 1 | -60901 | 196 | -60804 | 120 |
| $^{84}$As | -66299.68 | 1 | -66081.99 | 1 | -66082 | 300 | -65869 | 119 |
| $^{85}$As | -63394.92 | 2 | -63386.62 | 1 | -63323 | 196 | -63236 | 120 |
| $^{86}$As | -59242.80 | 3 | -59203.68 | 2 | -59150 | 298 | -58860 | 120 |
| $^{86}$Se | -59333.50 | 1 | -59542.07 | 1 | -59196 | 298 | -58955 | 120 |
| $^{70}$Br | -51077.43 | 1 | -51344.19 | 1 | -51426 | 306 | -51425 | 15 |
| $^{122}$Ag | -71045.66 | 1 | -71165.57 | 1 | -71231 | 205 | -71065 | 38 |
| $^{123}$Ag | -69781.58 | 2 | -69781.58 | 1 | -69955 | 205 | -69548 | 30 |
| $^{124}$Ag | -66221.55 | 3 | -66311.87 | 2 | -66471 | 196 | -66200 | 250 |
| $^{138}$Te | -65903.88 | 1 | -66048.61 | 1 | -65931 | 205 | -65755 | 122 |
| $^{140}$I | -64009.51 | 1 | -64077.94 | 1 | -64273 | 196 | -63596 | 121 |
| $^{141}$I | -60430.17 | 2 | -60430.17 | 1 | -60519 | 196 | -60301 | 128 |
| $^{143}$Xe | -60376.90 | 1 | -60284.83 | 1 | -60445 | 196 | -60253 | 124 |
| $^{213}$Tl | 1651.70 | 3 | 1639.27 | 2 | 1763 | 61 |
| $^{221}$Po | 20069.08 | 3 | 20208.92 | 3 | 19783 | 58 |
| $^{222}$Po | 23085.32 | 3 | 22476 | 67 |
| $^{224}$At | 28046.06 | 3 | 27706 | 59 |
| $^{236}$Ac | 51548.90 | 2 | 51508 | 499 | 51267 | 68 |

Table 4. Selected data among our predicted mass excesses (in units of keV). These unknown masses are either important in the context of astrophysics and nuclear structure or to be measured in the near future. $M_{\text{pred(1)}}$ and $M_{\text{pred(2)}}$ are as explained in the caption to table 3. AME2003 corresponds to the AME2003 database, and AME2011-preview corresponds to the results in tables of Ref. [18], which is a preview of the recent evaluation by Audi et al. Taken from Ref. [20].

| Nucleus | $M_{\text{pred(1)}}$ | $M_{\text{pred(2)}}$ | AME2003 | AME2011-preview |
|---------|---------------------|---------------------|----------|-----------------|
| $^{84}$Mo | -55687 ± 394 | -55681 ± 368 | -55806 ± 401 | -54502 ± 401 |
| $^{86}$Tc | -50969 ± 184 | -51359 ± 247 | -53207 ± 298 | -51297 ± 298 |
| $^{88}$Ru | -54277 ± 276 | -54314 ± 184 | -55647 ± 401 | -54399 ± 298 |
| $^{90}$Rh | -52378 ± 315 | -52163 ± 207 | -53216 ± 503 | -51959 ± 401 |
| $^{92}$Pd | -54962 ± 295 | -54722 ± 166 | -55498 ± 503 | -55070 ± 503 |
| $^{94}$Ag | -52719 ± 465 | -52629 ± 285 | -53300 ± 503 | -52412 ± 641 |
| $^{129}$Cd | -63500 ± 179 | -63360 ± 131 | -63202 ± 298 | -63314 ± 196 |
| $^{135}$Sn | -61017 ± 279 | -61022 ± 215 | -60799 ± 401 | -60612 ± 401 |
| $^{204}$Pt | -17955 ± 221 | -17995 ± 111 | -18062 ± 401 |
3. Summary

Now I would like to explain why our method works well.

First, the p-n interactions that we exploit include 1p-1n, 1p-2n, and 2p-1n types. These interactions have been much less investigated than the 2p-2n-type proton-neutron interactions. Their systematics have been much less known.

Second, most extrapolation approaches assume that the one- and two-body interactions evolve very slowly and are more or less constant in local regions. In our approach, we go one step forward: we refine the systematics of the p-n interactions by considering shell effects.

Third, if the number of equations to predict the mass of a given nucleus is more than one, our predicted value is given by the average value of all predictions. This reduces the deviations from experimental values. Such an advantage was pointed out by Barea et al [16,17] for the Garvey-Kelson relations. The reason why averaging the predicted results reduces the deviations from experimental values has not yet been well understood.

A brief summary of this report is as follows.

(1) The present method is very easy and practical. The model error is ~150 keV.
The odd-even staggering of $\delta V_{1p-1n}$ is a good test stone to inspect mass models.

(3) Mass relations between four neighboring nuclei are exploited, and the uncertainties are accumulated more slowly than for the Garvey-Kelson relation.

(4) The odd-even staggering of $\delta V_{1p-1n}$ puzzles us because the pairing interaction is not enough to explain it.

(5) The empirical values of parameters determined by the $\chi^2$-fitting must be explained from the microscopic point of view. Especially the shell effect must be understood.

(6) The prediction of masses depends on the accuracy of experimental data very much.

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