

Improvement in a phenomenological formula for ground state binding energies

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Abstract

The phenomenological formula for ground state binding energy derived earlier (International Journal of Modern Physics E **20** (2011) 179) has been modified. The parameters have been obtained by fitting the latest available tabulation of experimental values. The major modifications include a new term for pairing and introduction of a new neutron magic number at $N = 160$. The new formula reduced the root mean square deviation to 363 keV, a substantial improvement over the previous version of the formula.

1 Introduction

The history of efforts to find a global formula for nuclear ground state binding energy, or equivalently mass, can be traced way back to 1935 when von Weizsäcker[1] used a charge liquid drop model (LDM) to obtain a global formula. There are different approaches in the theoretical quest to calculate the binding energies of nuclei. Microscopic approaches usually utilize mean field theories such as Skyrme Hartree-Fock or relativistic mean field approaches to calculate the mean field calculation. Microscopic-macroscopic calculations usually derive the shell-correction microscopically and use a variant of LDM. A prime example of such an approach is the Finite Range Droplet Model (FRDM)[2]. The various forms of the Duflo-Zuker mass formulas[3, 4] have been particularly successful. For example, a recent variant with 33 parameters[5] shows a root mean square (rms) deviation of 374 keV. In a related approach, local mass relations use the masses of known nuclei to predict the mass of unknown nuclei in the neighbourhood.

Recent attempts to obtain an improved formula can be found in many works and only a few representative ones can be cited here. Goriely *et al.*[6] used the Hartree-Fock-Bogoliubov(HFB) method to obtain an rms error of 580 keV for 2149 nuclei. Isospin effect was considered by Wang *et al.*[7] who took the microscopic-macroscopic approach and utilized the Skyrme density functional. The rms deviation in their work, for 2149 nuclei, was 516 keV. Using the constraints of mirror nuclei, the rms deviation was further reduced to 441 keV [8]. Wang and Liu[9] also introduced the radial basis function approach to obtain a mass formula which showed an rms deviation of 336 keV for 2149 nuclei. In a related approach, Bao *et al.*[14] proposed an empirical formula for nucleon separation energies which produced an rms deviation of 325 keV and 342 keV for neutron and proton separation energies, respectively. All these three works took advantage of a new pairing term proposed by Mendoza-Temis *et al.*[10]. Zhang *et al.*[11] used a Strutinsky-like procedure to estimate the shell and pairing effects and fixed the coefficients of their macroscopic-microscopic formula by fitting the known masses. In a very recent work, Bhagawat[12] proposed a mass formula based on trace formulas. This formula yielded an rms deviation of 266 keV. However, the number of parameters was very large. A total of 142 free parameters was used in the formula. The Garvey-Kelson local mass relations[13] were recently revisited by Bao *et al.*[14] and Cheng *et al.*[15]. Readers are also referred to reviews such as Lunney *et al.*[16] for more details.

In an earlier work[17], hereafter referred to as Ref I, a phenomenological formula was developed for the ground state binding energy of nuclei. The formula, based on the charged liquid drop model, uses a number of parameters to describe the shell correction and also utilizes the number of valence protons (N_p) and neutrons (N_n) to predict the binding energy of the ground state of a large number of nuclei. The error in the binding energy of 2140 nuclei from the mass Table of 2003 (AME2003)[22] was found to be 376 keV. This formula has been used to study proton rich nuclei[18], neutron rich nuclei and r-process nucleosynthesis[19] and rapid proton capture process[20, 21].

Recent attempts at a global binding energy formula have been looking for alternative formulation of various terms. A significantly enlarged compilation[23, 24] has been made available after Ref I was published. The new compilation lists the experimental binding energy of 2353 nuclei with $Z \geq 8$ and $N \geq 8$. In the present work, we modify the phenomenological mass formula in the light of the new form of the pairing term[10] and extend our calculation to the new compilation[23, 24].

2 Formalism

In the new version of the formula, the most significant change has been in the form of the pairing term. It is well known that the parameters of the mass formula are very much correlated [See *e.g.* Kirson[25]]. Hence the parameters have substantially been modified on changing the form of the pairing term. We also have included certain corrections in the forms of the other terms and dropped a few terms. The new version of the formula keeps the form invariant in the sense that it consists of a LDM component (B_{LDM}), a one body term which simulates the shell correction effects (B_{bunc}), a term corresponding to the effect of the valence protons and neutrons (B_{np}), a Wigner term (B_W) and an empirical term for the electronic binding energy (B_{el}).

$$B.E.(N, Z) = B_{LDM} + B_{bunc} + B_{np} + B_W + B_{el} \quad (1)$$

The form of the one body term, which describes the shell correction effect, remains unchanged. However, as will discuss later, an additional parameter has been included to describe the more recent measurements in superheavy region.

$$B_{bunc} = \sum_i^{1,2} \sum_{\alpha} \epsilon_{\alpha}^i \mathcal{N}^i n_{\alpha}^i \quad (2)$$

where $i = 1, 2$ refer to the neutron or proton, respectively. Briefly, the number of neutrons and protons in the nucleus are given by $\mathcal{N}^1 (= N)$ and $\mathcal{N}^2 (= Z)$, respectively. A shell model like filling of the energy levels have been assumed so that we have

$$n_{\alpha}^i = \begin{cases} \mathcal{N}_{\alpha+1}^i - \mathcal{N}_{\alpha}^i & \text{for } \mathcal{N}^i > \mathcal{N}_{\alpha+1}^i \\ \mathcal{N}^i - \mathcal{N}_{\alpha}^i & \text{for } \mathcal{N}_{\alpha}^i \leq \mathcal{N}^i \leq \mathcal{N}_{\alpha+1}^i \\ 0 & \text{for } \mathcal{N}^i < \mathcal{N}_{\alpha}^i \end{cases}$$

More details about this one body term may be obtained from Ref I.

The LDM component is given by

$$B_{LDM} = a_v \left(1 - 4k_v \frac{T(T+1)}{A^2}\right) A - a_{surf} A^{2/3} - B_{sym} - B_{Coul} + B_{pair} \quad (3)$$

where $A = N + Z$ is the mass number and the isospin asymmetry parameter is $I = |N - Z|/A = 2T/A$.

The volume and the surface terms are the usual ones used in the LDM. One part of the symmetry energy is included in the volume term. We find

that the surface symmetry energy term $I^2 A^{2/3}$, used in many works, does not have any appreciable effect in our approach. We also find that the term proportional to I used in Ref I, which may also be considered as another Wigner term, has very little effect. Hence, we have dropped it from the expression to get a modified expression for the symmetry term,

$$B_{sym} = WI^2 + a_s A^5 I^5 \quad (4)$$

The Coulomb term has been rewritten as

$$B_{Coul} = \frac{3}{5} \frac{(Z(Z-1) - 0.76Z(Z-1)^{2/3})e^2}{r_0 A^{1/3} (1 - \frac{I^2}{4})} + a'_c \left(\frac{Z^2}{A}\right)^{5/2} \quad (5)$$

The first term in the Coulomb interaction uses the charge radius

$$r_c = r_0 A^{1/3} \left(1 - \frac{I^2}{4}\right) \quad (6)$$

and a surface correction term. In the numerator the first and the second terms indicate the direct and the exchange contribution, respectively. Hence they are of opposite signs. This form has already been used elsewhere[10, 26]. The second term, used in Ref I to represent the Coulomb corrections such as volume rearrangement, exchange contributions, etc, has been retained.

We should note that there is an alternative way of representing the direct and the exchange terms for Coulomb interaction based on the FRDM[2] used in various works[7, 8]. This prescription, used in the present method, produces an rms deviation almost identical with the form in eqn. (5) that has been used in the present work.

As already mentioned, the most important change from the formula of Ref I is in the pairing term. In the present version, the pairing term consists of two parts.

$$B_{pair} = \frac{a_{pair}\delta_{np}}{A^{1/3}} + \frac{a_{ph}\delta_{ph}}{A^{1/3}} \quad (7)$$

The first one was introduced by Mendoza-Temis *et al.*[10] and has been used in a number of works. Here δ_{np} is given by

$$\delta_{np} = \begin{cases} 2 - |I| & : N \text{ and } Z \text{ even} \\ |I| & : N \text{ and } Z \text{ odd} \\ 1 - |I| & : N \text{ even } Z \text{ odd, and } N > Z \\ 1 - |I| & : N \text{ odd } Z \text{ even, and } N < Z \\ 1 & : N \text{ even } Z \text{ odd, and } N < Z \\ 1 & : N \text{ odd } Z \text{ even, and } N > Z \end{cases} \quad (8)$$

It has been observed that in odd-odd nuclei, there is a difference between the proton-neutron interaction when the particles are particle or hole types. interaction between last odd proton and neutron has a attractive component when they are of similar type *i.e* when they are both particles or both hole). On the other hand this component is repulsive if the last odd particles are of different nature. Keeping this in mind, we have included the second term in the pairing interaction, called particle-hole pairing term for convenience. We define

$$\delta_{ph} = \begin{cases} 1 & : N \text{ and } Z \text{ both odd, both are particles or holes} \\ -1 & : N \text{ and } Z \text{ both odd, one particle and the other hole} \\ 0 & : \text{otherwise} \end{cases} \quad (9)$$

The Wigner term B_W , which we find to be very important, depends on I and appears in the counting of identical pairs in a nucleus. There are various forms for the Wigner term. Goriely *et al.*[27] assumed an Gaussian dependence on I^2 . Royer *et al.*[28, 29] suggested two terms, one in of the Gaussian form, $\exp(-\lambda I^2)$, and the other, $IA \exp(-A/A_0)^2$. In the first case, they assumed $\lambda = 80$. We have assumed this expression in this work, although other forms produce nearly identical results.

$$B_W = a_w \exp(-80I^2) \quad (10)$$

The valence neutron-proton terms, which are microscopic in nature, have been used in various works[25, 30] as well as in Ref I.

$$B_{np} = a_n N_n + a_p N_p + a_{np}^{(2)}(N_p + N_n)^2 + a_{np}^{(3)}(N_p + N_n)^3 + a_{np}^{(4)}(N_p + N_n)^4 + a_{np}^{(5)}(N_p + N_n)^5 \quad (11)$$

In B_{np} , N_p and N_n refers to the number of valence protons and neutrons. In the present work, the last two terms have been added. While evaluating the number of valence protons and neutrons, the magic numbers have been taken as 8, 20, 28, 50, 82, 126, 160 and 184. The only point worth noting here is the proposed neutron shell closure at $N = 160$ and will be discussed later.

The electronic binding energy is estimated by the empirical relation

$$B_{el}(\text{MeV}) = 1.44381 \times 10^{-5} Z^{2.39} + 1.55468 \times 10^{-12} Z^{5.35} \quad (12)$$

3 Results

The parameters of the formula in the previous section have been obtained in the procedure outlined in Ref I through fitting the experimental binding

energy data[23, 24]. A least square fit of experimental binding energies for 2353 nuclei with $N \geq 8$ and $Z \geq 8$ yielded the parameters in Table 1. There is one exception which has been discussed later.

Table 1: Values of various parameters for the binding energy formula obtained in the present calculation. The parameters k_v is dimensionless while r_0 is given in fm . The rest of the parameters are in MeV.

		α	\mathcal{N}_α^1	ϵ_α^1	\mathcal{N}_α^2	ϵ_α^2
a_v	12.381	1	8	0.1414	8	0.1832
a_{surf}	9.684	2	14	-0.0229	14	0.0249
k_v	1.839	3	20	0.0641	20	0.0959
W	-226.07	4	24	0.0273	24	0.0496
a_s	3.037×10^{-8}	5	28	0.0386	28	0.0405
r_0	0.815	6	32	0.0212	40	0.0289
a'_c	-9.022×10^{-3}	7	40	0.0086	44	0.0344
a_{pair}	6.252	8	44	0.0227	50	0.0223
a_{ph}	0.3141	9	50	0.0092	64	0.0199
a_n	-1.121	10	60	0.0142	74	0.0175
a_p	-1.017	11	64	0.0095	80	0.0134
$a_{np}^{(2)}$	4.605×10^{-2}	12	76	0.0124	82	0.0092
$a_{np}^{(3)}$	-1.654×10^{-3}	13	82	0.0043	86	0.0104
$a_{np}^{(4)}$	5.387×10^{-5}	14	88	0.0086	96	0.0066
$a_{np}^{(5)}$	-7.137×10^{-7}	15	122	0.0051		
a_w	-1.441	16	126	0.0067		
		17	134	0.0096		
		18	140	0.0099		
		19	160	0.0125 [†]		

$\epsilon_8^1 = 0.0176$ MeV for $Z \leq 34; N \geq 45$

$\epsilon_2^2 = 0.0507$ MeV and $\epsilon_3^2 = 0.0319$ for $Z \leq 22; N \geq 29$

[†] Calculated fitting alpha-decay energies in heavy nuclei.

As pointed out in Ref I, a large part of the total energy is included in the bunching term. Hence, substantial modifications in the conventional mass formula, and particularly in the values of the standard parameters, are only to be expected. A method was presented in Ref I to find a correspondence of the present formula with the standard LDM. We found that the parameters of a LDM mass formula devised from the present one fall within acceptable ranges. For example, the coefficient of the volume term, a_v obtained in Ref I was 11.890 MeV, a value much smaller than the standard values. However,

the corresponding value in the LDM formula came out as 15.289 MeV, within the accepted range for the parameter. We expect that the parameters of the LDM mass formula will also have parameters within the expected range for all the parameters.

The significance of the bunching term and the \mathcal{N}_α^i values have been discussed in detail in Ref I. It should be noted that there are a few differences in the \mathcal{N} values for protons and neutrons from Ref I in very heavy mass region. This is a consequence of the fact that most of the newly available mass values are for very heavy nuclei. Thus, for protons, $\mathcal{N} = 88$ has been replaced by 86. For neutrons, $\mathcal{N} = 96$ has been dropped while $\mathcal{N} = 132$ has been replaced by 134. Two new numbers $\mathcal{N} = 140$ and 160 has been introduced. The parameter ϵ in eqn. (2), corresponding to $\mathcal{N} = 160$, cannot be calculated from the available binding energy systematics and has been obtained from alpha decay energies as will be discussed later.

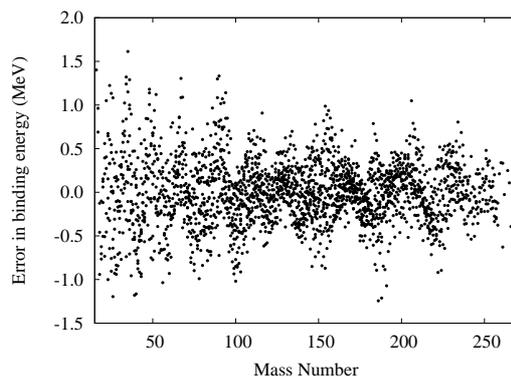


Figure 1: Deviations of binding energy for 2353 nuclei with $N, Z \geq 8$ from the predictions of the present formula.

The rms error in binding energies is 363 keV for 2353 nuclei. This is a significant improvement over the previous result of 376 keV for 2140 nuclei in Ref I. The total number of parameters, used to predict the binding energies of 2353 nuclei, is fifty one, one more than the previous version of the formula. There are 36 nuclei where error is 1 MeV. Only four of them lies in the region $A > 100$. Only in one nucleus the error is more than 1.5 MeV. In contrast, the results of the formula in Ref I had 39 nuclei with more than 1 MeV error in binding energy and 7 nuclei where the corresponding error was more than 1.5 MeV. The errors in binding energy for the present calculation are shown in Fig. 1 as a function of mass number.

To demonstrate the quality of fit, we have plotted our results for a number of elements ranging from very light to heavy, *viz.* O, F, Ca, Ni, Sn and Pb.

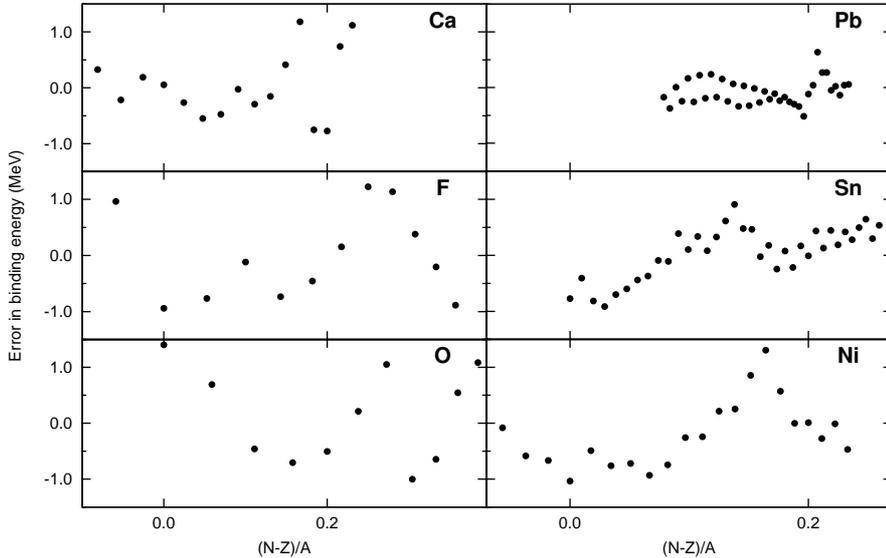


Figure 2: Deviations of binding energy for different isotopes of O, F, Ca, Ni, Sn and Pb.

The differences between the experimental measurements and prediction of the formula are plotted the errors as a function of $(N - Z)/A$ in Fig. 2. As we have already pointed out, the present formula provides a very good description, particularly beyond mass 100.

A major part of the improvement, particularly corresponding to the experimental data from AME2003[22] which were considered in Ref I, is due to the modification of the pairing term. We also note that the introduction of the new neutron magic number at $N = 160$ also plays an important role, obviously in very heavy nuclei. In Ref I, we found no evidence of any magic number beyond $N = 126$ except $N = 184$. However, in view of the new binding energy data in very heavy nuclei, the introduction of the new magic number at $N = 160$ improves the fit considerably decreasing the rms deviation from 369 keV to 363 keV for AME2012 data[23, 24]. The fact that $N = 160$ may be a new magic number is also supported by the alpha decay energy values predicted by this formula as discussed below.

All the magic numbers are of course expected to occur in the set of \mathcal{N} , as it represents shell effects. In view of this, we introduce an ϵ value corresponding to the neutron number 160 in eqn. (2). As the AME2012 data do not include any nuclei with $N > 160$, this value cannot be determined from the binding

energy data. However, alpha decay energies of superheavy nuclei above $N = 160$ are available and can be used to estimate the ϵ value corresponding to $N = 160$. The introduction of a new \mathcal{N} at 160 improves the alpha decay above mass 270 to a remarkable extent as indicated in Fig. 3.

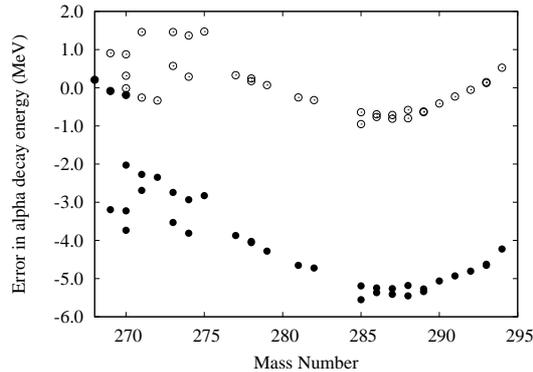


Figure 3: The effect of introducing a magic number at $\mathcal{N} = 160$ in errors in energy for alpha decays. Empty and filled circles indicate the errors in prediction of decay energy in presence and absence of the new magic number, respectively, in the formula. See text for details.

The introduction of the parameter discussed above takes the number of free parameters in the formula to 52. Though this appears to be quite large, one needs to consider that the number of data points that are being fitted is much larger. The justification for this purely phenomenological formula lies in the fact that, apart from the nucleon numbers, it requires no other input such as deformation, shell correction as used in most other works.

After the introduction of the fitted ϵ value corresponding to $N = 160$, the rms error in the predicted decay energies for 1175 alpha decay energies was found to be 299 keV. The differences between the experimental and calculated decay energies are shown in Fig. 4.

The effects of some of the new terms in the binding energy formula have also been studied and we present the salient points briefly. For this purpose, we modify only the relevant term, keeping others unchanged. As we have already stated, adding a new magic number at $N = 160$ decreases the rms deviation from 369 keV to 363 keV. Neglecting the last two terms in eqn. (11) increases the rms deviation to 368 keV and only the last term, to 365 keV. The particle-hole pairing term in eqn. (7) decreases the rms deviation by 2 keV. The effect of introducing the charge radius, rather than the radius, through the factor $(1 - I^2/4)$ in eqn. (5) is of the same magnitude.

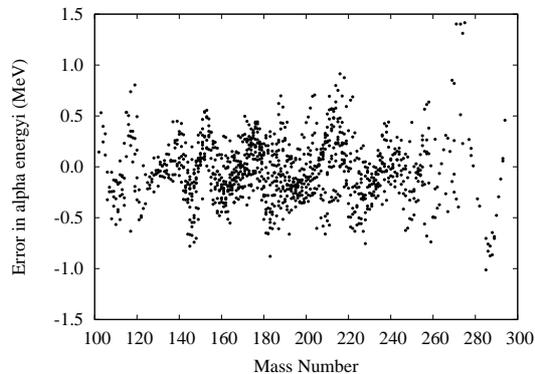


Figure 4: Errors in energy for 1175 alpha decays from the present formula.

4 Summary

The purely phenomenological formula of Ref I has been modified and the set of 52 parameters has been obtained by fitting the AME2012 values[23, 24]. Among the major modifications, the pairing prescription of Mendoza-Temis *et al.*[10] has been incorporated along with a term corresponding to pairing in odd-odd nuclei. A new magic number $N = 160$ has been introduced. The rms deviation for 2353 nuclei with $N, Z \geq 8$ is 363 keV.

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