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Revisiting Macro-microscopic Mass Formula using Atomic Mass Evaluation-2020 Data

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ABSTRACT

Background: The macro-microscopic model has been succesful in nuclear mass predictions and in obtaining various other properties of nuclear and nucleon matter. The present status of generalised liquid drop model (GLDM) has been based on atomic mass evaluation (AME)-2003 data..

Purpose: In this work, the co-ecients of most ecient mass formulae from Royer et.al., have been re-optimised for 2451 selected nuclei from AME-2020 data.

Methods: The root mean squared deviation (RMS) is minimized to optimize seven model parameters that correspond to various terms in the nuclear binding energy that come in powers of mass number A and square of relative neutron excess $I = \frac{N-Z}{A}$.

Results: The RMS between the theoretical and experimental binding energies has been obtained as 0.65 using both the formulae.

Conclusions: The best possible formula for nuclear binding energy has been obtained using AME-2020 data and it needs to be seen how this would eect the various nuclear properties and predictions.

1. Introduction

Bethe-Weizsacker mass formula[1-2] based on modeling of the nucleus as a charged liquid drop including asymmetry and pairing energies have been used to reproduce the nuclear masses using binding energies. But, in superheavy elements and near the proton and neutron drip lines, the binding energies of these nuclei are still not very accurately known [3]. So many other terms like coulomb diffuseness correction [4], charge exchange correction [5], different forms of Weigner energy term [6], shell effects [7], proximity energy [8] etc. are used to describe the masses, fission, fusion, cluster and alpha decay processes [9-11] more efficiently. ThomasFermi model has also been able to reproduce nuclear masses accurately [12]. Royer et al., [5] have arrived at the most efficient mass formulae to reproduce the most precisely known masses given in 2003 Atomic Mass Evaluation(AME) [13] data using different combinations of various terms. Even though different possible radii [14] are used to calculate the Coulomb energy term, the expression for radius given by $R_0 = 1.28A^{\frac{1}{3}} + 0.76 + 0.8A^{\frac{-1}{3}}$ as proposed in [8] and derived from the droplet model [15] is used here. Also, proximity energy is used, because these two terms work fairly well in both lower and heavier mass regions. In this work, we are re-optimizing the co-efficients of best mass formulae proposed by Royer [5] et.al., for the latest Atomic Mass Evaluation-2020 data [16]. The Coulomb diffuseness correction Z^2/A term or the charge exchange correction $Z^{\frac{4}{3}}/A^{\frac{1}{3}}$, are two terms which play main role to improve accuracy of the mass formula. So, these two combinations proposed by them are used to get the minimum Root Mean Squared (RMS) deviation between the theoretical and experimental binding energies(BE). The following nuclei have been taken into consideration while determining the theoretical BE.

- Nuclei with N, Z > 7 and
- Standard deviation in masses having value less than or equal to 150 keV

This resulted in a total of 2451 nuclei from AME-2020 data.

2. Methodology

2.1. Theoretical Binding Energies using Generalized Liquid Drop Model

Different studies have given different possible combinations of various energy terms of macro-microscopic mass formula to calculate the theoretical binding energies. The two best possible

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mass formulae with minimum RMS deviation, suggested by Royer et.al. are as mentioned in eqn1 and eqn2

$$B_{th} = a_v\left(1-k_v I^2\right)A - a_s\left(1-k_s I^2\right)A^{\frac{2}{3}} - \frac{3}{5}\frac{e^2Z^2}{R_0} + f_p\frac{Z^2}{A} - E_{shell} - E_{pair} - E_{wigner} \quad (1)$$

and

$$B_{th} = a_v\left(1-k_v I^2\right)A - a_s\left(1-k_s I^2\right)A^{\frac{2}{3}} - \frac{3}{5}\frac{e^2Z^2}{R_0} + a_{c,exc}\frac{Z^{\frac{4}{3}}}{A^{\frac{1}{3}}} - E_{shell} - E_{pair} - E_{wigner} \quad (2)$$

The only difference between eqn1 and eqn2 is in the fourth energy term with all other energy terms remaining the same. The various energy terms used in both the equations are as follows:

- I is the relative neutron excess given by

$$I = \frac{(N-Z)}{A}$$

- The first term corresponds to volume energy and asymmetry energy of Bethe-Weizsacker mass formula.
- The second term is the surface energy term. It takes into account the deficit of binding energy of the nucleons at the nuclear surface. The dependence of surface energy on relative neutron excess is given by the second part in this term which was not considered in the original Bethe-Weizscker mass formula.
- The decrease in binding energy due to the Coulomb repulsion is given by the third term. The radius of the nucleus R_0, that appears in the denominator of coulomb energy term, is considered as

$$R_0 = 1.28A^{\frac{1}{3}} - 0.76 + 0.8A^{\frac{-1}{3}} \quad (3)$$

  This has been derived from the droplet model so as to give best possible results for both lower and heavier mass regions.
- The Z^2/A term is the diffuseness correction to the basic sharp radius Coulomb energy term also called the proton form-factor correction to the Coulomb energy.
- The $Z^{\frac{4}{3}}/A^{\frac{1}{3}}$ is the charge exchange correction term.
- The theoretical shell effects obtained from TF model [17] have been used. They have been calculated from the Strutinsky [18] shell-correction method. We have taken the data from column 7 of Table, given in ref [17], directly for inclusion in our calculations.
- The pairing energy has been calculated with the following expressions used for spherical nuclei in the recent version [17] of the Thomas Fermi model:

$$\begin{aligned} E_p &= \frac{4.8}{N^{\frac{1}{3}}} + \frac{4.8}{Z^{\frac{1}{3}}} - \frac{6.6}{A^{\frac{2}{3}}} + \frac{30}{A}, && N = Z,\ odd \\ &= \frac{4.8}{N^{\frac{1}{3}}} + \frac{4.8}{Z^{\frac{1}{3}}} - \frac{6.6}{A^{\frac{2}{3}}}, && N\ \&\ Z - odd \\ &= \frac{4.8}{Z^{\frac{1}{3}}}, && N - even,\ Z - odd \\ &= \frac{4.8}{N^{\frac{1}{3}}}, && N - odd,\ Z - even \\ &= 0, && N\ \&\ Z - even \end{aligned} \quad (4)$$

- The Wigner energy allows to reproduce the kink in the nuclear mass surface. It depends on I and appears in the counting of identical pairs in a nucleus. Different expressions are considered. Royer has discussed the linear combination of four different forms given as, $W_1 = kw_1 |I|$, $W_2 = kw_2 |N-Z| e^{-(\frac{A}{50})^2}$, $W_3 = kw_3 |N-Z| e^{-(\frac{A}{35})}$, $W_4 = kw_4 e^{-80I^2}$. But in the best fitted mass formula only *W2* and *W4* have been considered and we are also considering the same two.

So in order to calculate the theortical binding energy given by eqn1, we have to optimize seven parameters which are a_v, k_v, a_s, k_s, f_p or $a_{c,exc}$, kw_2 and kw_4.

2.2. Optimization of Model Parameters

Theoretical binding energies have been determined by fitting the parameters so as to minimize the root mean squared deviation (RMS) [19], defined as

$$\sigma = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(BE_i^{\exp.} - BE_i^{th}\right)^2}\ MeV \quad (5)$$

Where $BE_i^{exp.}$ and BE_i^{th} are the experimental and theoretical binding energies and N is the number of nuclei considered in this work.

3. Results and Discussion

The total number of 2451 nuclei with N and Z > 7 and the standard deviation in masses having value less than or equal to 150 keV from Atomic Mass Evaluation-2020 data are used in this study. The values of optimized co-efficients and root mean square deviation(σ) (in MeV) between the

theoretical and experimental binding energies are shown in Table I. The Coulomb energy is determined by eqn6.

$$BE_c = \frac{0.6e^2Z^2}{1.28A^{\frac{1}{3}} - 0.76 + 0.8A^{\frac{-1}{3}}} \quad (6)$$

where the value of e^2 is substituted as 1.44 MeV. The charge exchange correction term and Columb diffuseness correction term which mainly effect the accuracy of the mass formula are used one by one to calculate the RMS value, while keeping all the other terms same. Although there are somewhat different values obtained for the co-efficients, but overall the RMS value remains same for both the terms, as can be seen from TableI. A similar result has also been obtained in [5] with formulae resulting in RMS value of 0.56 for a total number of 2027 nuclei. TableI gives the optimized co-efficients for best macro-microscopic mass formula, also called as the generalised liquid drop model (GLDM), with RMS devaiation of 0.65 for the latest 2020-AME data. It remains to be seen how our optimised parameters will perform when used over the same set of data as chosen in ref [5] for AME-2003 data.

Table I: Optimized co-efficient values and root mean square deviation (in MeV) between the theoretical and experimental binding energies for AME-2020 data table. The theoretical shell and pairing energies are taken into account.

a_v	k_v	a_s	k_s	f_p	$a_{c,exc}$	kw_1	kw_2	*RMSE (MeV)*
15.5019	1.8767	18.4914	2.0368	-	1.6661	0.4000	3.7447	0.65
15.7219	1.8686	18.4922	2.0379	1.7650	-	0.40001	3.7531	0.65

Conclusion

The best macro-microscopic mass formulae proposed by Royer et.al., for Atomic Mass Evaluation-2003 data have been re-optimised for 2451 selected nuclei from Atomic Mass Evaluation-2020 data. The root mean squared error is minimized to optimize seven model parameters that correspond to various terms in the nuclear binding energy that come in powers of mass number A and square of relative neutron excess $I = {}^{N}{}_{A}{}^{-Z}$. The effect of charge exchane correction term and Columb diffuseness correction term which mainly effect the accuracy of the mass formula along with pairing and shell energies have been studied. The root mean square deviation between the theoretical and experimental binding energies has been obtained as 0.65. The best possible formula for nuclear binding energy has been obtained using AME-2020 data which can be used to analyse changes in the various nuclear properties and predictions with the latest data.
data.

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Authorship Contribution

Swapna Gora: Data curation; formal analysis; investigation; methodology; resources; software; validation; visualization; writing-original draft. **S.K.Soni:** Discussions on methodology; supervision. **O.S.K.S. Sastri:** Conceptualization; formal analysis; investigation; methodology; project administration; resources; software; supervision; validation; visualization; writing-review & editing.

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Conflict of Interest

There is no conflict of interest whatsoever.

Declaration

The research work presented here is not published partially or in total, anywhere else, by me or someone else. It is our original work.

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