Energy and Deformation Signatures of Shell Evolution at N = 40, 50, and 58

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Introduction

Accurate prediction of nuclear masses is a cornerstone of nuclear structure theory, astrophysical modeling, and the study of nuclei far from stability. The Bethe–Weizsäcker (BW) mass formula provides a foundational macroscopic framework, yet its conventional form falls short in capturing local structural features, particularly near shell closures and in regions of large isospin asymmetry. Over the past decades, several refinements have been developed, introducing microscopic corrections such as pairing, shell effects, deformation, and isospin-dependent asymmetry terms [1-4]. Motivated by these developments and guided by the Fermi gas model, we propose a modified BW mass formula that includes an additional higher-order symmetry term proportional to $(N-Z)^4/A^3$. This term is designed to enhance the model's sensitivity to deformation and non-linear isospin effects, particularly in mid-mass and neutron-rich nuclei.

To test the efficacy of the proposed formulation, we apply it to the Zirconium (Zr) isotopic chain (N = 31 to N = 60), which encompasses the well-established magic number at N=50 and the previously suggested sub-shell closure near N=40 & 58 [5-8]. By analyzing binding energy per nucleon (B.E./A), two-neutron separation energies (S_{2n}), and their differentials (dS_{2n}), we demonstrate that the modified model captures essential shell features and yields improved agreement with experimental systematics.

Methodology

The starting point of our analysis is an augmented version of the BW mass formula, as reported by Xu et al. [9]. The model assumes a macroscopic-microscopic separation of the nuclear binding energy (B.E.):

$$\mathbf{BE}_{Xu\ et\ al.} = \alpha_v A + \alpha_s A^{\frac{2}{3}} + \alpha_c \frac{Z^2}{A^{\frac{1}{3}}} + \alpha_t \frac{(N-Z)^2}{A} + \alpha_{XC} \frac{Z^{\frac{4}{3}}}{A^{\frac{1}{3}}} + \alpha_w \frac{|N-Z|}{A} + \alpha_{st} \frac{(N-Z)^2}{A^{\frac{4}{3}}} + \alpha_p \frac{\delta(N,Z)}{A^{\frac{1}{2}}} + \alpha_R A^{\frac{1}{3}} + \alpha_m p + \beta_m p^2 + \frac{b(N-Z)^4}{A^3} \quad (1)$$

where the coefficients are (in MeV) as follows:

α_v	α_s	α_c	α_t	α_{XC}	α_w
16.58	-26.95	-0.774	-31.51	2.22	-43.40
α_{st}	α_p	α_R	α_m	β_m	b
55.62	9.87	14.77	-1.090	0.140	-1.30

To improve predictive accuracy, we introduced deformation corrections through a multiplicative factor accounting for quadrupole (β_2) and hexadecapole (β_4) [10] components:

$$\mathbf{BE}_{modified} = \alpha_v A + \alpha_s A^{\frac{2}{3}} + \alpha_c \frac{Z^2}{A^{\frac{1}{3}}} + \alpha_t \frac{(N-Z)^2}{A} + \alpha_{XC} \frac{Z^{\frac{4}{3}}}{A^{\frac{1}{3}}} + \alpha_w \frac{|N-Z|}{A} + \alpha_{st} \frac{(N-Z)^2}{A^{\frac{4}{3}}} + \alpha_p \frac{\delta(N,Z)}{A^{\frac{1}{2}}} + \alpha_R A^{\frac{1}{3}} + \alpha_m p + \beta_m p^2 + \frac{b(N-Z)^4}{A^3}\left(\beta_2^2 + \beta_4^2\right) \quad (2)$$

where the coefficients are taken same as of Eq. 1, except b selected as -0.22 MeV for Eq. 2.

To analyze nuclear shell structure, we also calculate several key observables [12-18]:

(i) $\mathbf{S_n(Z,N) = BE(Z,N) - BE(Z,N-1)}$

(ii) $\mathbf{S_{2n}(Z,N) = BE(Z,N) - BE(Z,N-2)}$

(iii) $\mathbf{dS_{2n} = \frac{S_{2n}(Z,N+2) - S_{2n}(Z,N)}{2}}$

(iv) The goodness of fit was assessed using the RMSD [9] of the extraction from the measured binding energies as follows:

$$\mathbf{RMSD} = \sqrt{\frac{\sum_i (M_i - F_i)^2}{n}},$$

Where M_i denotes the theoretical value, F_i is the experimental value, and n is the total number of data points.

Results and Discussion

The modified mass model was applied to Zr isotopes (Z=40) across neutron numbers N=31 to N=60. The calculated binding energy per nucleon (BE/A) exhibits a peak at N=50, confirming the canonical shell closure which is shown in **Fig. 1**. Local maxima are also evident at N=40 and N=58, suggestive of subshell structures.

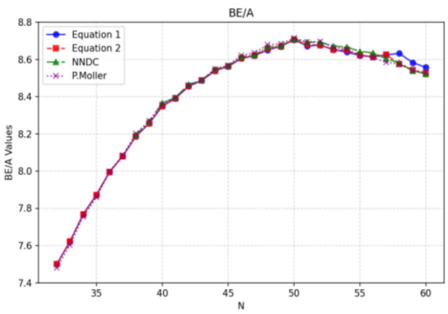

Fig. 1: The graph between B.E./A verses Neutron number of Zr isotopes (Z=40). The data of NNDC and P. Moller taken from [10, 11].

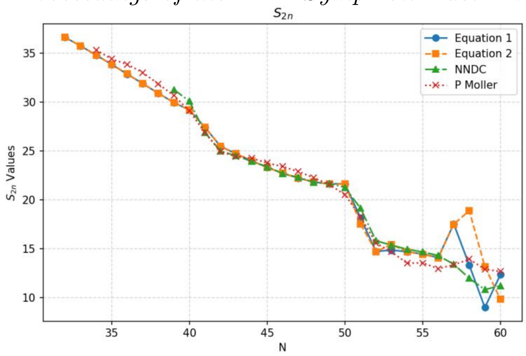

Fig.2: The graph between two neutron separation energy verses neutron numbers of Zr isotopes (Z=40).

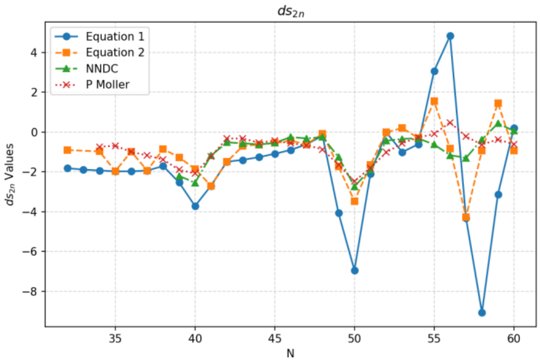

Fig.3: The graph between dS_{2n} verses neutron numbers of Zr isotopes (Z=40).

Two-neutron separation energies (S_{2n}) show pronounced drops at N=50, and slope changes at N=40 and N=58, which is shown in **Fig. 2**. The differential separation energies dS_{2n} also exhibit noticeable discontinuities at these neutron numbers which is shown in **Fig. 3**, reinforcing the shell or subshell effects. The consistent appearance of these signatures in multiple observables supports the physical significance of these shell structures.

To quantitatively assess the predictive power of both models (Eq. 1 & 2), root-mean-square deviation (RMSD) values were calculated by comparing the theoretical and experimental binding energies. The RMSD for Equation 1 (with fermi energy) is found to be 5.985, whereas the RMSD of our modified Equation 2 (including deformation corrections) is 5.706. This reduction demonstrates that the inclusion of deformation parameters improves the accuracy of the mass formula.

Conclusion

In this study, we have proposed an improved semi-empirical mass formula by incorporating higher-order isospin asymmetry and deformation-dependent corrections into the extended Bethe–Weizsäcker framework. The modified model, which includes a quartic $(N-Z)^4/A^3$ term and a deformation factor proportional to $\beta_2^2+\beta_4^2$, was systematically applied to Zr isotopes across the neutron-rich region.

The calculated observables: binding energy per nucleon (B.E./A), one and two-neutron separation energies (S_{1n}, S_{2n}), and differential separation energies (dS_{2n}) exhibit pronounced signatures of shell or subshell closures at N=40, the traditional magic number N=50, and the proposed subshell closure at N=58. These features are consistent with experimental trends and theoretical expectations [5-8, 11], affirming the physical relevance of the introduced deform corrections. A comparative analysis of root-mean-square deviations demonstrates that the deformation-enhanced model (Equ. 2) offers improved predictive accuracy over the simpler quartic isospin formulation (Equ. 1), with RMSD values of 5.706 and 5.985, respectively. This improvement highlights the importance of incorporating deformation effects into macroscopic mass models, especially for transitional and mid-shell nuclei.

Overall, the findings validate the extended formalism as a meaningful step toward bridging macroscopic mass models with local structural phenomena. Future work will involve applying this approach to other isotopic chains and integrating microscopic deformation inputs for improved global reliability.

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