An Investigation of the Accuracy of the Semi-Empirical Mass Formula and Binding Energies

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1. Background

From Ernest Rutherford, to Niels Bohr, to Erwin Schrödinger have physicist sought to understand the strange world of the atom. In exploring the various properties governing the laws of the atomic and subatomic world, it was understood that atomic nuclei made up individual constituents (protons, neutrons, and electrons) had been forged deep within stellar furnaces, continually smashing these particles together creating the very elements we observe in the modern age. It is this simple idea, transmuting seemingly fundamental building blocks found within nature into every piece of matter that surrounds us, that suggests the question: How does nature do it? What follows is a detailed investigation of binding energy and its empirical cousin, the Carl Friedrich von Weizsäcker mass formula, named after the physicist himself, and its accuracy to observations made within nature.

Binding energy is to be understood as the energy that keeps an atomic nuclei together, and thanks to the pioneering work of early 20th century physicist, can be calculated in the following simple manner:

$$\mathrm{BE} = [\ Z \cdot m_H + N \cdot m_N - \text{ Atomic Mass }]\, c^2$$

The fascinating complexities one finds within the details of this rather simple equation is the suggestion that binding energy is the physical process of mass-energy transfer. It fits, then, that by convention the measurement of an atom's binding energy should always be positive, as the rise of a negative binding energy would infer the continual use of energy to keep the atom together rather than tear it apart. This is an important assumption for which I based my calculations upon, as the nonphysical quantity negative binding energy provides can be ignored. Understanding binding energy provides key insight into the nuclear structure itself, which in turn served as the basis for Weizsäcker to begin his journey to understand the nature of binding energy in his own terms.

2. History of the Semi-Empirical Mass Formula

The semi empirical mass formula has its roots embedded within early 20th century nuclear physics, specifically the new line of thinking (at the time) that nuclei could be though of as incompressible drops of liquid - thus, the liquid drop model was born [1]. Early pioneering physicist suggesting this liquid drop model view of atomic nuclei, namely George Gamow and Niels Bohr, blazed the trail for eventual contemporary Weizsäcker to propose his theory of an alternative to traditional thought to be the energy in the binding of a nucleus. In 1935, Weizsäcker, along with his colleague Hans Bethe, published what would later be known as the Weizsäcker-Bethe formula, or semi-empirical mass formula [1]. In its full glory:

$$\mathrm{BE} = a_{vol}A + a_{surf}A^{2/3} + a_{coul}Z(Z-1)A^{-1/3} + a_{sym}\frac{(N-Z)^2}{A} + a_{pair}A^{-3/4}$$

3. Investigation

What prompts my exploration of the semi-empirical mass formula (SEMF) is the motivation to discover previously unknown complexities for my personal understanding that otherwise appear superficial masked in the terms of the equation. The start of my investigation begins with the most basic of question pertaining to fundamental nuclear physics, in that the nuclear makeup and arrangement of the nuclear constituents. A logical first step is to explore nuclear makeup of the 3,167 nuclear isotopes provided by the Nation Nuclear Data Center (NNDC) [2], namely the number of either nucleon as the other increases, otherwise coined as the “line of stability” graph.

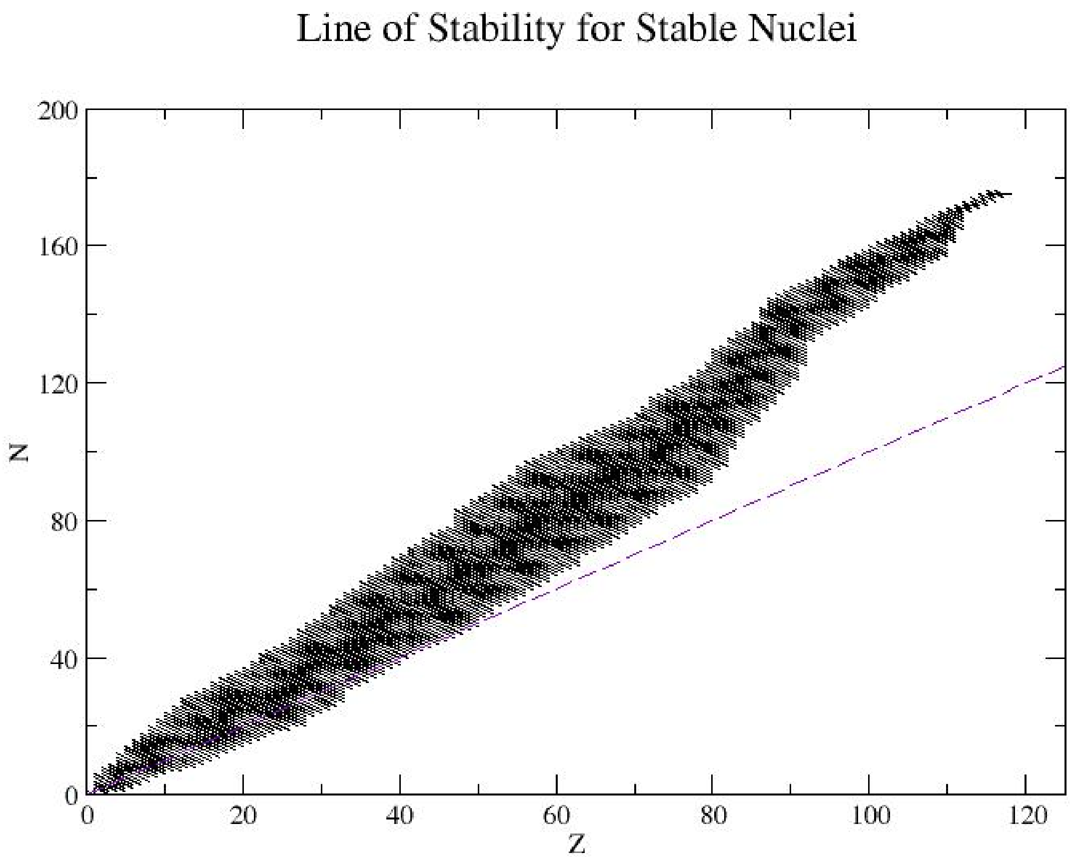

Figure 1: Line of stability graph generated from NNDC data of 3,167 isotopes

The peculiarities in the line of stability graph become quite prevalent in the heavier nuclei, namely Z > 60. What the data suggests is larger deviations for heavy nuclei away from the line of stability: what physical processes in nature account for such curvature bending away from the stability line? Delving further, another question that may be of interest is the fit of binding energy per nucleon in comparison to the beloved graph commonly referenced in nuclear chemistry and physics while computing the graph using the SEMF. [3]

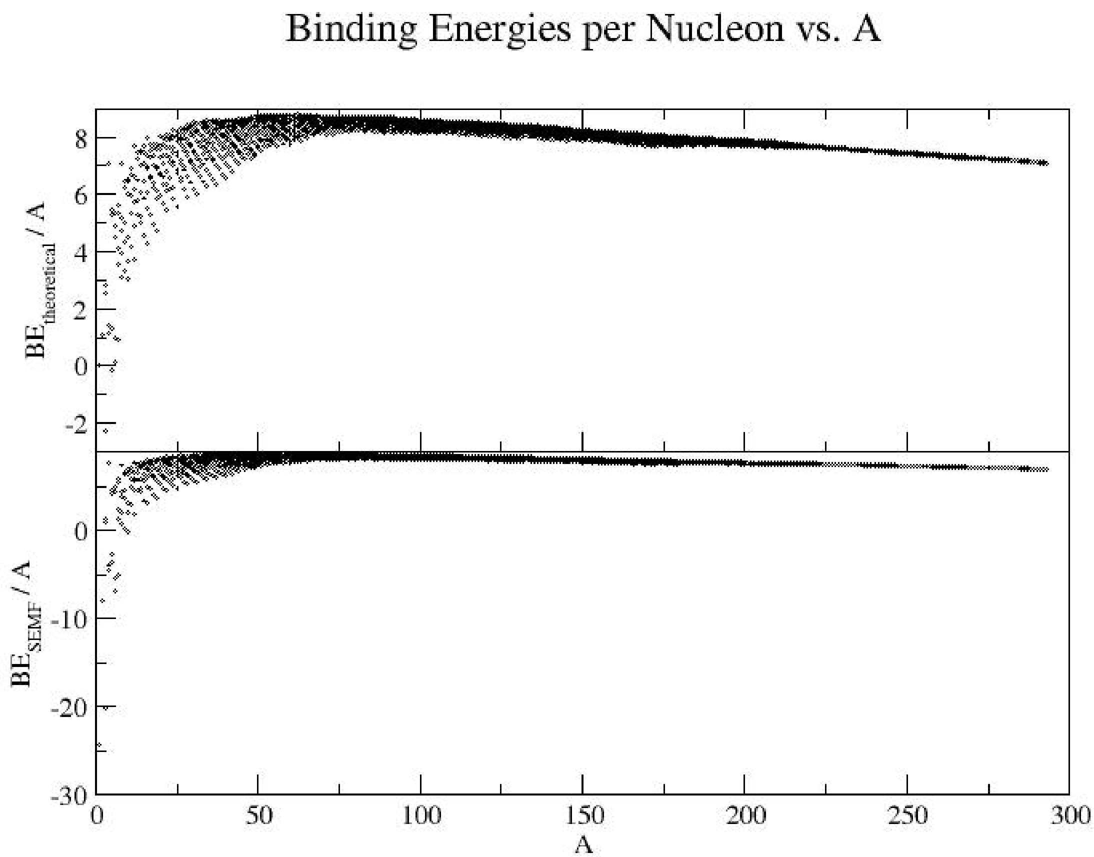

Figure 2: Binding energy per nucleon vs. A for theoretical and SEMF calculations

Examining either graph, one notes the incredible match in structure the SEMF has when compared to theoretical values of binding energies for heavy nuclei. Although, what becomes apparent is the approximate 6 MeV difference when comparing the two graphs. Should such a difference exist, the question of the absolute accuracy of the SEMF comes into play, in particular for light nuclei approximation. A natural succession in the investigation of the SEMF is examining the effect of each energy term in the equation. Even more interesting, one may discern, are the individual effects of the SEMF energy terms in their derivatives with respect to A: what would be implied by the result?

Next, natural curiosity brought forth the question of the various derivatives of the SEMF, with hopes of providing insight on the effect on the equations of varying nuclear properties would have. Due to the pairing term, three derivatives were calculated due to the variance the pairing term takes on depending on odd values of A along with even and odd values of Z and N. For graphing the derivatives, the following was used:

Differentiating the SEMF with respect to A,

$$\frac{\partial \mathrm{BE}}{\partial \mathrm{A}} = a_{vol} + \frac{2}{3}A^{-1/3} - \frac{1}{3}a_{coul}Z(Z-1)A^{-4/3} - a_{sym}\frac{(N-Z)^2}{A^2} - \frac{3}{4}a_{pair}A^{-7/4}$$

where

$$a_{pair} = \begin{cases} -34 \text{ MeV} & \text{for Z, N odd,} \\ +34 \text{ MeV} & \text{for Z, N even,} \\ 0 \text{ MeV} & \text{for A odd,} \end{cases}$$

A modular division technique was used to sort the derivatives in terms of odd pairings of N, and Z and even/odd A:

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IF ( MOD(Z(j),2) == 0 .AND. MOD(N(j),2) == 0 ) THEN
pairing_A = 34.

ELSE IF ( MOD(Z(j),2) == 1 .AND. MOD(N(j),2) == 1 ) THEN
pairing_A = -34.

ELSE IF ( MOD(A(j),2) == 1 ) THEN
pairing_A = 0.

END IF
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Graphing the various derivatives of A for the fluctuating conditions a_{pair} yields the following graphs. From the graphs, it is observed that the asymptotic behavior of each derivative for large A appears similar in each calculation.

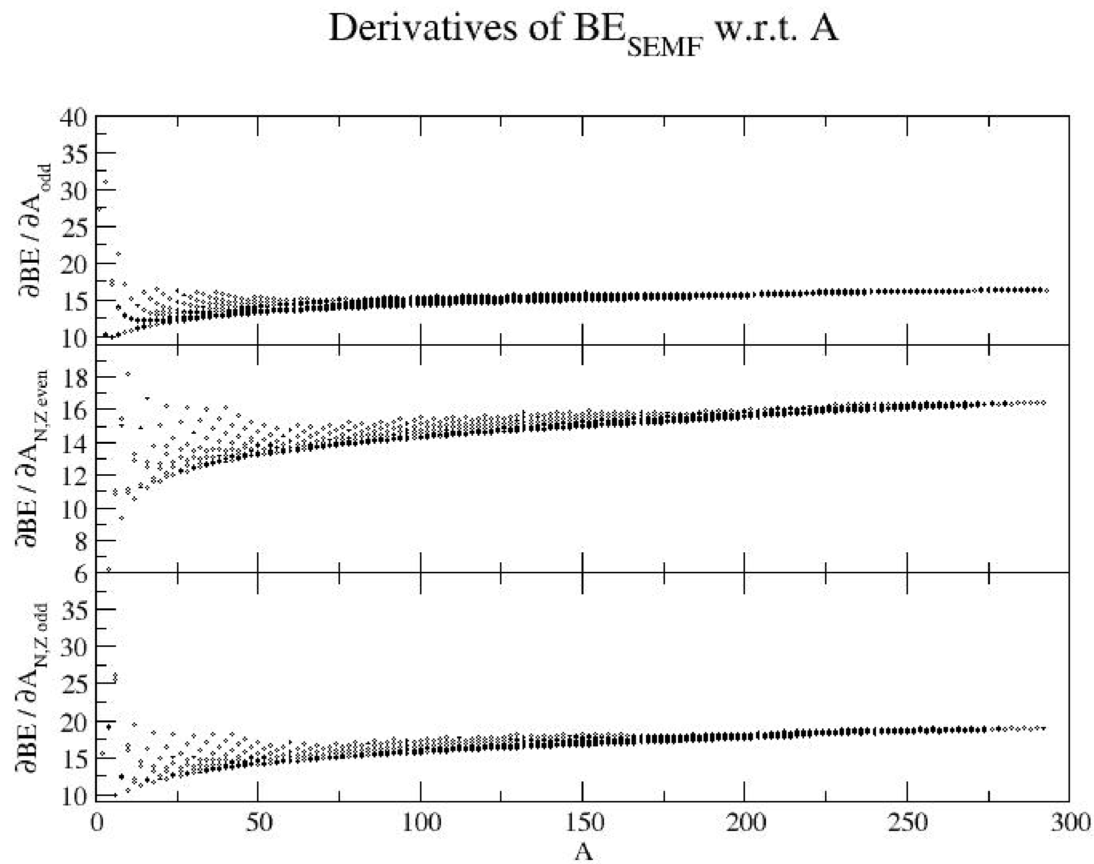

Figure 3: Derivatives taken with respect A for each value of the pairing term.

The structure of the derivative graphs present interesting information: there seems to be a logarithmic, near asymptotic, approach a stabilizing binding energy around 15 MeV/nucleon. The interpretation of this result is the positively branching off the derivatives approach, which suggests an increasing binding energy as nucleon number increases. Next, in graphing the derivatives of the SEMF with respect to Z and N, the same asymptotic structure appears:

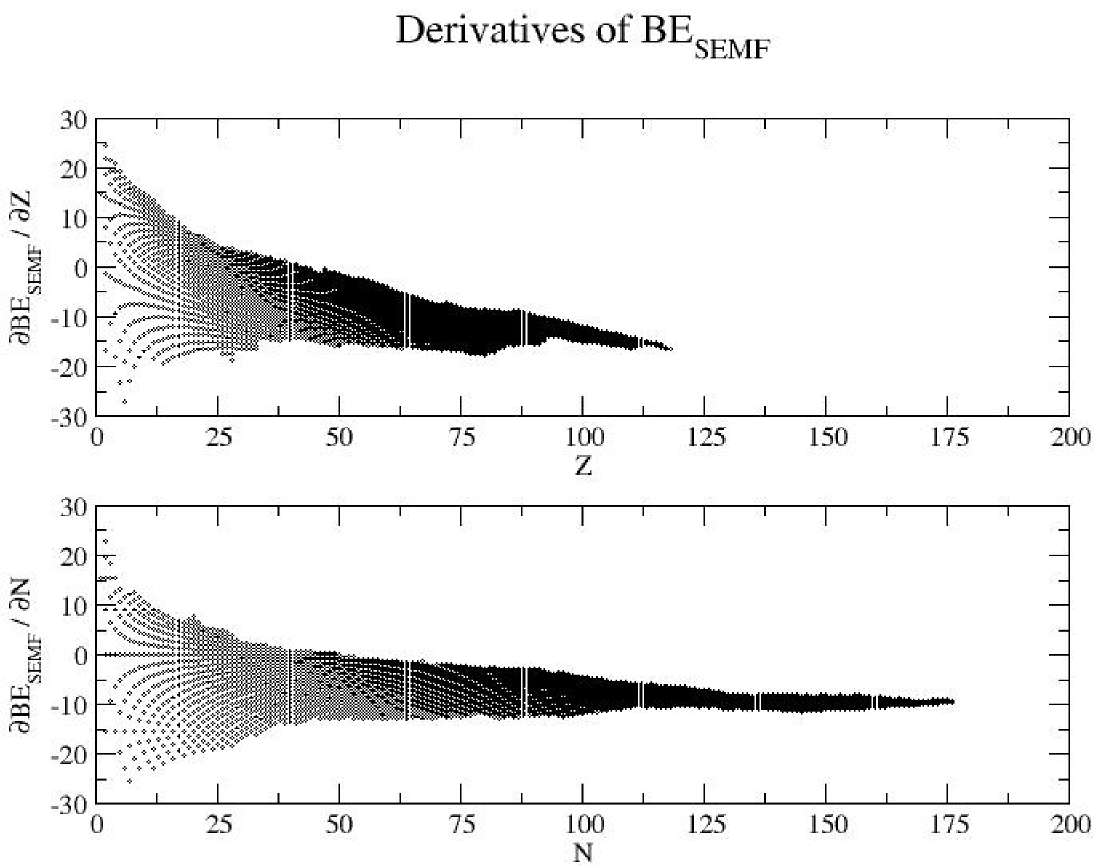

Figure 4: Derivatives of the SEMF with respect to Z and N

Again, as we observe the leveling off of the derivative seemingly approaching a finite number, some questions are raised. Obtaining derivatives of the SEMF with respect to Z and N yields the result,

$$\frac{\partial \mathrm{BE}}{\partial \mathrm{Z}} = a_{coul}(2Z-1)A^{-1/3} - \frac{2a_{sym}}{A}(N-Z)$$
$$\frac{\partial \mathrm{BE}}{\partial \mathrm{N}} = \frac{2a_{sym}}{A}(N-Z)$$

What strikes me immediately is the isochrone lines that light nuclei seem to follow, eventually plunging asymptotically with the group to the -10 MeV/nucleon value. What this data seems to suggest is the trend, possibly for particular decays of similar isobars, that follow predetermined decay paths while increasing the number of protons or neutrons in their nucleus. Noticeably, the derivatives of N and Z appear to approach values of -10 MeV/nucleon, but when comparing this to the derivative with respect to A, we notice the slow approach to 15 MeV/nucleon. If my interpretation of this result is correct, it would suggest that while increasing the number of nucleons *on the whole*, i.e. increasing the number of neutrons and protons simultaneously, binding energy is increased.

In contrast, increasing neutron number <u>or</u> proton number while holding the other constant, as observed in several decay modes discussed in class such as $\beta^{\pm}$-decay and γ-decay, the binding energy decreases. It seems as though the data suggests that certain decays *should* happen, as changing proton or neutron number decreases the binding energy allowing the decay to happen in the first place. Again, this is my personal interpretation of this result.

In examining the binding energy difference between the SEMF and the classical formulation, the most striking and perhaps astounding result arises, in that the peculiar peaks formed coincidentally around the nuclear magic numbers. This would seem to suggest that perhaps Gamow's model of the liquid drop, while being an incredible insight to early nuclear physics, was an approximation to the physical structure; a shell model structure, which gives rise to the magic numbers, seems to align closely with predictions made by the SEMF as represented graphically below. What is peculiar about the nature of this graph is the interpretive power it provides in *predicting* simple magic numbers, indicating closed shells in the nucleus. The interpretation of each peak is the local maximum of binding energy difference for a particular nuclei, or the local error maximum in the SEMF when compared to the theoretical outcome. This peak, or local maximum, in binding energy difference, as I elucidate, suggests the within the nucleus, certain values of A (magic numbers) reach a binding energy maximum for that particular configuration where the nucleus is prone to become less bound. Thus, new shells are created by the nucleus to ensure lower energy states may become occupied and allow the nucleus to dodge the danger of becoming less bound.

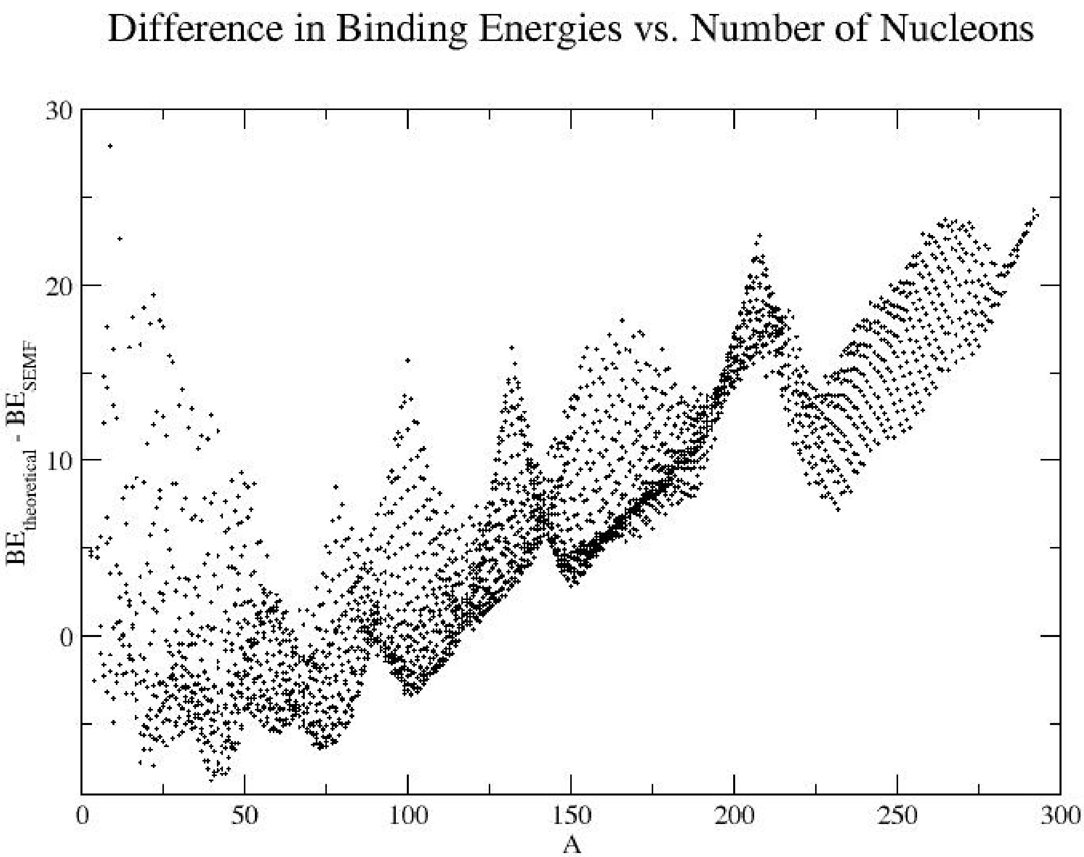

Figure 5: Graphical representation of the binding energy difference plotted against increasing value of A.

The scatter of binding energy differences for lighter nuclei seem inconclusive with data by just looking at the graph, as their seems to be a trend of peaking around 50 as predicted from the shell model. To obtain a better view of this peaking, I have binding energy differences for Z, N, and A below. These peaks, however, lie closely with predicated magic numbers of 50, 82, and 126 with suggestions of *another* magic number just past 200. These, however, only give the clear picture for heavier nuclei with A > 50. To obtain the full picture, we examine the graph of all three binding energy differences.

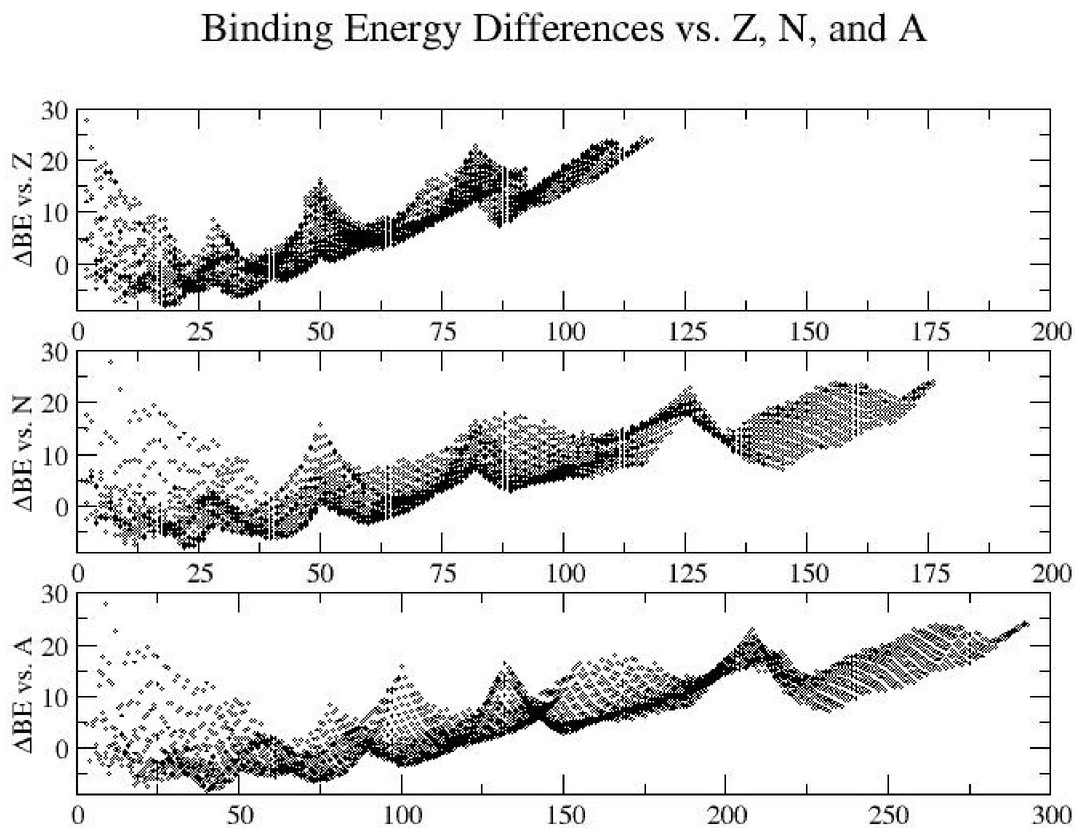

Figure 6: Binding energy differences graphed against various nuclear properties.

As the graphs suggest, clear peaks at 50, 82, 100, and 126 become easily recognizable. For light nuclei, however, the data presents too much spread to accurately interpret graphically from numerical calculation in this brief investigation. Looking closely at the binding energy difference versus nucleon number, though, seems to suggest a mysterious number just past 200 for another closed shell.

4. Conclusion

After investigating the SEMF to an intermediate extent, it is clear that its accuracy is closely aligned with theoretical binding energies predicted in nature. The power of the formula, although, lies in its exploration of derivatives and comparison to the theoretical calculations, as mentioned earlier with the suggestion of binding energy increase/decrease with various nucleons and magic numbers. It is prevalent that further studies could be done to fully investigate some of the lingering questions tied to the SEMF, such as the investigation of the effect of each term to obtain a higher accuracy with the refinement of the experimental constants.

References

[1] D. Kleppner, "A short history of atomic physics in the twentieth century," *Rev. Mod. Phys.*, vol. 71, pp. S78–S84, Mar 1999.

[2] J. Jänecke and T. W. O'Donnell, "Symmetry energies, pairing energies, and mass equations," *Nuclear Physics A*, vol. 781, pp. 317–341, Jan. 2007.

[3] G. Audi, C. Thibault, and A. H. Wapstra, "Atomic mass adjustment," *National Nuclear Data Center*, Dec. 2003. Table of tabulated masses.