The appearance of a superheavy nucleus: Investigating shape-dependent nuclear stability

Zara Andhyarujina

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Abstract: Superheavy elements have been widely researched for years. Known to be extremely unstable, their nuclei have half-lives of mere milliseconds. Several shapes have been extrapolated for which the nuclei could be more stable. Two of these include the sphere and torus. By identifying the most stable shape of a superheavy nucleus, new forms of energy could be provided and new discoveries made. This paper compares the stability of the spherical nuclei and the toroidal nuclei of elements with different atomic numbers, ranging from 300 to 500 using Python through established numerical methods such as Rejection Sampling and Poisson Disc Sampling. This paper concludes that the stability of the toroidal nuclei of elements with atomic numbers ranging from 300 to 500 is higher than

that of the spherical nuclei.

1 INTRODUCTION

Several years have been dedicated to the investigation of the most stable shape of the nucleus of a superheavy element. Identifying this shape and the resultant stability of the nucleus could lead to several developments in technology and nuclear science, as well as pave the way for new discoveries and provide new forms of energy. Such energy could be used to replace the conventional forms of providing energy like coal or wood. This could thus help us as humans to be more sustainable.

The elements with an atomic number equal to or larger than 104 [1] are known as superheavy elements. They allow the exploration of the island of stability, an area of proposed long-lived superheavy elements that still awaited discovery were located here and “magic numbers” of nucleons, which would provide for a stable nucleus, which are useful in understanding why some nuclei may be more stable than others [2]. The island of stability is known as a set of isotopes of superheavy elements predicted to have considerably longer half-lives [3]. These nuclei with magic numbers [4] have several configurations extrapolated such as bubble nuclei [5], toroidal [6], pear nuclei [7] and band-like nuclei [8] along with the already known spherical shape of nuclei.

The stability of an atomic nucleus is affected by different forces. These forces are the Coulomb force [9], the strong nuclear force [10] ,and the weak interaction force [11]. The number of nucleons and the neutron-proton ratio [12] also affect the stability of the nucleus. Many possible nuclear configurations and forces are distance-dependent, which thus makes stability difficult to assess. When a nucleus is not stable, decay would occur primarily by α decay (the emission of α particles) as well as spontaneous fission caused by electrostatic repulsion. β decay (the emission of electrons) is usually caused by the weak interaction force [13]. Both types of decay would change the number of protons in the nucleus, thus changing that atom to a different element.

This paper first explores the known literature on this subject and then describes the process of simulating a superheavy nucleus. Data was generated through rejection sampling to determine the number of particles in each shape, using Poisson Disc Sampling to help create randomised positions of nucleons. In the end, the two forces were defined and the results of the shape-dependent stability for different atomic numbers are calculated through a stability metric using the dot product.

2 LITERATURE REVIEW

2.1 The Stability of Nuclei

2.1.1 Forces

The nucleus consists of protons and neutrons held together by forces which are the Coulomb force, the nuclear strong force and the weak interaction force. It is important to note that force vectors are additive. Taking an example of three particles, the force on one particle will be equal to the sum of the forces applied by the other two particles.

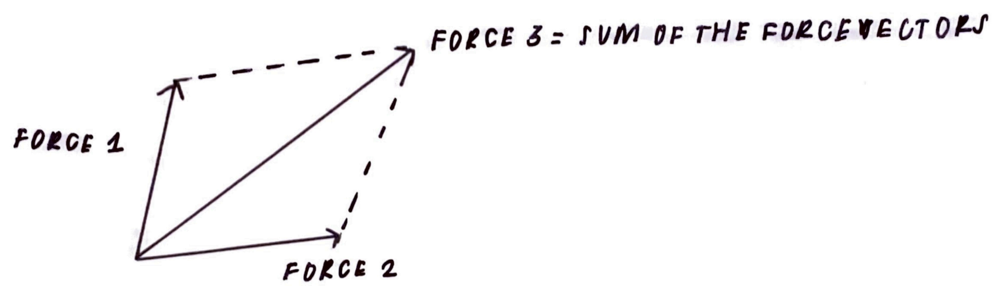


Figure 1: A diagrammatic representation of the additive property of force vectors.

The Coulomb Force: The Coulomb force can be defined through the Coulomb law as the force of attraction or repulsion acting along a straight line between two electric charges is directly proportional to the product of the charges and inversely to the square of the distance between them [15]. Since protons are positively charged, they are affected by the Coulomb force (the attraction or repulsion due to the electric charge of a particle). However, neutrons, being neutral particles, are not. The magnitude of this force (F) can be described using the following formula where k_e = Coulomb constant, q_1, q_2 = charges, r = distance of separation. Here $k = 8.988 \times 10^9\ \mathrm{N\,m^2\,C^{-2}}$.

$$F = k_e \frac{q_1 q_2}{r^2} \tag{1}$$

The Strong Nuclear Force: The strong nuclear force is responsible for holding the neutrons and protons together to form an atomic nucleus. It is partly responsible for the stability of the atom. Even though the strong nuclear force is one of the strongest fundamental forces, it acts over a short range of 10^{-15}m. All nucleons are affected by the nuclear strong force. This force also prevents the electrostatic repulsion from causing the protons to fly apart. The strong force can be approximately described by the Reid Potential along the line between two nucleons where $\mu = 0.7\ fm^{-1}$ and the potential is given in MeV.[15].

$$V_{\text{Reid}}\left(r\right) = -10.463\frac{e^{-\mu r}}{\mu r} - 1650.6\frac{e^{-4\mu r}}{\mu r} + 6484.2\frac{e^{-7\mu r}}{\mu r} \tag{2}$$

As the Reid Potential has been expressed in MeV while the Coulomb Force is expressed in $\mathrm{N\,m^2}$ .To resolve this, the Reid Potential is first converted to units of joules, which is the SI Unit of Potential Energy. By dividing the strong force expressed through the Reid Potential, it returns a new value, the Reid Force which is in $\mathrm{N\,m^2}$.

The Weak Interaction Force: The weak interaction force is a fundamental force of nature that underlies some forms of radioactivity, governs the decay of unstable subatomic particles such as mesons and initiates the nuclear fusion reaction that fuels the sun [11]. All nucleons are affected by the weak interaction force. Just like the strong nuclear force, this force only acts over a short range of around 10^{-17} m to 10^{-16}m. However, this force is not considered as it is inconsequential to the

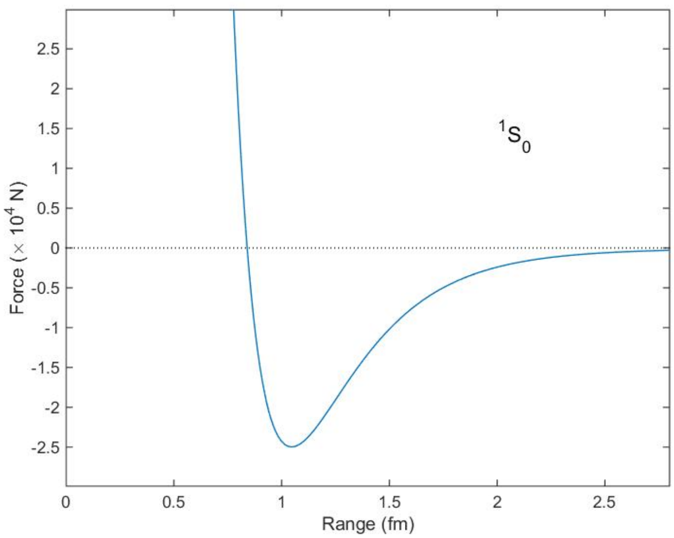


Figure 2: Through this graph, we can see that the strong force is attractive at distances of 1 fm or greater. This graph has been taken from [16]

calculations due to its relatively small magnitude compared to the other forces.

2.1.2 Number of Nucleons

The neutron-proton ratio is also an important factor that plays into the stability of the nucleus [12]. The more the number of protons in the nucleus, the higher the number of neutrons required to maintain the stability of the nucleus. Too many protons (or too few neutrons) in the nucleus can result in an imbalance between forces. This is because it results in too high of a charge concentration, which leads to the domination of the Coulomb force. Thus, this can cause the atom to be ripped apart, leading to nuclear instability. Stable nuclei are mostly known to have even numbers of both protons and neutrons and a neutron-to-proton ratio of at least 1, however, it can differ from element to element.

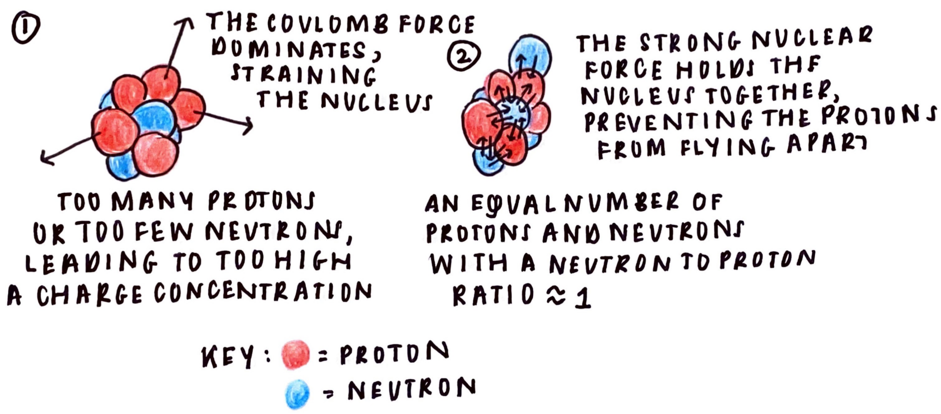


Figure 3: A diagrammatic representation of the impact of the number of nucleons on nuclear stability. In 1, too many protons or too less neutrons leads to a high charge concentration, which leads to the domination of the Coulomb force. In 2, an equal number of protons and neutrons with a neutron-to-proton ratio of approximately 1 leads to stability. The strong nuclear force prevents the Coulomb force from causing the protons to fly apart.

2.1.3 The Island of Stability

The stable isotopes are hypothesised to be found in the "Island of Stability." This has now been explained as a set of isotopes of superheavy elements predicted to have considerably longer half-lives than the known isotopes of these elements. It was also proposed that long-lived superheavy elements that still awaited discovery were located here [3]. This would be because these elements would have "magic numbers" of protons and neutrons, which would provide for a stable nucleus. Magic numbers are those number of nucleons (either protons or neutrons) that can be arranged into complete shells within the atomic nucleus [4]. These numbers are 2, 8, 20, 28, 50, 82, and 126 which correspond to Helium, Oxygen, Calcium, Nickel, Tin, Lead and Unbihexium (a hypothetical element).

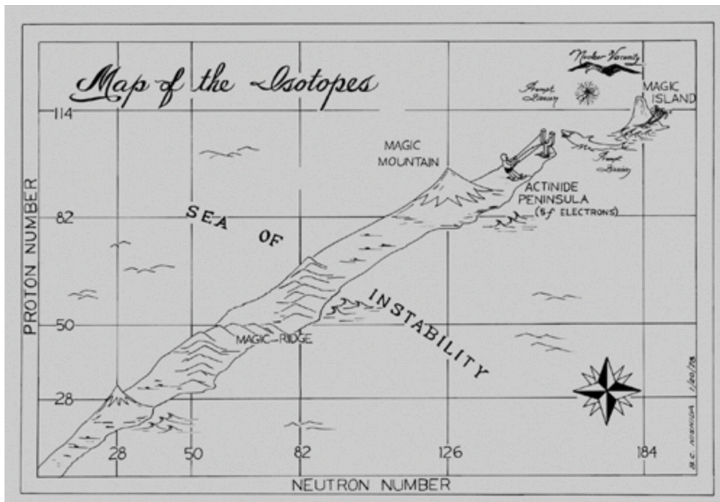


Figure 4: "Map of the isotopes, showing the 'magic island' of stability, drawn for Glenn Seaborg by B.C. Nishida in 1978. The 'magic mountain' shows the increased stability of lead compared with the rest of the elements." - *Superheavy, K. Chapman*

2.2 Known and Theorised Shapes of the Nuclei

Apart from the well-known spherical shape of the nucleus, several other shapes of nuclei have been observed, including the derivative spherical, triaxial [?] and reflection asymmetric (pear-like) shapes [7]. Several exotic shapes of the nuclei have been extrapolated, including shapes such as bubble [5], toroidal [6] and band-like [8]. Not much is still known about the nuclei of these shapes. Different studies and research have different outcomes, however, it is clear that they all support the idea that the nucleus of superheavy elements may be stable in a non-spherical shape.

For example, toroidal nuclei were claimed as stable shapes in a theoretical analysis done in 2021 by S. E. Agbemava and A. V. Afanasjev, shown in Figure 5[18]. This paper establishes the general trends in the evolution of toroidal shapes in the Z≈130–180 region of the nuclear chart and discusses ”fat” and ”thin” toroidal nuclei shapes.

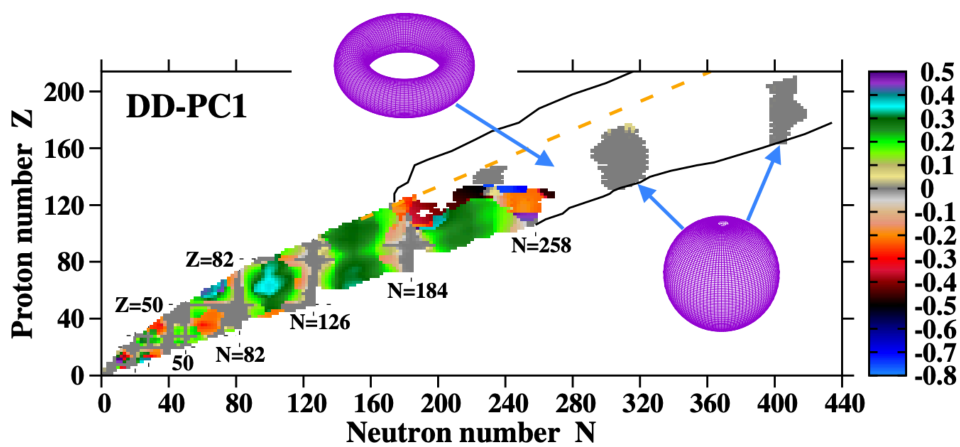


Figure 5: The toroidal shape of nucleus as discovered by S. E. Agbemava and A. V. Afanasjev.

Figure taken from [18]

However, experiments in 2013 discovered that certain heavy unstable atomic nuclei were distorted into a pear shape [19] as shown in Figure 9. This could also imply that the stability of superheavy nuclei could be better suited as ’octuple deformed’ i.e., pear-shaped.

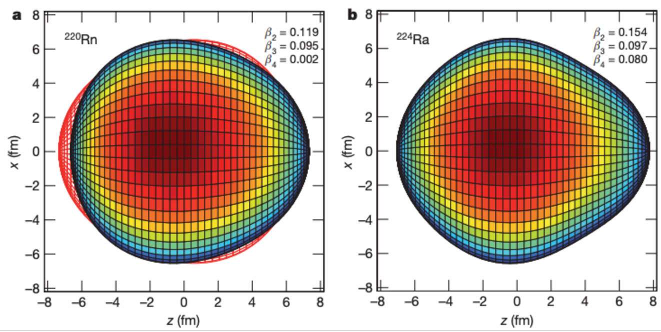


Figure 6: Graphical representation of the shapes of ^{220}Rn and ^{224}Ra, where a represents ^{220}Rn and b represents ^{224}Ra Figure taken from [19]

3 SIMULATIONS

The goal of this research paper is to compare the shapes mentioned for different atomic numbers by simulating realistic configurations of nucleons. Taking a particular atomic number with a given number of neutrons and protons and using the packing arrangement in the shape of a sphere or torus, its stability was evaluated for both shapes and then they were compared. This section involves the process of data generation and data analysis. All simulations have been carried out in Python.

3.1 Data Generation

The data being generated is simply the positions of neutrons and protons in a nucleus of realistic size. The charges of particles were ”scrambled” to ensure their positions are realistic as well as random. To find out the number of particles that would be present in a certain shape, the established numerical methods of Rejection Sampling and Poisson Disc Sampling were used.

3.1.1 Finding the number of particles in the shape

Rejection Sampling: Rejection sampling is a method to simulate random samples from an unknown distribution or distribution which is difficult to sample from, known as the target distribution. These samples are then generated by using random samples from a similar, more convenient probability distribution [20].

Generating random particles could cause them to cluster, leading to the Coulomb force dominating, which would not be realistic. Generating particles which would be uniformly distributed would also not be realistic. Thus, to make sure the particles were reasonably distanced apart to imitate a nucleus, the method of Poisson Disc Sampling was chosen.

Poisson Disc Sampling: In a Poisson disc sample, no two points are too close together where the radius is defined by the Poisson Disc Radius (half the distance between the two closest points) and provides a much more uniform sample distribution over the sampling domain [21].

The steps have been quoted from the paper, Bridson, R. (2007) [23]:

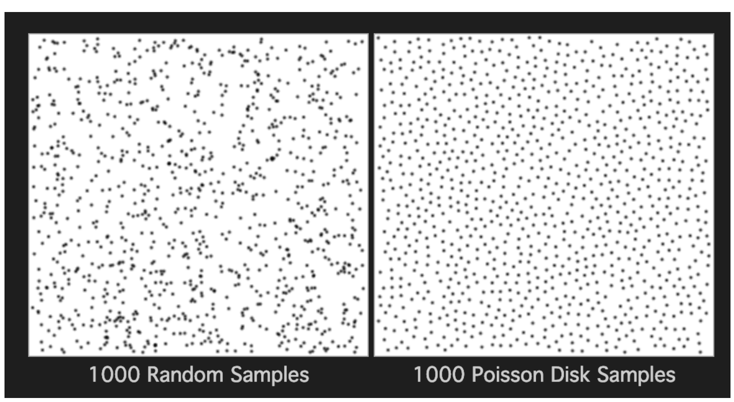
1. Initialize an n-dimensional background grid for storing samples and accelerating spatial searches. We pick the cell size to be bounded by r/$\sqrt{n}$, so that each grid cell will contain at most one sample, and thus the grid can

be implemented as a simple n-dimensional array of integers: the default -1 indicates no sample, a non-negative integer gives the index of the sample located in a cell.

2. Select the initial sample, x_0, randomly chosen uniformly from the domain. Insert it into the background grid, and initialize the "active list" (an array of sample indices) with this index (zero).

3. While the active list is not empty, choose a random index from it (say *i*). Generate up to k points chosen uniformly from the spherical annulus between radius *r* and *2r* around, x_i. For each point in turn, check if it is within distance *r* of existing samples (using the background grid to only test nearby samples). If a point is adequately far from existing samples, emit it as the next sample and add it to the active list. If after *k* attempts, no such point is found, instead remove i from the active list.

Figure 7: A comparison to show why generating sample through Poisson disc sampling allows for less clustering of particles



[21]

Furthermore, realistic spacing of a certain number of particles was obtained by looking at how big the nucleus should be by finding the diameter of a nucleus using the following formula [**?**] where R stands for the radius and A, the mass number (i.e. total number of nucleons) and $R_0 = 1.2 \times 10^{-15}$m. R_0 was doubled as the diameter, not the radius, was the desired value.

$$R = R_0 A^{1/3} \tag{3}$$

3.1.2 Sampling

Larger simpler figures, such as a cube, were used to bound the more complex nuclei geometry. Taking a cube for a sphere and a rectangular prism for the torus, the number of test samples in the shape could be found. As the nuclear strong force has a short range on the order of 10^{-15}m (also equal to 1 femtometre), all calculations have been done in units of femtometres. By putting in coordinates for the shape, the samples which were in the shape were determined and those which were not in the shape using the formulae mentioned were eliminated.

The following formula was used for the sphere, where r is the radius.

$$r^2 > x^2 + y^2 + z^2 \tag{4}$$

For the torus, the following formula was used where a is the major radius, and b, the minor radius.

$$a > (x^2 + y^2 + z^2 + a^2 - b^2)^2 - 4a^2(x^2 + y^2) \quad (5)$$

The minor radius *b* was taken as a constant, while the major radius *a* was 1.5 times *b*. This helped in keeping the torus uniform when we would test it for a larger number of particles.

3.2 Data Analysis

3.2.1 Determining the Forces

Particles interact in a pair-wise manner. When multiple pairs of particles are interacting and acting upon other pairs in terms of forces, the forces scale with the square of the number of particles. The Coulomb force only comes into action when the pair of particles are charged. However, the nuclear strong force comes into action for any pair of particles. As mentioned earlier, force vectors are additive and thus these forces on the particles were added to yield a net force.

3.3 Stability Metric

A dot product is equal to the product of the magnitude of each vector and the cosine of the angle between them shown in Figure 8[24].

In the end, the final stability of an atomic number was found by finding out the dot product of the position and force of each particle and then adding it up. Keeping

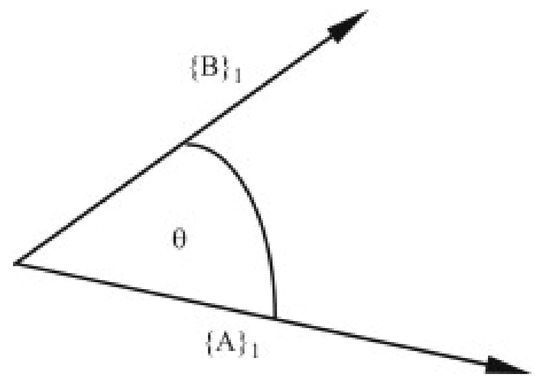


Figure 8: An explanation of the dot product. The dot product of vectors A_1 and B_1 yields a dot product equal to $A_1 \cdot B_1 \cdot \theta$

the number of neutrons and protons constant, this simulation was run several times due to the randomised labelling of particles and then averaged over fifty. This dot product gave the overall stability metric of the nucleus of a given atomic number and neutron number. By taking the minimum value of the stability and averaging it over 3, an overall stability for each shape was obtained.

Assuming that the most stable nucleus would have a stability metric of 0, the higher the stability metric below 0 was, the more would be its stability, while the lower the stability metric was, the stability would be considerably lower, resulting in radioactive decay.

4 RESULTS

The results have been displayed in the graphs as shown below. The graphs of the shape-dependent stability of the sphere and toroidal nucleus have also been given in 9 and 10. Purple represents Z = 300, blue represents Z = 400 and pink represents

Z = 500.

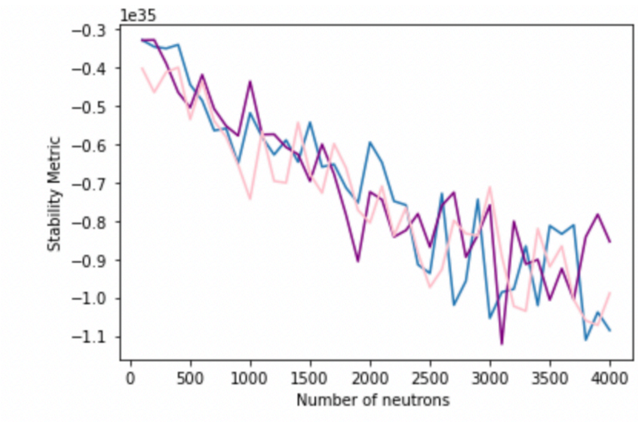


Figure 9: The stability metric of a Toroidal Nucleus of Z=300,400,500. As it can be seen, the trend for the stability metric is non-linear as the metric is not a straight line but varies greatly.

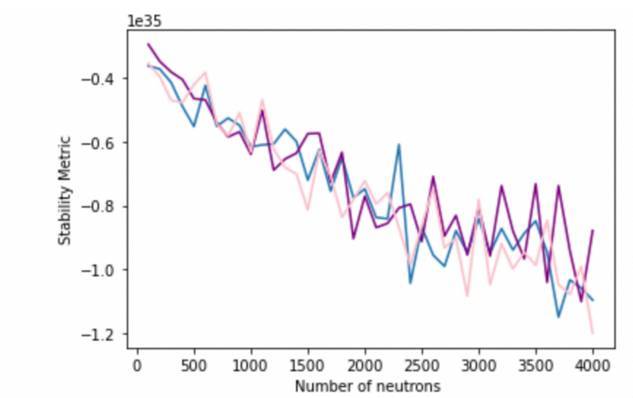


Figure 10: The stability metric of a Spherical Nucleus of Z=300,400,500. As it can be seen, the trend for the stability metric is non-linear as the metric is not a straight line but varies, but less than that of the toroidal nucleus.

5 DISCUSSIONS AND LIMITATIONS

5.1 Analysis of the Results

As mentioned in the literature review, stable nuclei are mostly known to have even numbers of both protons and neutrons and a neutron-to-proton ratio of at least 1. The goal of the stability metric of the two differently shaped nuclei was to achieve one stability metric that was closer to 0.

Upon calculation, the stability of a toroidal nucleus is closer to 0 than that of a spherical nucleus, implying that the toroidal nucleus is more stable than the spherical nucleus for atomic numbers of 300 to 500.

Another thing to note is that even with the addition of one neutron, the stability increases and decreases. This could indicate the sensitivity of the stability of a nucleus.

5.2 Limitations

The primary limitation of this study was that quantum mechanics was not accounted for and the forces taken were classical. The stability metric, which is an arbitrary number relied on the configuration stability and not a dynamic simulation. Nuclear stability is governed by numerous factors such as the strong force, Coulomb force, quantum electrodynamics, and quantum chromodynamics simultaneously and is quantum. Given the fact this paper has mainly been theoretical with a few simulations to compare the sphere and torus, it only takes into account a limited number of factors. However, these assumptions allow the study to be done with reasonable computational power.

6 CONCLUSION

The toroidal shape of a nucleus is more stable than the spherical shape of a nucleus for atomic numbers of 300 and above. With further study, a clear trend can be established of whether the nuclear stability of a toroidal nucleus increases with the increase of atomic number or neutron number. Further research could be the stepping stone to moving forward in understanding nuclear stability and paving the way for new discoveries.

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