Nuclear HW 2
Critical Mass for U-235 Fission

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November 5, 2025

1 Problem Statement

This project asks you to consider the question of the mass of U-235 required such that it becomes "super-critical" and explodes in a manner similar to the atomic bomb detonated over Hiroshima that was nick-named "Little Boy".

You should feel free to approach this project in a manner of your own choosing. The important issue is that you make thoughtful choices in your calculations, and that you present your reasoning clearly.

As you will quickly discover (if you haven't already), there is considerable information available that purports to describe in detail the actual design of Little Boy. For example, the Wikipedia article on Little Boy draws heavily from a book written by John Coster-Mullen that has received fairly positive reviews from experts in the field. I actually saw him speak at an APS conference.

Rather than trying to duplicate or analyze the precise design that was purportedly used, one framework you might consider is a spherical mass of U-235 under the assumption that it has been assembled quickly enough that you don't need to consider the time period prior to it being assembled. Your goal is to determine the mass at which the uranium becomes "super critical". That is, the mass at which a chain reaction proceeds quickly enough that the sphere of U-235 explodes. Toward that end, you can assume that upon the assembly of the super-critical mass, a burst of neutrons is released at the center of the sphere. The exact number of neutrons is up to you, but you certainly want more than one, as a single neutron has a reasonable statistical chance of producing no chain reaction at all or a chain reaction that quickly fizzles out.

An important and subtle issue is the difference between a critical mass and a super-critical mass. A useful parameter in this regard is the average number of fissions, k, that occur due to the neutrons released by each fission. If k=1 a critical mass has been achieved and a sustained chain reaction will occur. Such a situation, however, would not result in a sufficiently fast release of energy that a significant explosion occurs. What is needed is the release of a large amount of energy before the device blows itself apart. A mass sufficient to do so is often referred to as "super-critical". Various sources suggest that a super-critical mass is achieved if k=2. While you are welcome to develop your own criterion for a super-critical mass, you should feel free to use the criterion of k=2.

Most accounts of the design of fission weapons describe the use of a neutron-reflecting material surrounding the fissile material. Feel free to include such a detail or not as you wish. Your choice on this issue will influence the outcome of your results, which is fine.

As you proceed with this project, you will need to establish various inputs to your calculations. Some of the questions you will need to answer for your calculations are likely to include:

1. What is the cross-section for fission (of U-235) as a function of the energy of the incident neutron?

2. What other scattering processes can occur and what are their cross sections?

3. How many neutrons are released from each fission and what are their energies?

4. How much energy is released by each fission? How much variation is there?

5. If you include a neutron reflector, what are the relevant cross sections?

   Depending on how you structure your calculations, there are additional questions you might consider. Assuming you use k=2 to establish super criticality here are a few more questions you might ask yourself.

6. It is possible to establish a value for k by looking at the results of a single "seed" neutron. For a U-235 mass of a given size, what type of variation do you see in the values of k resulting from multiple trials of single seed neutrons?

7. Can you estimate the fraction of the U-235 that has fissioned when your idealized device has produced the energy equivalent of 15 kTons of TNT? (1 kTon equivalent is approximately equal to 4.18×10^9 Joules.) How can you compute such a number?

2 Outline

To talk about fission, we must first talk about the interaction cross section. The path length a neutron can cover inside a spherical mass of U-235, before interacting with a U-235 atom, is called the mean free path. In Lecture 9, we derived the probability of interaction upon traveling a distance x inside the sphere as given by

$$P(x) = e^{-\sigma n x} \tag{1}$$

Here n is the number density of U-235 atoms and σ is the cross section for the interaction. Consequently, the mean free path, x is given by

$$x_f = \frac{-1}{n\sigma} \ln(P) \tag{2}$$

where P is a random number between $0 - 1$.

There are several processes that can occur when a neutron interacts with a U-235 atom, each with their own cross section, some of which are elastic or inelastic scattering, fission, or absorption. The interaction cross section for each process depends on the energy of the interacting neutron. If the neutron initiates a fission reaction, then the U-235 atom emits 2 or 3 neutrons. Tracking the number of fissions per generation is done using a variable called k, defined as the ratio of the number of child neutrons to the number of parent neutrons. For example, $k = 2$ would mean that the number of neutrons in the sphere doubles every generation.

Thus, to model fission reactions, a simple procedure would be as follows: track the interactions of a bunch of neutrons and compute k for each generation. The average of these k values would be the k for a given radius of a U-235 sphere.

3 Assumptions

The actual modeling of a fission chain reaction is quite challenging. To make our lives (and code) simpler, we make certain assumptions:

1. Consider spheres of pure U-235. Realistically, there should be U-238 present at different levels of U-235 enrichment. However, U-238 has different interaction cross sections, which we ignore. To consider different enrichment levels of U-235, we simply multiply the number density by a fraction (for example $n \to 0.8n$ for 80% enrichment).

2. For a U-235 bomb, $k = 2$. This is usually done using reflectors, which are highly effective at keeping neutrons inside the fissile sphere to cause more fissions. In this model, we use a crude design for a reflector, which simply stops the neutron from exiting the sphere with a certain probability. the presence of U-238 also has a significant effect on the number of fission reactions, which in turn affects k. The assumptions in this model thus make it difficult to achieve $k = 2$. Thus the aim will be to attain supercriticality at $k > 1$.

3. A neutron will be assumed to be able to interact with a U-235 atom in only four possible ways: elastic scattering, inelastic scattering, fission and absorption. Each of these interactions has a separate energy dependent cross section as shown in fig. 1

4. The energies of neutrons in the fissile sphere will be divided into three broad ranges, each with a separate probability distribution [2]. These are 'thermal' ($E < 1\ eV$), 'epithermal' ($1\ eV < E < 0.1\ MeV$) and 'fast' ($E > 0.1\ MeV$). The probability distributions are given as follows:

   (a) Thermal neutrons follow a Maxwellian distribution. The probability distribution function is given by ($T = 293K$):

   $$\mathrm{PDF}(E) = \frac{2}{\sqrt{\pi}(k_B T)^{3/2}}\sqrt{E}e^{-E/k_B T} \tag{3}$$

   (b) Epithermal neutrons follow a $1/E$ distribution. The probability dis-

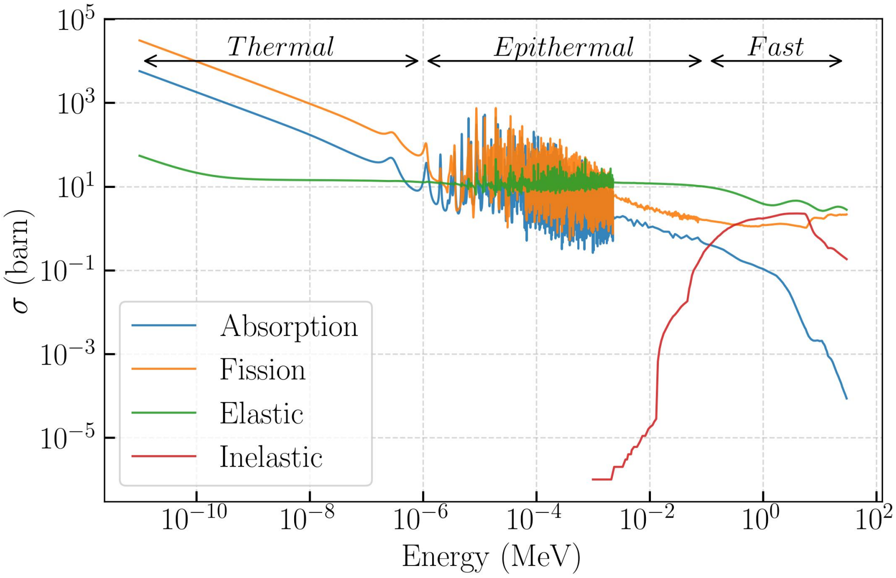

Figure 1: Energy dependent cross sections for the four types of interactions considered in this model. The data was obtained from ENDF [1]

tribution function is given by:

$$\mathrm{PDF}(E) = \frac{1/E}{\ln(E_{max}/E_{min})} \tag{4}$$

(c) Fast neutrons follow a Watt distribution. The probability distribution function is given by [3]:

$$\mathrm{PDF}(E) = 0.4865 \sinh\left(\sqrt{2E}\right) e^{-E} \tag{5}$$

These distributions are shown in fig. 2

5. The energy of a neutron will be assumed to be the same after an elastic collision. After an inelastic collision, which is relevant mostly for fast neutrons, the neutron energy will be set to a randomly sampled energy from either thermal or epithermal distributions with equal probability. A fission will cause the release of 2 or 3 neutrons. The energy of these will be sampled from the fast energy distribution.

6. The direction of a neutron after elastic scattering is heavily dependent

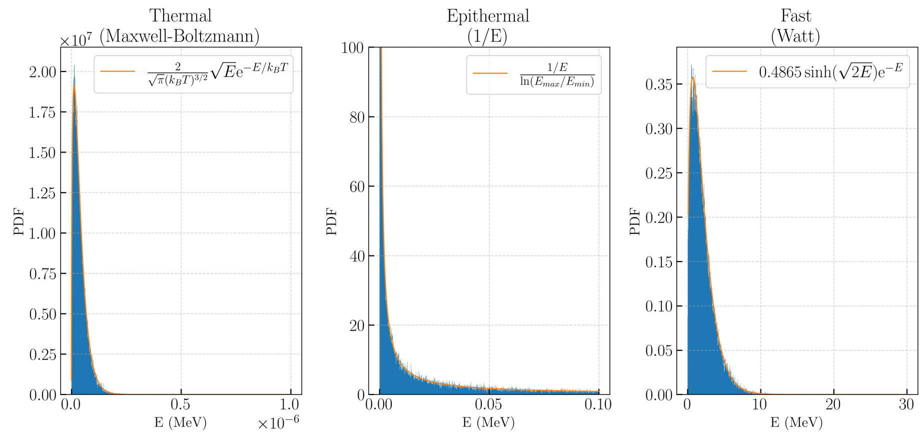

Figure 2: PDFs of energy distributions for the three energy ranges in this model

on the energy of the neutron. High energy neutrons are mostly forward scattered while low energy neutrons scatter isotropically. For the model, we will consider a crude angular dependence. For neutron energy, $E < 0.05\ MeV$, elastic scattering will be isotropic. For $0.05\ MeV < E < 0.1\ MeV$, the scattering angle will be restricted to $130°$. For $E > 0.1\ MeV$, scattering angle will be restricted to $50°$. This is shown in fig. 3

4 Algorithm and Logistics

This section describes the algorithm used for the code to find the supercritical mass of U-235. For a U-235 sphere of radius R, having mass density $\rho = 19.05\ g/cm^3$, and enrichment 'ench', we first find the number density of U-235 atoms as

$$n = \rho \times \frac{N_A}{235.044} \times \text{ench} \tag{6}$$

where N_A is the number of moles and 235.044 is the molar mass of U-235. We then populate the sphere with 100 neutrons in the center of the sphere at $r = 0$, where r is the radial position of the neutron. These neutrons have randomly sampled thermal or epithermal energies. Let us talk about how to track a single neutron.

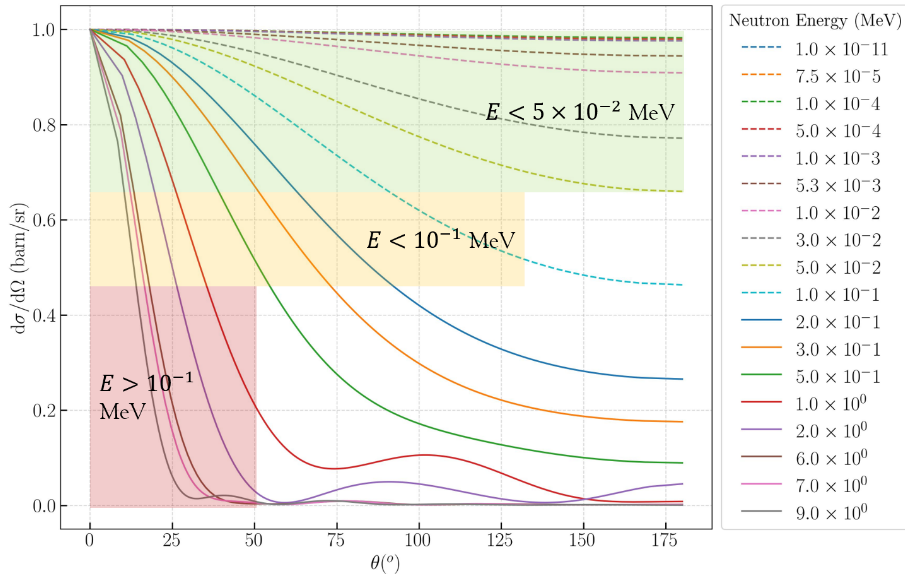

Figure 3: Angular dependence of elastic scattering for different neutron energies. The highlighted ranges are the crude angular dependence ranges used in this model.

1. We first compute the mean free path for each of the 4 processes p using

$$x_{f,p} = \frac{-1}{n\sigma_p} \ln(RND)$$

where RND represents a random number between 0 and 1, and each process has a separate distribution to sample RND from. The process that has the smallest $x_{f,p}$ is the process that is chosen as the interaction type.

2. Choose random uniformly distributed directions θ and ϕ applying the crude energy dependent bounds for θ in case of elastic scattering. ϕ is always assumed to be isotropic.

3. Move the neutron a distance x_f in the sampled direction. If the new radial position is greater than the radius of the sphere, R, then sample a random number between 0 and 1. If this number is greater than the reflection probability, then stop tracking the neutron. Else, keep tracking.

4. If the process is absorption, stop tracking the neutron

5. If the process is elastic, do nothing and continue tracking the neutron
6. If the process is inelastic, change the energy of the neutron to a randomly sampled energy between thermal and epithermal. Keep tracking the neutron.
7. If the process is fission, then stop tracking the neutron. Create 2 or 3 neutrons having Watt sampled energies at this position. Add these neutrons to the next generation.

Thus, a neutron generation only ends when it escapes, is absorbed, or causes a fission. Since we start with 100 neutrons, k per run will be the average of the number of neutrons in gen_{i+1} divided by the number of neutrons in gen_i. k_{eff} is calculated as the average k over 500 runs. Thus, k_eff is the average k after tracking 50000 neutrons. To make the code less computationally intensive, we only track up to 30 generations at max. Further, at each generation, we track at most 100 neutrons. If the number of neutrons doubles to 200 in a generation, then we randomly sample 100 from these to continue in the next generation.

For the results, we do this for 100 different radii of the U-235 sphere and vary the reflection probability and enrichment percentage.

5 Results

Following the algorithm detailed above, the simulation was performed for 100 different radii between $0 - 25cm$. The enrichment percentages were taken to be 65%, 85% and 100%, and the reflection percentage was taken to be 0% or 70%. fig. 4 shows the dependence of k_eff with the radius and mass of the U-235 sphere. For larger enrichment, since there are more U-235 atoms to interact with, k_eff increases faster.

fig. 5 shows the same dependence of k_{eff} with radius and mass, but for a reflection probability of 70%. For the smallest radii, instead of the neutron escaping immediately, it stays in the sphere 70% of the time, increasing the possibility of fission. This is why the beginning of the graph looks flat, after which it looks similar to fig. 4. Again, as expected, k_{eff} grows quicker with a reflector than without.

Finally, the importance of the angular dependence of elastic scattering was also examined at 100% enrichment and without a reflector. This is shown in

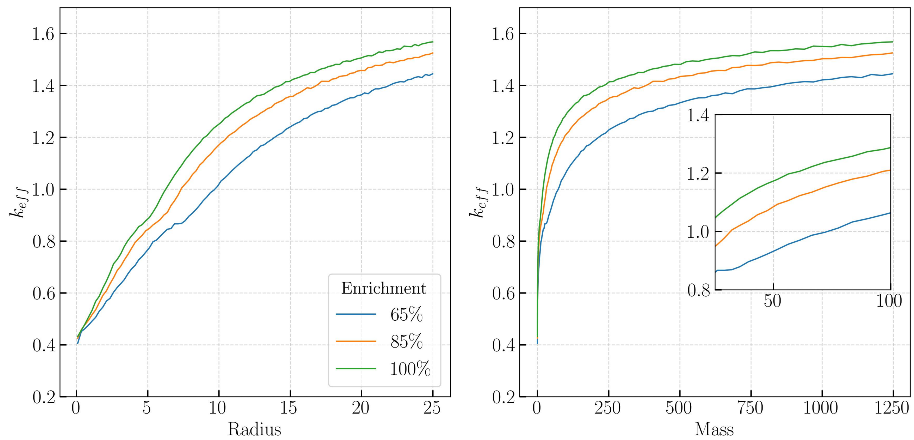

Figure 4: k_{eff} plotted against radius and mass for no reflector

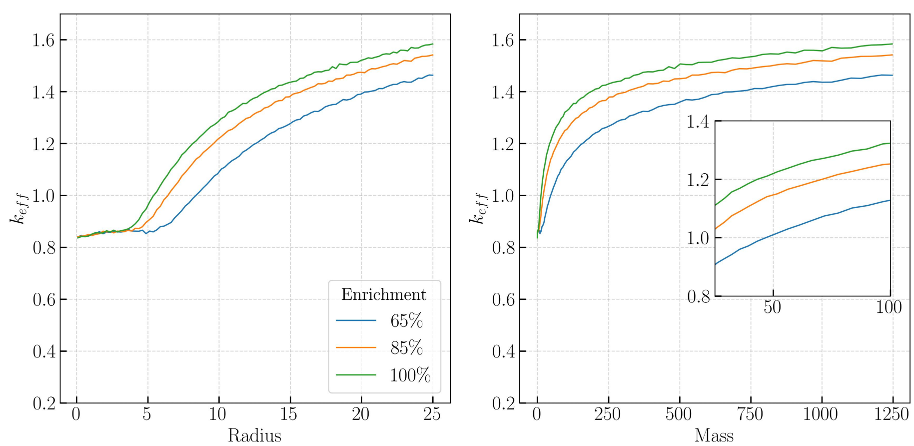

Figure 5: k_{eff} plotted against radius and mass for 70% reflection

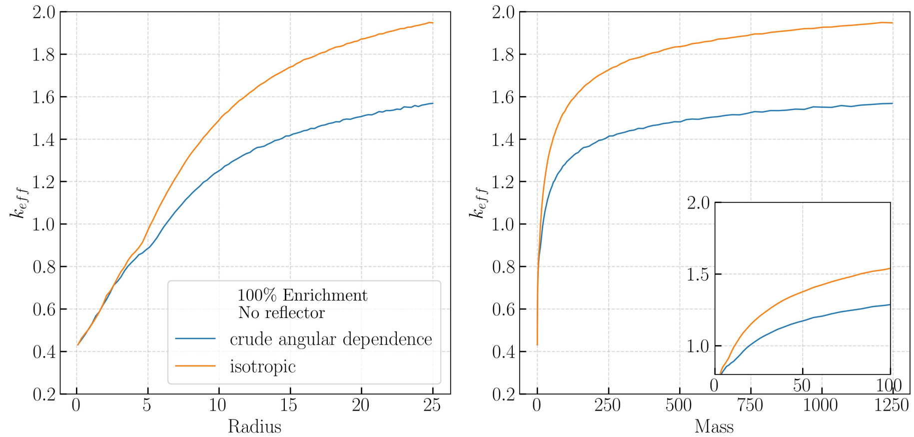

Figure 6: Importance of angular dependence of elastic scattering. With isotropic scattering, $k_{eff} = 1$ is attained faster.

Enrichment (%)	Reflection (%)	M for k_{eff}=1 (kg)	R for k_{eff}=1 (cm)
65	0	73.3	9.72
85	0	31.7	7.35
100	0	19.8	6.28
65	70	47.0	8.38
85	70	21.1	6.42
100	70	12.7	5.42

Table 1: Simulated mass for which $k_{eff} = 1$ for various simulation parameters. True value is 46.7 kg

fig. 6. Isotropic elastic scattering keeps the neutron in the sphere for longer, increasing the possibility of fission. As expected, without angular dependence, criticality is reached significantly at a smaller radius.

The critical mass for a bare U-235 metal without a reflector is 46.7 kg [4]. table 1 shows the results of this simulation for $k_{eff} = 1$.

Finally, let's address the question:

Can you estimate the fraction of the U-235 that has fissioned when your idealized device has produced the energy equivalent of 15 kTons of TNT? (1 kTon equivalent is approximately equal to 4.18×10^9 Joules.)

In class, we estimated that each fission produces on average 184 MeV energy. To produce 15 kTons (3.917×10^{26})of energy, we would thus need 2.129×10^{24}

fissions. Considering the case of 65% enrichment and 70% reflection, i.e. a U-235 sphere of mass 46.7 kg and radius 8.38 cm, the number of U-235 atoms in this mass are:

$$N = \rho \times \frac{N_A}{235.044} \times \frac{4}{3}\pi R^3 \times 0.65 \tag{7}$$

$$= 19.05 \times \frac{6.022 \times 10^{23}}{235.044} \times \frac{4}{3}\pi \times 8.38^3 \times 0.65 \tag{8}$$

$$= 7.8 \times 10^{25} \tag{9}$$

Thus fraction of U-235 that has fissioned is $2.129 \times 10^{24}/7.8 \times 10^{25} = 0.027$ So only 2.7% of the U-235 sphere has to fission to release 15 kTon of energy.

6 Conclusions

From table 1, it seems that this simulation suggests that 65% enrichment and 70% reflection estimates the critical mass of a bare U-235 sphere most closely. There are several reasons for this discrepancy and most go back to the assumptions that we made. Assuming a crude angular dependence was seemingly not enough to accurately model the elastic collisions, and this overestimated the duration a neutron was inside the sphere, leading to a larger k_{eff} at a lower mass. We also get incorrect values since we ignore the presence of U-238 which has significant fission and elastic scattering cross sections especially for higher neutron energies. In our simulation, we did not reach $k_{eff} = 2$. This is most likely due to poor reflector design. Realistic nuclear weapons are almost always surrounded by a highly efficient reflector which keeps fast and thermal neutrons inside the U-235 sphere for longer. Further, the number of fission products is also energy dependent, and the neutron energy after an inelastic collision also follows a more complicated distribution. All these factors combined allow for nuclear weapons to reach $k_eff = 2$ in a short amount of time, thus causing a devastating explosion. These factors haven't been accurately considered in this simple simulation, thereby leading to incorrect critical mass estimates.

References

[1] Evaluated nuclear data file (endf) database. https://www.nndc.bnl.gov/endf/.

[2] Nuclear-power: What are fission neutrons. https://www.nuclear-power.com/nuclear-power/reactor-physics/atomic-nuclear-physics/fundamental-particles/neutron/fission-neutron/.

[3] J. watterson, 2007. https://indico.cern.ch/event/145296/contributions/1381141/attachments/136909/194258/lecture24.pdf.

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