A Monte-Carlo Simulation of Gamma Rays in a Sodium Iodide Detector

A Senior Project

By

Ben Kessler

Advisor, Dr. Tom Bensky

Department of Physics, California Polytechnic University SLO

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Abstract

Gamma rays principally interact with matter through Compton scattering, photoelectric effect, pair production, and triplet production. The focus of this simulation is to study the theoretical energy spectrum created by gamma rays from a Cesium-137 source, which produces gamma photons with an energy of 0.662 MeV. At this energy level, most interactions are results of Compton scatters and the photoelectric effect. Therefore, this simulation only models those two effects on gamma rays. Using Monte Carlo methods and the Metropolis algorithm to sample the probability distributions of the two effects allowed for the simulation of gamma rays in a Sodium Iodide detector. Using these methods produced a theoretical spectrum for Cesium-137 that closely matches those from other simulations, as well as an actual spectrum. The spectrum lacks certain features, such as a backscatter peak and the energy smearing that is seen in an actual spectrum, but it does model the Compton shelf and the principal photopeak. This allows for accurate modeling of different size detectors and gamma rays under one MeV.

Introduction

Gamma ray interactions are well studied and modeled; therefore, the goal of this research was to use Python to reproduce an accurate spectrum by utilizing Monte Carlo methods. Gamma ray attenuation is an exponential decay process that is dependent on the energy of the gamma ray, the linear attenuation coefficient, and the depth of penetration. This process models the major effects that can attenuate gamma rays in a material. There are four primary processes through which gamma rays are attenuated; however, for energies lower than 1 MeV only Compton Scattering and the Photoelectric effect are likely to occur, as Pair Production and Triplet Production require a higher energy of $2m_ec^2$.

The photoelectric effect is the mechanism by which a photon is completely absorbed as it interacts with an electron. This causes the electron to be ejected from the atom and carry away the energy of the incident photon. This process results in the creation of the photopeak for a spectrum, as the electrons that are ejected carry the energy of the incident gamma rays. The second mechanism, Compton scattering, describes the interaction of a gamma ray with a valence electron in an atom. Similar to the photoelectric effect, the electron is freed from the atom and the gamma ray is scattered. However, the scattered electron only carries away a certain fraction of the energy of the incident photon. This process is dependent on the incident energy of the gamma ray and the angle at which the gamma ray is deflected. The angle at which the gamma ray is deflected is governed by the Klein-Nishina cross-section, which gives the likelihood for the scattering angle depending on the energy of the incident photon.

The goal of simulating these mechanisms is to produce a theoretical spectrum for gamma rays emitted by Cs-137 and compare it to an actual spectrum created by a scintillation detector. Doing this will highlight the effects that are a direct result of the physics, as well as show which effects are results of the detector and the environment. It is expected that the theoretical spectrum will have a characteristic photopeak at 0.662 MeV and a Compton shelf that extends to .478 MeV, while it will not have the energy smearing, backscatter peak, and x-ray emission that appear in a scintillation detector spectrum.

Methods

Simulating gamma rays in a detector using Python involves leveraging the power of scientific libraries and mathematical models to accurately replicate the behavior of these high-energy photons. To achieve this, NumPy, Matplotlib, and the Random libraries were used within the code. As gamma emissions and attenuation are inherently probabilistic in nature, Monte-Carlo methods were applied along with the use of the Metropolis algorithm to model the behavior of the gamma rays.

To begin, the gamma rays must be created from a source. In the lab, a source will constantly give off gamma rays in all directions, therefore the beginning direction is chosen randomly.

The random emission was simulated by randomly selecting an angle between zero and two pi. After verifying the direction of each photon, the simulation begins for each photon that is projected towards the detector.

The first usage of Monte-Carlo techniques occurs when calculating the attenuation length of the gamma ray, or the amount of distance that the photon will travel once it enters the detector. To calculate this, the simulation begins with $I(z) = I_0 e^{-\lambda z}$ (1) which models the attenuation of gamma rays in a material. In (1) I(z) is the intensity of the gamma ray after traversing a distance z, I_0 is the initial intensity of the gamma ray, and λ is the linear attenuation coefficient. For gamma rays, the linear attenuation coefficient is dependent on the energy of the photon and the detector composition. For a Sodium Iodide (NaI) detector and 0.662 MeV photon, λ equals 8.2208 cm^{-1}. To produce a normalized probability distribution of interaction (1) is rewritten as $f(z) = \lambda e^{-\lambda z}$ (2). Integrating (2) over the length of the detector, L, produces the cumulative probability distribution $F(L) = 1 - e^{-\lambda L}$ (3). Rearranging and utilizing Monte-Carlo methods to pick a value for F(L) provides $L = -\frac{1}{\lambda}\ln(1 - r)$ (4), where L is the distance travelled by the gamma ray and r is a random number between zero and one. (4) gives the distance that a gamma ray will travel inside the detector before it is attenuated.

Fig. 1 illustrates this, by showing a histogram of the penetration depth of gamma rays, given a sample of 10,000 equal energy gamma rays.

Fig. 2 shows the path of a group of gamma rays through a detector, where a red x signifies the photon leaving the detector and a black star signifies a photon that is photoelectrically absorbed.

Fig. 1 and (4) detail the distance that a photon will travel inside a detector before interacting with the detector, to determine what occurs at this point, the cross-sections for the photoelectric effect and Compton scattering are calculated. The cross-sections for the two effects describe the probability of the effect occurring. The photoelectric cross-section is described by $\sigma_{ph} = 8\sqrt{2}\pi r_e^2 \alpha^4 \frac{Z^5}{k^{3.5}}$ (5) (Siegbahn) where r_e is the classical electron radius, α is the fine structure constant, Z is the atomic number of the absorber, and k is the ratio of the gamma ray energy and the Electron rest mass energy. The Compton cross-section is described by the Klein-Nishina equation (Klein and Nishina, 2014), which produces

$$\sigma_C = Z2\pi r_e^2 \left\{\frac{1+k}{k^2}\left[\frac{2(1+k)}{1+2k} - \frac{\ln(1+2k)}{k}\right] + \frac{\ln(1+2k)}{2k} - \frac{1+3k}{(1+2k^2)}\right\} (6)$$

for energies greater than .1 MeV and

$$\sigma_C = Z\frac{8}{3}\pi r_e^2 \frac{1}{(1+2k)^2}\left(1 + 2k + \frac{6}{5}k^2 - \frac{1}{2}k^3 + \frac{2}{7}k^4 - \frac{6}{35}k^5 + \frac{8}{105}k^6 + \frac{4}{105}k^7\right) (7)$$

(Hubbel, 1969) for energies less than .1 MeV.

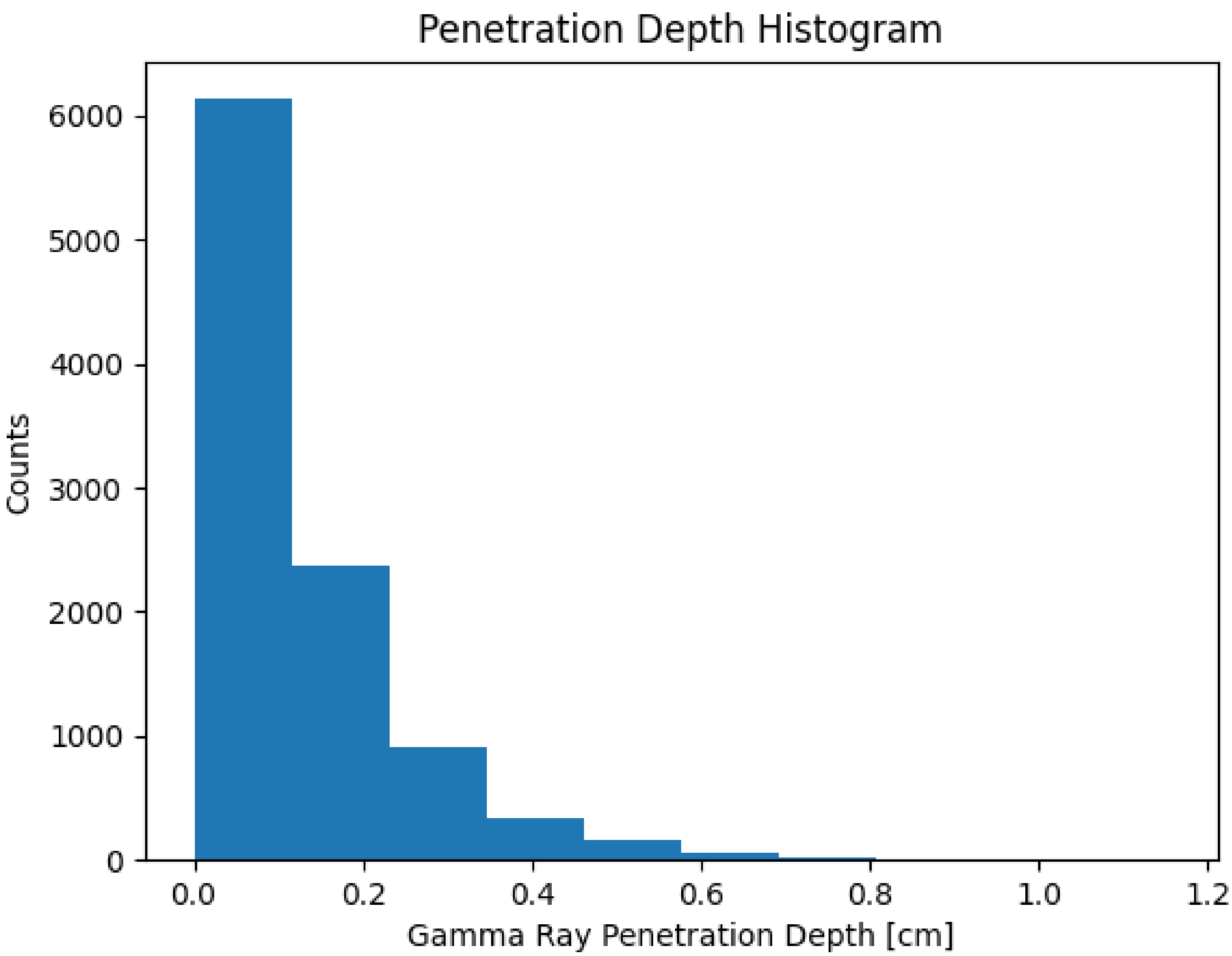

Figure 1: Penetration Depth Histogram

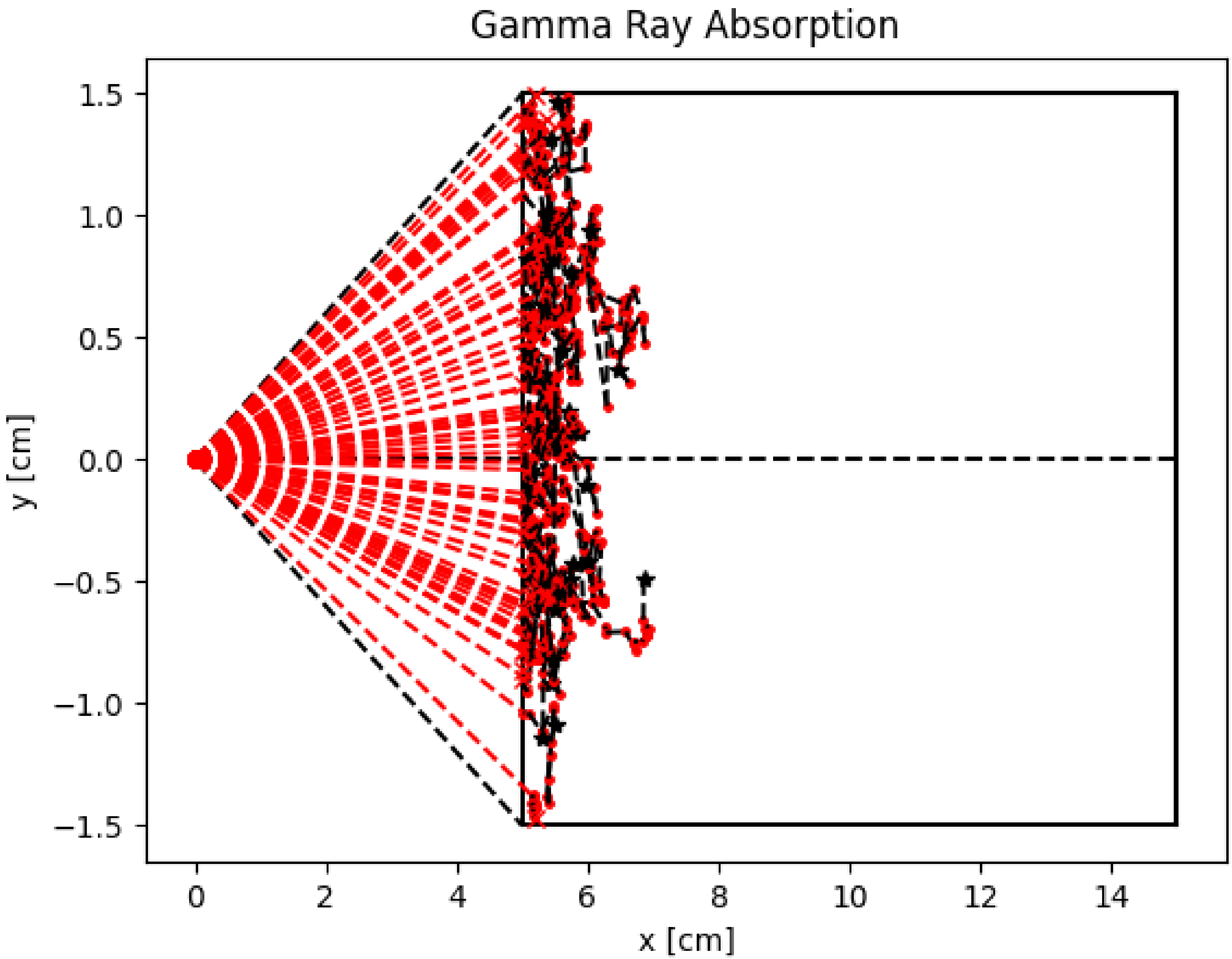

Figure 2: Gamma Ray Absorption

Plotting these cross-sections over a span of energies from .01 MeV to 1 MeV produces Fig. 2, which shows the probability of a gamma ray interacting with an atom versus its energy. This figure shows that the cross-section for attenuation stays approximately constant, even as the photoelectric effect cross-section drops off steeply as energy increases. For each simulated photon, (6) and (7) were used to calculate the cross-sections.

As each cross-section provides the probability for an event, the total probability of a photoelectric absorption occurring is the cross-section of an absorption divided by the sum of the cross-sections. The Metropolis algorithm is then used to determine whether the event would occur by computing a random number between zero and one and comparing it to the total probability of the event occurring. If the random number is less than the total probability, then the gamma ray is photoelectrically absorbed; if it is greater than the photon is Compton scattered. This scattering imparts energy onto an electron and the gamma ray energy is decreased accordingly,

$$E' = \frac{E}{1+\frac{E}{.511}(1-cos\theta)} \text{ (8).}$$

In (8), E' is the final energy of the gamma ray, E is the initial energy, and θ is the angle at which the photon is scattered. Therefore, the energy

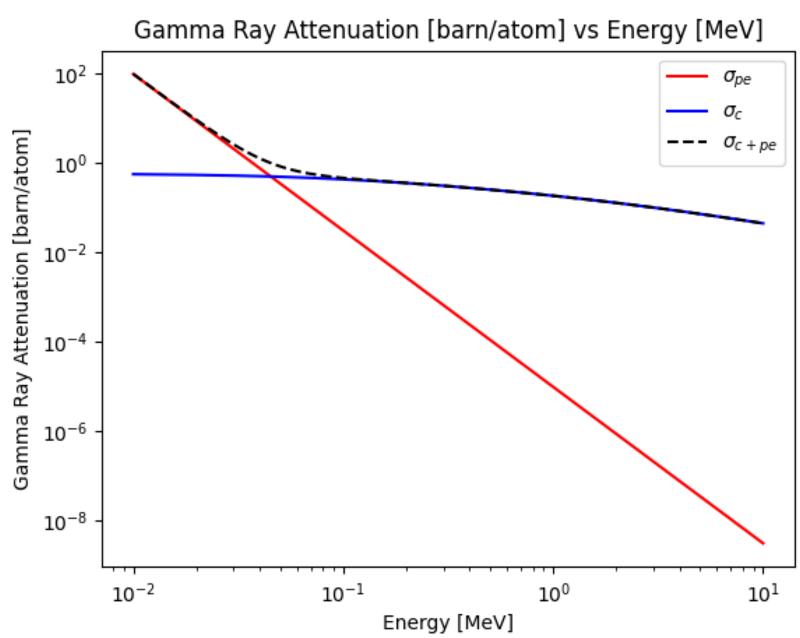

Figure 3: Gamma Ray Attenuation

imparted on the electron is $E_e = E - E'$(9).

When Compton scattering occurs, an angle must be chosen for the photon to be scattered at to calculate the energy. This process is not random but is instead based on the Klein-Nishina cross-section. Fig. 3 shows the probability for each angle, for multiple different photon energies. As gamma ray energy increases, there is a forward scattering bias. This results in the Compton shelf, as there are certain angles that are heavily favored and others that are extremely unlikely. The Klein-Nishina distribution comes from the previously mentioned Klein-Nishina equation and is used to calculate the Klein-Nishina cross-section (Klein and Nishina, 2014),

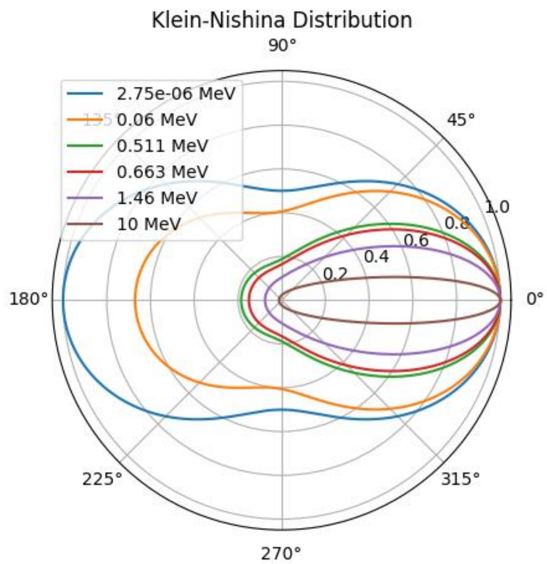

Figure 4: Klein-Nishina Distribution

$$\sigma_{KN}(E,\theta) = \left(\frac{1}{1+\alpha(1-cos\theta)}\right)^2 \left(\frac{1+\cos^2\theta}{2}\right)\left(1 + \frac{\alpha^2(1-cos\theta)^2}{(1+\cos^2\theta)[1+\alpha(1-cos\theta)]}\right. \quad (10)$$

where α = E/.511 MeV. This cross-section gives the probability that a gamma ray with a certain energy will scatter at an angle. This cross-section is calculated for each gamma ray in the simulation and the Metropolis algorithm is utilized again. When a Compton scattering event occurs, a random angle between zero and two pi and a random number between zero and one are chosen.

The Klein-Nishina cross-section is then calculated for that angle and the energy of the incident photon. If the random number is less than the cross-section, the angle is accepted. If the random number is greater than the cross-section new random angles and numbers are chosen, and the cross-section is calculated again. This continues until an accepted angle is found. Fig 5 shows a histogram of accepted angles for a 0.662 MeV gamma ray.

The complete path for a gamma ray in the simulation begins with its creation, where a random angle is chosen. Assuming this angle takes it into the detector it will then travel a distance that is calculated with (4), at which point the photon will either Compton scatter or be photoelectrically absorbed. To determine which occurs, (6) and (7) are used to calculate σ_c and σ_{ph}.

The Metropolis algorithm once again is used to determine which event occurs. If the gamma ray is absorbed via the photoelectric effect, its entire energy is added to the detector and a new gamma ray is created. If the photon is Compton scattered, the energy that it imparts on the electron is calculated using (8) and (9), and the angle at which the photon is scattered is calculated using (10). Following the Compton scatter, the penetration depth for the gamma ray is calculated again and if the photon remains in the detector, the process above is repeated. If the photon leaves the detector, a new gamma ray is created, and the process is repeated.

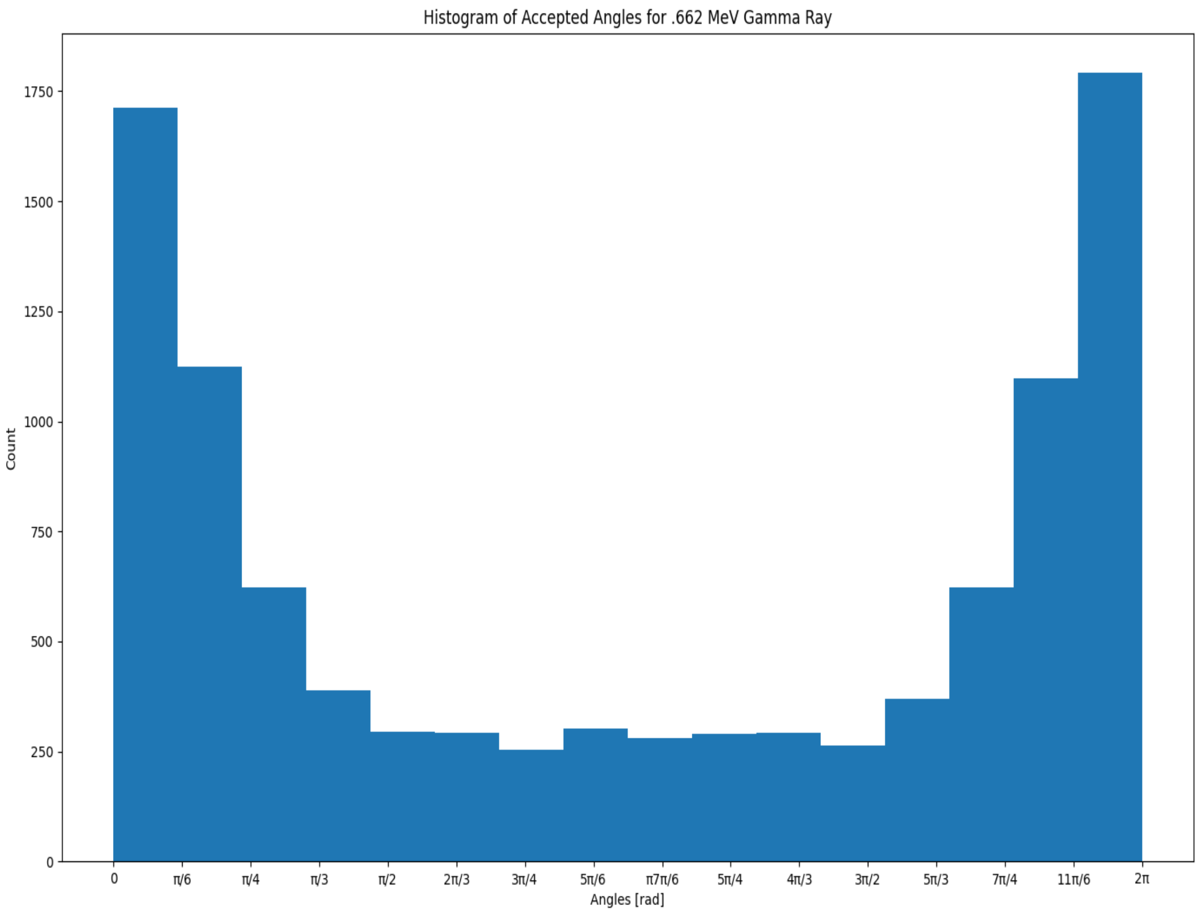

Figure 5: Histogram of Accepted Angles

Results

After simulating one million gamma rays, a spectrum was produced that closely matches the theoretical spectrum for Cs-137. Fig. 6 shows the simulated spectrum, Fig. 7 shows a close-up view of the Compton shelf, and Fig. 8 shows an actual spectrum. Comparing the two spectra shows that the characteristic photopeak at 0.662 MeV is present, as is the Compton shelf. The zoomed in view of the Compton shelf shows the energy drop-off at .48 MeV, as is seen in an actual spectrum. The small hump seen on actual spectrum at approximately .2 MeV is a result of backscatter and the sharp spike at .032 MeV is a result of x-ray emissions by Cs-137 as it decays. These effects were not modeled in the simulation as the goal of the simulation was to explore the effects that Compton scattering and Photoelectric absorption have on the spectrum. Another aspect of the spectrum that is missing is the energy smearing. Energy smearing is a result of the composition of the detector; therefore, it does not appear on the simulation.

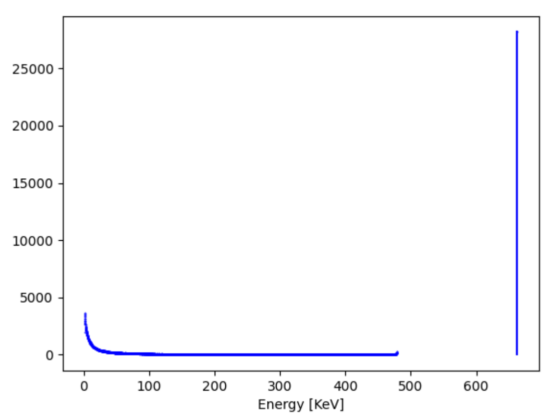

Figure 6: Simulated Cs-137 Spectrum

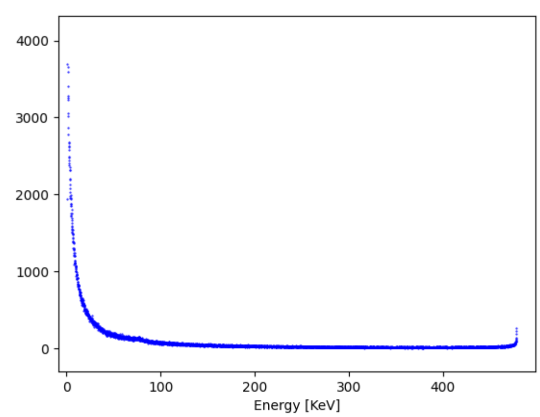

Figure 7: Simulated Cs-137 Spectrum Compton Shelf

An advantage of simulating gamma rays is that it allows for changing the detector sizes and visualizing how the size of the photopeak and the Compton shelf are affected. Fig. 9 and Fig. 10 show two simulations of 100,000 gamma rays for detector sizes of one cm by one cm and ten cm and ten cm respectively. These spectra show that a smaller detector has a larger Compton shelf with a smaller photopeak, as more of the photons exit the detector, while the larger detector has a smaller Compton shelf with a larger photopeak, as most of the gamma rays are absorbed by the detector. The spikes present at zero are a result of rounding and are not indicative of the behavior of the gamma rays, as some photons are scattered away at 180 degrees and impart only a miniscule amount of energy on the detector. There are more counts near zero in the larger detector due to the larger number of initial photons that enter the detector and are backscattered.

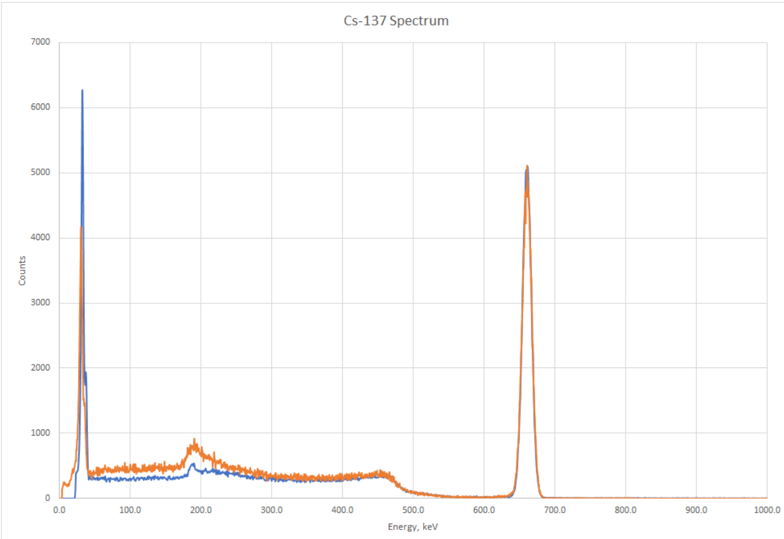

Figure 8: Actual Cs-137 Spectrum (Fomitchev, 2022)

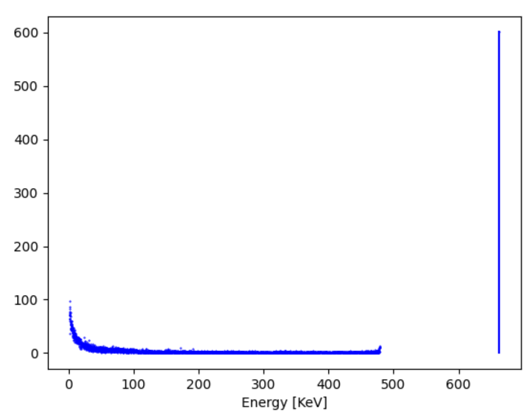

Figure 9: Small Detector Simulated Cs-137 Spectrum

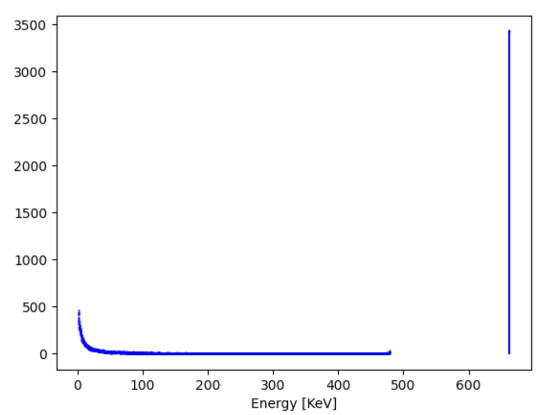

Figure 10: Large Detector Simulated Cs-137 Spectrum

Works Cited

Fomitchev, Max. “The Rich Physics of CS-137 Gamma Spectrum.” *Maximus Energy*, 20 Oct. 2022, maximus.energy/index.php/2020/10/24/the-rich-physics-of-cs-137-gamma-spectrum/.

Hubbell, J H. *Photon Cross-sections, Attenuation Coefficients, and Energy Absorption Coefficients from 10 keV to 100 Gev*, 1969, https://doi.org/10.6028/nbs.nsrds.29.

Klein, O., and Y. Nishina. “On the Scattering of Radiation by Free Electrons According to Dirac’s New Relativistic Quantum Dynamics.” *The Oskar Klein Memorial Lectures*, 2014, pp. 253–272, https://doi.org/10.1142/9789814571616_0015.

Siegbahn, Kai. *Alpha-, Beta- and Gamma-Ray Spectroscopy*. North-Holland Publ, 1979.

Code/Data

Kessler, Ben. "SeniorProject." GitHub, 2023, github.com/bnkessler/SeniorProject.