TFY4235/FY8904: Computational Physics

Assignment 3: Radioactivity and photon transport
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1 Introduction

On this assignment we will create a very simple Monte Carlo (MC) based particle transport algorithm to study how gamma radiation (photons) behaves when moving though matter. To do so we will:

- Briefly study how random (or pseudorandom) number generators work.
- Create a MC algorithm to replicate nuclear decay. Study the uncertainty of this results.
- Model two (photoelectric effect and Compton scattering) of the three interactions that photons undergo when moving through matter. Study photon trajectories and energy losses.
- Combine the nuclear decay with the photon interaction simulations to look at how the energy loss distributions from primary photons look like when a radioactive source is placed within a homogeneous medium.

Much more complex versions of the algorithm that will be made in this assignment are key in the study of cosmic rays that reach the earth and are considered to be the "gold standard" at the time of performing radiotherapy treatment recalculations.

2 Random number generator

A random number generator (RNG) lays a sequence of numbers or symbols that cannot be reasonably predicted better than by random chance. However, by means of a computer it is not possible to create such RNGs. Instead computes use what is known as a pseudorandom number generator (PRNG) which are algorithms that use a sequence to create long runs of numbers with good random properties but eventually the sequence repeats. Two PRNGs are the **middle square method** and the **linear congruential method** [1].

2.1 Middle square method

To generate a sequence of n-digit pseudorandom numbers, an n-digit starting value is created and squared, producing a 2n-digit number. If the result has fewer than 2n digits, leading zeroes are added to compensate. The middle n digits of the result would be the next number in the sequence and returned as the result. This process is then repeated to generate more numbers.

1. We start with an n-digit seed: $seed = 1234$ ($n = 4$).
2. We calculate the square of the original seed: $seed^2 = 1522756$ ($n_{new} = 7 < 2n$).
3. If $n_{new} < 2n$ we add zeros until $n_{new} = 2n$: 01522756.
4. We take the center n digits: $\underline{01}5227\underline{56} \rightarrow 5227 = Randomnumber$.
5. We make $seed_{new} = Randomnumber$ and repeat from step 1.

Note: The value of n must be even in order for the method to work. Also, the value of n and the seed will affect the efficiency of the algorithm.

2.2 Linear congruential method

To generate a sequence of pseudorandom numbers we use a relatively simple relation:

$$X_{n+1} = (aX_n + c) \cdot (mod)(m) \tag{1}$$

Where X is the random number being X_0 the initial seed, m is the modulus, a is the multiplier and must fulfill $0 < a < m$, and c is the increment and must fulfill $0 \leq c < m$.

1. We select an initial X_0 (seed) and the corresponding m, a and c parameters.
2. We solve equation 1 and make X_1 the new seed.
3. We repeat from step 1.

Note: The values of X_0, m, a and c will affect the performance level of the algorithm. You can find several examples (with different performance levels) for these parameters in `https://en.wikipedia.org/wiki/Linear_congruential_generator`.

3 Nuclear decay

In general, atomic nuclei are not stable and they "look for" more favorable energy states transforming into other nuclei by emitting particles or groups of particles. There exist different types of decay, alpha decay, beta decay, nuclear fision and gamma decay for example.

Independently of the type of decay, we can study the statistical aspect of nuclear decay. If we consider that at a time t we have N radioactive nuclei, the change with time of the number of nuclei will be $-dN/dt$. If we now define a **decay constant** λ as the probability per unit time for any nucleus to decay, we define the **exponential law of decay** as

$$\lambda = -\frac{1}{N}\frac{dN}{dt} \rightarrow N(t) = N_0 e^{-\lambda t}, \tag{2}$$

where N_0 is the number of nuclei at $t = 0$, and we define a **half-life** as $t_{1/2} = \ln(2)/\lambda$. The half-life represents the amount of time needed for the initial number of nuclei to halve. At the same time, the mean time that takes a nucleus to decay is known as the **mean life** and it corresponds to $\tau = 1/\lambda$.

In nature, a nucleus can undergo several decay processes until the stable most favorable energy state is reached. This results in what is known as a radioactive or decay chain. In a decay chain each decay process will be described by a different decay constant. In a process like this the exponential law of decay would vary depending on the "step" of the decay chain that we look at. If we assume that at $t = 0$, we only have nuclei from the father nucleus (type 1) we find the general solution to be:

$$N_i(t) = N_1(0) \left(\sum_{k=2}^{k=i} h_k e^{-\lambda_k t} \right), \tag{3}$$

where

$$h_k = \frac{\lambda_1 \lambda_2 ... \lambda_{k-1}}{(\lambda_1 - \lambda_k)(\lambda_2 - \lambda_k)...(\lambda_{k-1} - \lambda_k)}. \tag{4}$$

3.1 Secular equilibrium

In the case of a 3-step decay chain (3 nuclei) if we have $\lambda_1 \ll \lambda_2$ we will find that after a sufficiently enough large time we will find a transient state in which the number of nuclei 2 (N_2) stays constant and follows $N_2(t) = N_1(0)\frac{\lambda_1}{\lambda_2}$. This state is known as secular equilibrium.

4 Photon interactions with matter

When photons interact, they transfer energy to charged particles (usually electrons) and the charged particles give up their energy via secondary interactions (mostly ionization). During this task we will focus on the photon-matter interaction and there are three main mechanism that describe photon interaction with matter [2]:

- Photoelectric (PE) interactions.
- Compton scattering.
- Pair production.

The interaction of photons with matter is a probabilistic phenomenon and the probability of a photon undergoing any of these tree processes depends on:

- The photon energy.

- The atomic number and density of the material (i.e., the electron density of the absorbing matter).

For the sake of simplicity, on this task we will only consider photoelectric interactions and Compton scattering.

4.1 Interaction probabilities (cross-sections)

In very simplistic terms, a projectile particle will interact with a target particle if it gets "close enough". What exactly "close enough" is, would then depend on the energy of the incident particle and various properties of the target (e.g., the atomic number). If we now think about this "close enough" distance and project it into a plane, we will get an effective surface around the target particle. If the projectile particle hits this effective surface the projectile and the target would interact (if it doesn't there will be no interaction). This effective surface is referred to as a **cross-section**, see Figure 1 for a simple sketch. These cross-setions are measured in barns being $1\text{barn} = 10^{-28}\text{m}^2$.

Different interaction mechanisms (e.g., PE and Compton scattering) will have different cross-sections and therefore different interaction probabilities.

4.2 Photoelectric Interactions

During PE interactions the incident photon is absorbed by an inner shell atomic electron. During this absorption the electron absorbs all the photon energy (the electron disappears). The electron that absorbs the photon gets ejected from the atom creating a vacancy on the electronic shell originally occupied, see Figure 2. Some of the photon energy is used to overcome the binding energy of the ejected electron and the rest is transformed into the kinetic energy of the photon.

The PE interaction is most likely to occur for:

- Low energy photons (below 50 keV).
- High atomic number of the target.

Usually, the cross section of the PE interaction can be approximated by the simplified equation of

$$\sigma_{PE}(Z, E_\gamma) \approx 3 \cdot 10^{12} \frac{Z^4}{E_\gamma^{3.5}}, \tag{5}$$

where Z is the atomic number of the target element and E_γ is the incident photon energy in eV [3].

4.3 Compton scattering

In Compton scattering, a photon transfers a portion of its energy to a loosely bound outer shell electron of an atom (the binding energy of the electron is considered negligible). After the photon-electron collision the photon loses energy and changes direction, see Figure 3.

Compton scattering is most likely to occur for, and it is given by equation 6 [4]:

- Intermediate energies (between 100 keV and 10 MeV).
- High atomic number of the target (even though its dependence with Z is much weaker than the one from PE interactions).

$$\sigma_C(Z,k) = \begin{cases} Z 2\pi r_e^2 \left(\frac{1+k}{k^2} \left[\frac{2(1-k)}{1+2k} - \frac{\ln(1+2k)}{k} \right] + \frac{\ln(1+2k)}{k} - \frac{1+3k}{(1+2k)^2} \right) & \text{if } k \leq 0.2 \\ Z \frac{8}{3}\pi r_e^2 \frac{1}{(1+2k)^2} \left(1 + 2k + \frac{6}{5}k^2 - \frac{1}{2}k^3 + \frac{2}{7}k^4 - \frac{6}{35}k^5 + \frac{8}{105}k^6 + \frac{4}{105}k^7 \right) & \text{if } k > 0.2 \end{cases} \tag{6}$$

Where k is the ratio of the photon energy and the electron's rest mass energy ($k = E_\gamma / E_e$) and r_e is the classical electron radius ($r_e = e^2/E_e$).

The resulting energy of the incident photon after undergoing Compton scattering is given by the following equation:

$$E'_\gamma = \frac{E_\gamma}{1 + k(1 - \cos\theta)}. \tag{7}$$

Making the energy loss to be $E_\gamma - E'_\gamma$, being E_γ the photon energy before Compton scattering and E'_γ the photon energy after Compton scattering. In equation 7 we also find a dependence with an angle θ. This is the deflection angle of the photon after undergoing Compton scattering. The "probability distribution" of is given by the Klein-Nishina formula, see equation 8 (where $\alpha \approx 1/137.035$ is the fine-structure constant).

$$\frac{d\sigma}{d\Omega}(E_\gamma, E'_\gamma, \theta) = \frac{\hbar^2\alpha^2c^2}{2E_e^2}\left(\frac{E'_\gamma}{E_\gamma}\right)^2\left[\frac{E'_\gamma}{E_\gamma} + \frac{E_\gamma}{E'_\gamma} - \sin^2\theta\right] \tag{8}$$

Note: With equation 7 and equation 8 we can calculate $d\sigma/d\Omega$ for every angle θ for a particular incident photon energy E_γ (or k):

$$\frac{d\sigma}{d\Omega}(k, \theta) = \frac{\hbar^2\alpha^2c^2}{2E_e^2}\left[\frac{1}{1+k(1-\cos\theta)}\right]^2\left[\frac{1}{1+k(1-\cos\theta)} + 1 + k(1-\cos\theta) - \sin^2\theta\right] \tag{9}$$

The quantity $d\sigma/d\Omega$ is defined as a **differential cross-section**. But for the assignment at hand, we will look at it as an angle probability distribution. In other words, we will use it to answer the following question: For an incident photon energy of E_γ, what is the likelihood of having a deflection of θ in the trajectory of the photon?

5 Particle transport and Monte Carlo implementation

To create our simple particle transport code, first we will have to:

1. Implement nuclear decay.
2. Use the nuclear decay results to create a specific discrete gamma spectrum.
3. Use the Klein-Nishina equation and the energy variation equation to implement Compton scattering (calculate the resulting energy and deflection angle of the incident photon after interaction).
4. Study the probability of a photon of undergoing PE interaction and being absorbed.

At this point we should be able to see that the physical processes that photons during their generation, and their movement through matter until they get absorbed are of random nature. Therefore, we will rely on Monte Carlo methods to create a program for particle transport calculation.

5.1 Monte Carlo implementation of nuclear decay (points 1 and 2)

From the exponential decay law we can define the probability of a nucleus of **not** decaying in a time interval Δt as $P_{no-decay}(\Delta t) = e^{-\lambda \Delta t}$. Consequently, the decay probability in a time interval Δt of a nucleus will be $P_{decay}(\Delta t) = 1 - P_{no-decay}(\Delta t) = 1 - e^{-\lambda \Delta t}$.

To replicate this phenomena we will go from 0 to $t_{max} = n \cdot \Delta T$ in Δt steps (n would corrspond to the total number of steps to take). At every step we will draw a random number and use $P_{decay}(\Delta t)$ or $P_{no-decay}(\Delta t)$ to determine whether we have a decay or not. The we will do:

- In the case of having a decay we will reduce by one the amount of initial nuclei ($N_1(n_i \Delta t) = N_1(n_{i-1} \Delta t) - 1$) and increase by one the amount of new nuclei ($N_2(n_i \Delta t) = N_2(n_{i-1} \Delta t) + 1$).

- In the case of **not** having a decay we will do $N_1(n_i \Delta t) = N_1(n_{i-1} \Delta t)$ and $N_2(n_i \Delta t) = N_2(n_{i-1} \Delta t)$ and go to the next step.

Note: the time step and max time should be chosen accordingly to the decay constant of the nucleus at hand.

5.1.1 Gamma decay spectrum

In gamma decay the initial nuclei transforms emitting a photon. The reaction that we get corresponds to $X_1 \rightarrow X_2 + \gamma$ where X_1 is the initial nucleus, X_2 is the nucleus resulting from the decay and γ is the emitted photon. The energy spectrum of these emitted photons is discrete, this means that during evey decay event the emitted photon would have an E_1 energy with a P_1 probability, a E_2 energy with a P_2 probability and so on. Randomly drawing an energy value from the corresponding discrete $P(E)$ distribution every time we have a decay we would replicate the energy spectrum.

5.2 Monte Carlo implementation of particle transport

In a Monte Carlo simulation of particle transport the path that a particle follows when moving thorugh matter is discretized. At every step of the particle's path it can be subject of physical interactions (the particle's probabilities of undergoing different interactions will be different). Depending on the inteaction that the particle undergoes, its energy and direction will change. A Monte Carlo algorithm will allow us to track individual particles at every step of its path and record/save data on its energy loss and deflection angles.

In our photon transport case we will track individual photons when moving through a known medium (known Z) in steps of size l.

1. The initial energy E_0 of the tracked photons will be determined by gamma decay energy spectrum. And for simplicity the initial position of the photon will be $(x_0 = 0, y_0 = 0)$ with a $\theta_0 = 0$ rad.

2. For this E_0 we will solve the Klein-Nisina equation (equations 8 and 9) to obtain the corresponding $d\sigma/d\Omega$ for θ from 0 rad to 2π rad. The $d\sigma/d\Omega$ results to to create a probability distribution for θ.

3. Using the corresponding cross-sections/interaction probabilities we will determine if the tracked photon undergoes PE interaction or Compton scattering.

   (a) If the photon undergoes PE interaction it will be absorbed all its energy will be lost (stopping the particle tracking and getting out of the algorithm).

   (b) If the photon undergoes Compton scattering we will draw a deflection angle θ_{def} from the probability distribution created in step 2. With this angle, E_0 and equation 7, we will calculate the energy lost by the photon, the corresponding new energy of the photon (E_{new}) and the new direction that the photon follows ($\theta_{new} = \theta_0 + \theta_{def}$). We will now calculate and store the new position of the photon following $x_{new} = x_0 + l * \cos\theta_{def}$ and $y_{new} = y_0 + l * \sin\theta_{def}$, store the energy loss, and repeat from point 1 making the initial conditions $E_0 = E_{new}$, $\theta_0 = \theta_{new}$, $x_0 = x_{new}$ and $y_0 = y_{new}$ until we the photon is absorbed (i.e., until point 3(a) is reached).

In order to get good statistics and ”reliable” results we will have to track a very large number of photons and agregate the results.

6 Questions

1. Implement the middle square method and the linear congruential method, test them for different model parameters, study their limitations and compare them with a built-in random number generator.

2. Implement a Monte Carlo algorithm for a nuclear decay of an element of $\lambda = 0.3$ s^{-1} and compare your simulation results with the analytical solution given by equation 2 (use a built-in random number generator to do so). Study the uncertainties of the results when you perform the same simulation several times and agregate the results. What is the error of $N(t)$? Do you find a time dependence in it? How do the $N(t)$ results for a specific t from all simulations distribute around the analytical $N(t)$ value?

3. Adapt your nuclear decay algorithm to simulate a 3-step decay chain where the last nucleus is stable and we have $N_1(0) = N_0$ and $N_2(0) = 0$. If you use $\lambda_1 = 0.3$ s^{-1}, for what value of λ_2 do you find secular equilibrium?

4. Solve the Klein-Nishina equation for θ from 0 rad to 2π rad (equations 8 and 9) and plot $d\sigma/d\Omega$ for various incident photon energies (try to replicate Figure 3 and Figure 4 from [5]). How do these curves change if you introduce an initial angle different from zero?

5. Use the $d\sigma/d\Omega$ results to to create a probability distribution for θ. Test your probability distribution: if you randomly draw θ enough times, can you create a histogram that matches the original $d\sigma/d\Omega$ curve?

6. Implement a **particle trasport algorithm for photons** to study photon trajectories and energy loss distributions around a photon source placed whithin a material of Z between 0 and 92. Use your nuclear decay algorithm to generate random draws from a discrete gamma energy spectrum and assume that all photons are emitted in the same direction (i.e., same initial angle). These will consitute the initial conditions for the tracked photon. Select two values for Z, a low one (to imitate a gas medium) and

a high one (to imitate a solid medium). Perform and compare some range estimations (distance that the photon travels from emission to absoption) and compare them, do your results make sense? If not, why? Plot some of the resulting trajectories from the photons. Can you show the amount of energy lost and where it has been lost by the photons?

Note: In order to make this simulation feasible we will have to make several asumptions:

- The discrete spectrum from our gamma decay will be: $E_1 = 135$ keV with 850 counts, $E_2 = 525$ keV with 13600 counts and $E_3 = 615$ keV with 2550 counts. Use the counts given to create a probability distribution.

- The photons move on the XY-plane.

- We only consider PE interactions and Compton scatering. And we will encounter one of these interactions at every step.

- The probability of a photon of being absorbed (undergoing a PE interaction) will go as $1 - \exp(-\sigma_{PE}(Z, E) \cdot l)$. Equation 5 lays $\sigma_{PE}(Z, E)$ and l is the step size used in our photon path discretization.

- The step size will be set as constant (Note: it could be approximated using $l = 1/\mu$ as a reference with μ being the linear attenuation coefficient. Use `https://physics.nist.gov/PhysRefData/XrayMassCoef/tab3.html` to find μ for elements up to $Z = 92$. Take the value of the 2nd coulumn for the initial energy of the photon and remember to multiply this number by the density of the chosen element).

7. Modify your particle transport algorithm to include some variability in the step size: make $l_i = l_0(1-\eta_i)$ with l_0 equal to the step size from question 6 and η_i a random number between 0 and 1.

8. Modify your particle transport algorithm to account for photons being emitted in any direction from the gamma decay source.

References

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[2] Shahmohammadi B.M., Krstic D., Nikezic D., Yu K.N. (2018). Monte Carlo studies on photon interactions in radiobiological experiments. PLOS ONE **13**(3):e0193575. `https:doi.org/10.1371/journal.pone.0193575`

[3] Fornalski, Krzysztof W (2018). Simple empirical correction functions to cross sections of the photoelectric effect, Compton scattering, pair and triplet production for carbon radiation shields for intermediate and high photon energies. *Journal of Physics Communications*. **2**(3):035038.

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[5] Davisson, C. M., Evans, R. D. (1952). Gamma-Ray Absorption Coefficients. *Reviews of Modern Physics*. **24**(2):79–107.

7 Figures

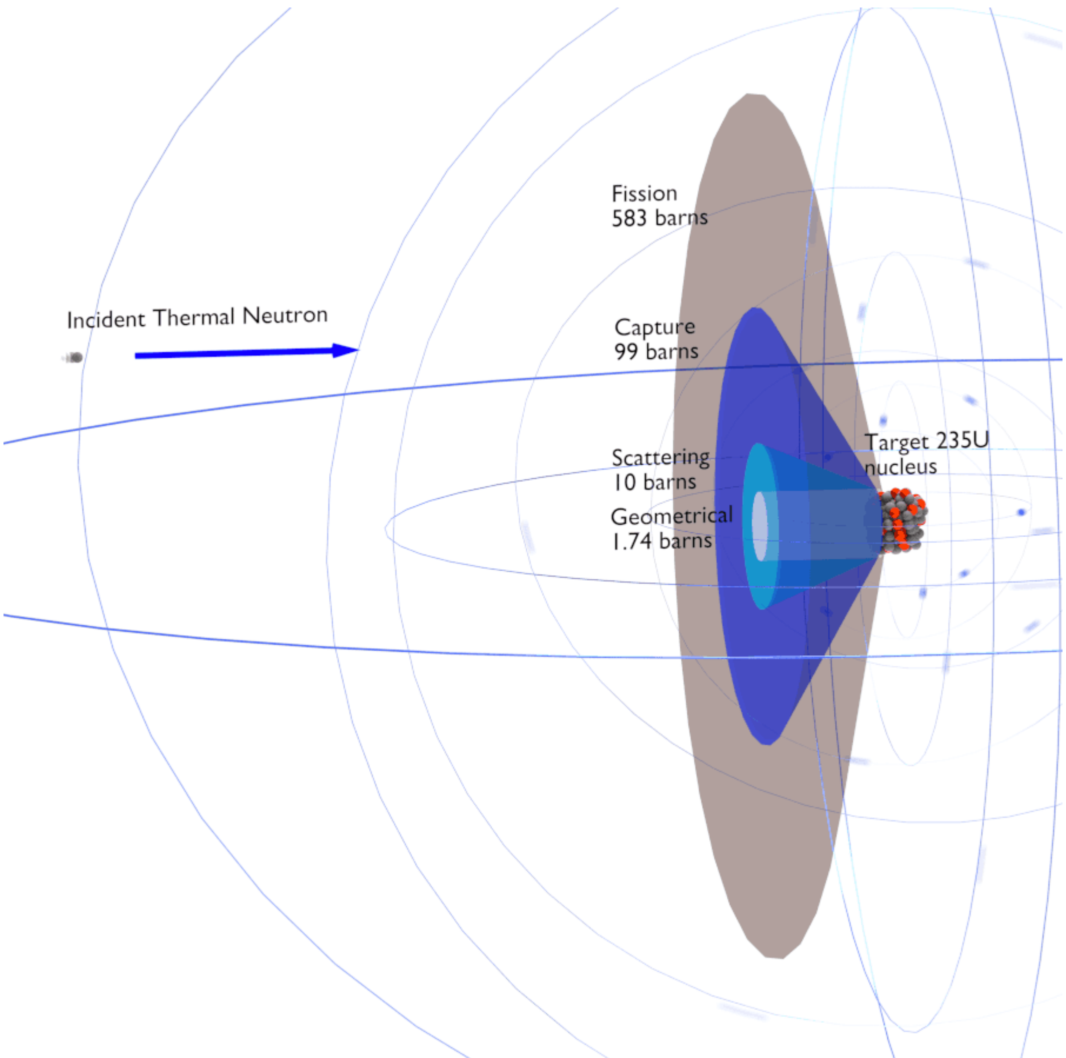

Figure 1: Sketch of an interaction cross-section for a neutron interacting with a nucleus of Uranium-235.

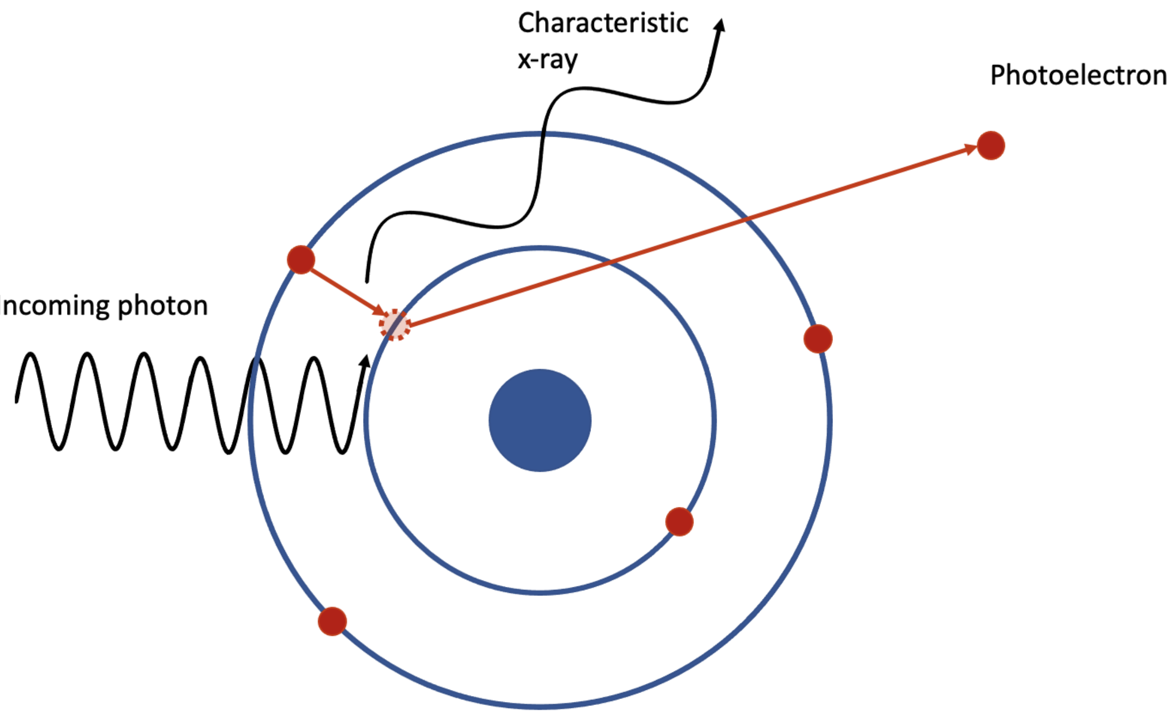

Figure 2: Sketch of a photoelectic interaction between an incoming photon and an atom.

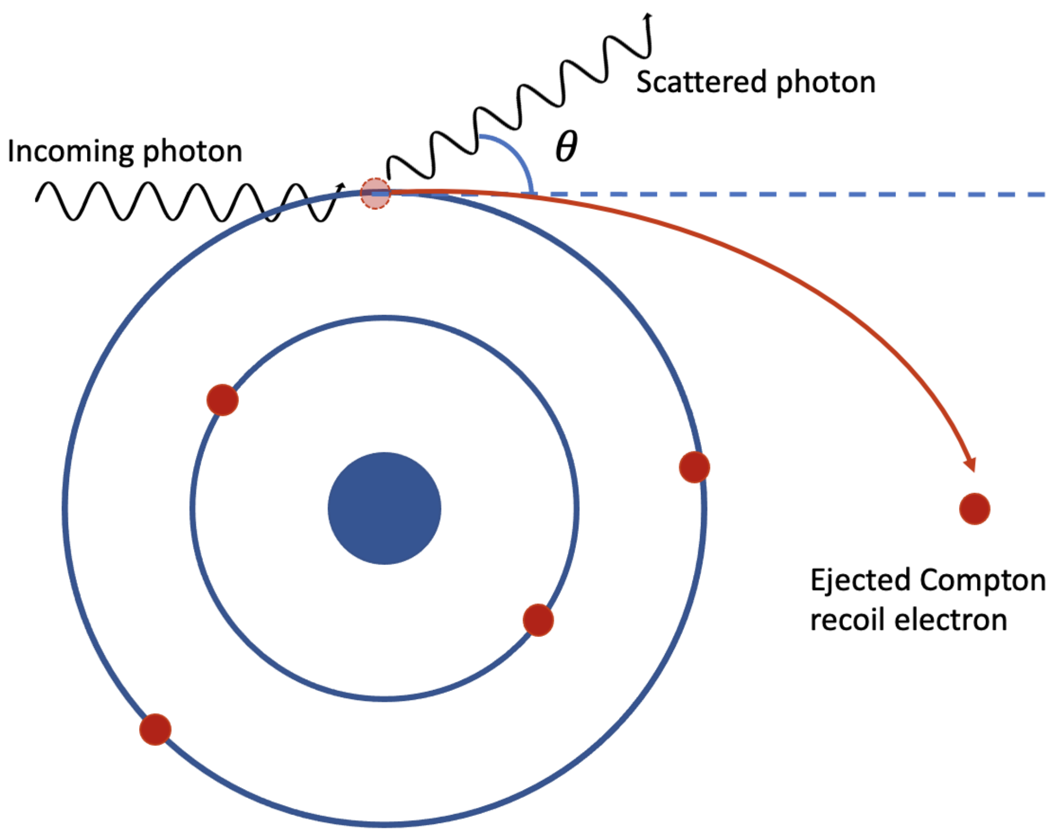

Figure 3: Sketch of a Compton scattering event between an incoming photon and an atom.