APPENDIX D

Calculating Scintillator Compton Spectra

(this text is from the Sophomore Lab Mathematica *application* Compton_Spectra1.nb *available on the lab network drive)*

Compton Scattering Formulas

Calculation of the probability of the scattering of a single high-energy photon by a single free electron initially at rest requires a fairly sophisticated quantum theory called *Quantum Electrodynamics*. The resulting equation is known as the *Klein-Nishina* formula, first derived jointly by Oskar Klein and Yoshio Nishina in 1929. The differential cross section for such scattering (integrated over all polarization states of the photon and electron) is given by the simple formula:

$$\frac{d\sigma}{d\Omega} = \frac{r_e^2}{2}\left(\frac{k}{k_0}\right)^2\left(\frac{k}{k_0} + \frac{k_0}{k} - \sin^2\theta\right) \tag{1}$$

Where θ is the angle from the inital photon path to the scattered photon path, $d\Omega = \sin\theta\, d\theta\, d\phi$ is the differential solid angle about the angles θ and ϕ (defining the outgoing photon direction), $k_0 = \hbar\omega_0$ is the initial photon energy, k is the outgoing photon energy, r_e is the *classical electron radius*, and σ is the scattering cross section. Even though expression (1) is simple, its derivation is subtle and is beyond the scope of this text.

The length r_e is one of the natural units of length for the electrodynamics of the electron and is formed from the electron's rest energy and charge. In Gaussian units, it is given by:

$$r_e = \frac{e^2}{m_e} = 2.817\times 10^{-13}\ \text{cm}$$

It is called the *classical electron radius* because a thin spherical shell of total charge e and radius r_e would have a total Coulomb potential energy of $m_e = 0.511$ MeV, the rest energy of the electron. The situation for an actual electron is much more complex — this classical calculation doesn't include Planck's constant $\hbar$, and, as you might therefore expect, r_e is not relevant to a full quantum mechanical description of the electron. Interestingly, however, r_e turns out to be of the same order as the radius of a typical atom's nucleus.

The outgoing photon energy k can be derived from the incoming photon energy k_0 and the electron rest energy m_e using simple relativistic kinematics of an elastic collision of two point particles (that is, using conservation of energy and linear momentum), where the photon's rest mass is 0:

$$\frac{k_0}{k} = 1 + \frac{k_0}{m_e}(1 - \cos\theta) \tag{2}$$

The recoil kinetic energy of the target electron is simply the difference $t_e = k_0 - k$. The maximum recoil kinetic energy the electron could receive happens when $\theta = \pi$; in this case we have:

$$k_{\text{min}} = \left(\frac{1}{k_0} + \frac{2}{m_e}\right)^{-1} \tag{3}$$
$$(t_e)_{\text{max}} = k_0 - k_{\text{min}}$$

The minimum outgoing photon energy k_{min} is called the *backscatter energy* and approaches $m_e/2$ for large k_0. The maximum electron recoil kinetic energy defines the *Compton edge*, the maximum energy observed in a scintillator Compton scattering spectrum. The minimum electron recoil kinetic energy is, of course, 0 (when $\theta = 0$) The functions **`BackscatterEdge[]`** and **`ComptonEdge[]`** are provided to calculate k_{min} and $(t_e)_{\text{max}}$.

To calculate the expected Compton scattering spectrum observed in a scintillation detector, we need to know the probability of scattering as a function of the electron's recoil kinetic energy, since it is this energy to which the detector responds. To convert equation (1) to an expression for $d\sigma/dt_e$, we note that:

$$\frac{d\sigma}{dt_e} = \frac{d\sigma}{d\Omega}\,\frac{d\Omega}{dt_e} = \frac{d\sigma}{d\Omega}\,\frac{d\Omega}{d\theta}\,\frac{d\theta}{dt_e} = -\frac{d\sigma}{d\Omega}\,\frac{d\Omega}{d\theta}\,\frac{d\theta}{dk}$$

Now, since we want $\Omega(\theta)$ in this expression, we must integrate over the azimuth angle ϕ, so that $d\Omega(\theta) = 2\pi\sin\theta\;d\theta$, and from equation (2):

$$\frac{d\theta}{dk} = \frac{d}{dk}\left(\frac{k_0}{k}\right)\Big/\frac{d}{d\theta}\left(\frac{k_0}{k}\right) = -\left(\frac{k_0}{k^2}\right)\Big/\left(\frac{k_0}{m_e}\sin\theta\right) = -\frac{m_e}{k^2\sin\theta}$$
$$\therefore \frac{d\sigma}{dt_e} = \frac{2\pi m_e}{k^2}\,\frac{d\sigma}{d\Omega} \tag{4}$$

From equation (2), we can get an expression for θ to substitute into (1) and then (4):

$$\cos\theta = 1 - \frac{m_e(k_0-k)}{k_0\,k} = 1 - \frac{m_e\,t_e}{k_0\,k}$$
$$\therefore \sin^2\theta = 2\left(\frac{m_e\,t_e}{k_0\,k}\right) - \left(\frac{m_e\,t_e}{k_0\,k}\right)^2$$

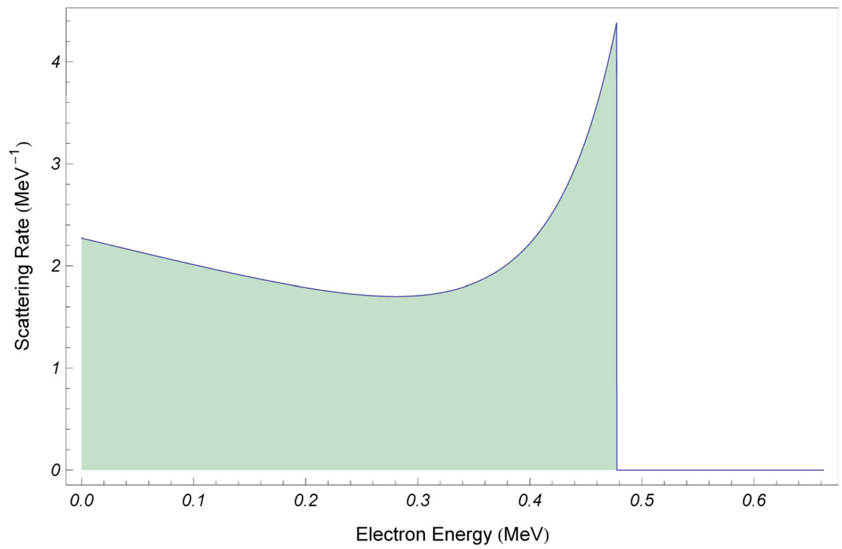
$$\therefore \frac{d\sigma}{dt_e} = \left(\frac{\pi m_e r_e^2}{k_0^2}\right)\left(\frac{k}{k_0} + \frac{k_0}{k} - 2\left(\frac{m_e\,t_e}{k_0\,k}\right) + \left(\frac{m_e\,t_e}{k_0\,k}\right)^2\right);\; k = k_0 - t_e \tag{5}$$

To convert the expression (5) into a probability density for observing Compton scattered electrons with various recoil energies t_e, we note that the probability density is proportional to the differential cross section $d\sigma/dt_e$, but must be normalized so that the total probability is 1:

$$P(t_e\,;k_0)\,dt_e \propto \left(\frac{k}{k_0} + \frac{k_0}{k} - 2\left(\frac{m_e\,t_e}{k_0\,k}\right) + \left(\frac{m_e\,t_e}{k_0\,k}\right)^2\right)dt_e$$
$$\int_0^{(t_e)_{\max}} P(t_e\,;k_0)\,dt_e = 1$$

$$\therefore P_{\text{Compton}}(t_e\,;k_0) = \frac{1}{A}\left(\frac{k}{k_0} + \frac{k_0}{k} - 2\left(\frac{m_e\,t_e}{k_0\,k}\right) + \left(\frac{m_e\,t_e}{k_0\,k}\right)^2\right);\; k = k_0 - t_e$$
$$A \equiv \left(2\left(k_0^3 + 9\,k_0^2\,m_e + 8\,k_0\,m_e^2 + 2\,m_e^3\right)\right)\Big/(2\,k_0 + m_e)^2 + \left(2\,k_0 - 4\,m_e - \frac{4\,m_e^2}{k_0}\right)\tanh^{-1}\!\left(\frac{k_0}{k_0 + m_e}\right) \tag{6}$$

The following figure shows a plot of $P(t_e)$ from equation (6) for an incoming photon with $k_0 = 0.662$ MeV (this plot was generated using the function `ComptonPDF[]`):



Detector Resolution

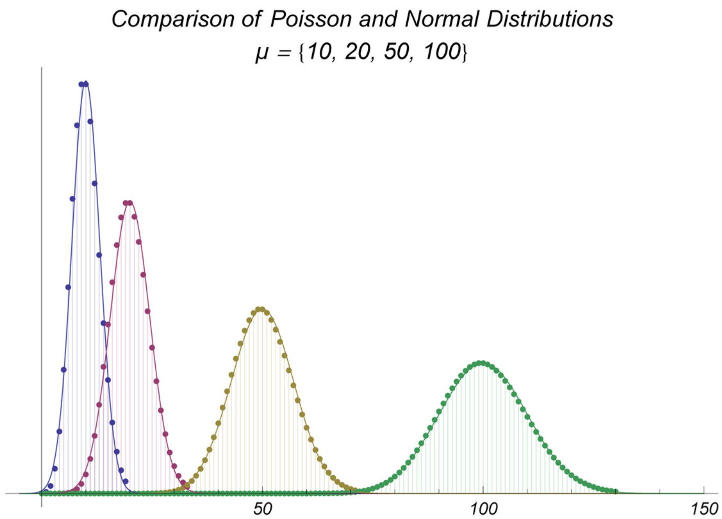
Following a Compton scattering event in a scintillation detector the outgoing electron loses most of its kinetic energy by ionizing other atoms in the scintillator material. Eventually most of the original energy deposited by the incoming photon is converted to the total ionization energy of many slowly-moving electrons in the material (the electrons are near the bottom of the *conduction band* of the scintillator material). The scintillator material is engineered so that these electrons recombine with the ionized atoms mainly through the efficient production of visible-light photons. Many of these photons are detected by a photomultiplier tube attached to the scintillator, and it is the photomultiplier's output signal which is amplified and analyzed to estimate the energy deposited in the scintillator material by the incoming photon.

Unfortunately, only a fraction of the visible-light photons generated by the scintillator are absorbed by the photomultiplier's *photocathode* (this fraction defines the *quantum efficiency* of the detector). Nearly all of the absorbed photons cause a *photoelectron* to be emitted by the photocathode. The collection of photoelectrons comprise the signal which is then amplified by the photomultiplier to produce its output. The absorption of any particular photon is random; the statistics of the absorption process are well-described by the *Poisson distribution*, a discrete distribution with the single parameter μ, the expected (mean) number of events. Equations (7) and (8) give the probability density functions of the Poisson and the familiar normal (Gaussian) distributions:

$$\text{Poisson Distribution}: \quad P_P(k\,;\mu) = \frac{e^{-\mu}\,\mu^k}{k\,!} \tag{7}$$

$$\text{Normal Distribution}: \quad P_G\left(x\,;\mu,\,\sigma^2\right) = \frac{1}{\sqrt{2\pi\sigma^2}}\,e^{-\frac{(x-\mu)^2}{2\sigma^2}} \tag{8}$$

The variance of the Poisson distribution is equal to its mean, μ. For $\mu \gg 1$, the Poisson distribution approaches that of a normal distribution with mean and variance both equal to μ, as illustrated by the following figure:



Since the standard deviation grows only as $\sqrt{\mu}$, the family of Poisson distributions is characterized by peaks which are relatively more well-defined for larger μ values.

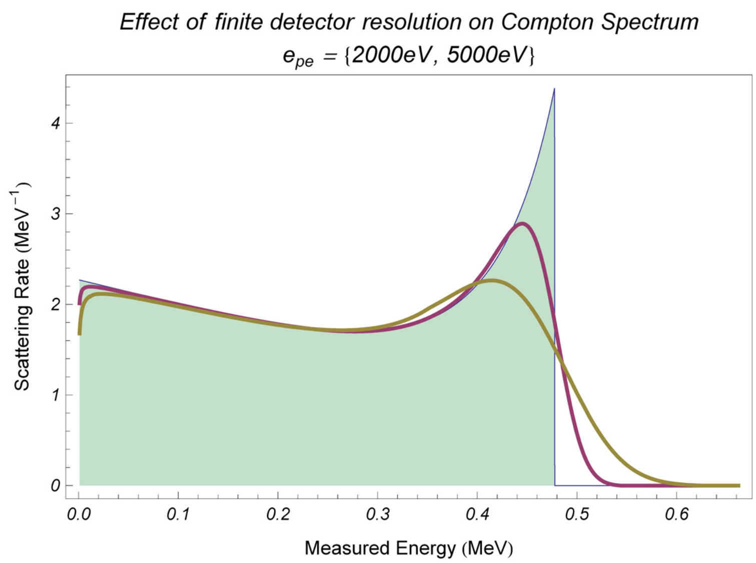
A well-engineered scintillation detector produces a number of visible-light photons which is very nearly proportional to the energy deposited by an incoming high-energy photon over a wide range of energies. The quantum efficiency of the system is also nearly independent of the number of visible-light photons produced, so that a scintillation system's resolution as a function of energy may be accurately characterized by a single parameter: the *average energy per photoelectron*, or e_{pe}. The kinetic energy a high-energy photon imparts to a scintillator electron during a Compton scatter, t_e, will on average result in the generation of $\mu = t_e / e_{\text{pe}}$ photoelectrons by the photomultiplier's photocathode. The actual number of photoelectrons produced by events with energy t_e will vary randomly, as samples of the Poisson distribution with mean t_e / e_{pe}. This distribution has a fractional standard deviation of $\sqrt{\mu} / \mu = \sqrt{e_{\text{pe}} / t_e}$, so the resolution of the scintillation detector improves as e_{pe} is made smaller. Typical values for e_{pe} range from $\lesssim 1000\,\text{eV}$ for a good sodium iodide (NaI) scintillator to $> 5000\,\text{eV}$ for a plastic (organic) scintillator.

The finite resolution of the detector can be modeled by its *response function*, $R(t\,;\,t_e,\,e_{\text{pe}})$. The response function is a distribution which gives the probability density that the detector will respond with an output corresponding to energy t as a result of energy t_e actually being deposited in the scintillator. Since the detector output is characterized by the discrete Poisson distribution, the response function $R(t\,;\,t_e,\,e_{\text{pe}})$ must be discrete as well. We will, however, make use of the similarity of the normal and Poisson distributions for large μ and consider $R(t\,;\,t_e,\,e_{\text{pe}})$ to be well represented by the continuous normal distribution, equation (8), with mean and variance determined by the values of t_e and e_{pe}, as shown in equation (9).

$$R(t\,;\,t_e,\,e_{\text{pe}}) = P_G(t\,;\,t_e,\,e_{\text{pe}}\,t_e) = \frac{1}{\sqrt{2\pi\,e_{\text{pe}}\,t_e}}\,e^{-\frac{(t-t_e)^2}{2\,e_{\text{pe}}\,t_e}} \tag{9}$$

With the response function R in hand, the observed Compton spectrum of an incoming photon with energy k_0, which includes the effects of the finite detector resolution, may be calculated. The expression for the probability density of the measured energy t involves a generalization of a *convolution integral* of the Compton scattering distribution (6) and the response function (9), as shown in expression (10).

$$P_{\text{observed}}(t\,;k_0,\ e_{\text{pe}}) = \int_0^{(t_e)_{\max}} R(t\,;t_e,\ e_{\text{pe}})\, P_{\text{Compton}}(t_e\,;k_0)\, dt_e \tag{10}$$



The figure above shows the results of the convolution on the measured Compton scattering distribution for an incoming photon with $k_0 = 0.662$ MeV. This figure was generated using the functions **`ComptonPDF[]`** and **`SmoothedComptonPDF[]`**.