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Title: Doppler Energy Broadening for Incoherent Scattering in MCNP5, Part I

Author(s): Avneet Sood (X-5, LANL)

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ABSTRACT

Incoherent scattering of an incident photon can occur with a bound electron in a shell of a material and will generate a Compton electron and a scattered photon. The electron binding effects become important when the incident photon energy is near a few hundred keV. The result of the binding effects on the angle and energy of the scattered photon must be taken into account for accurate simulation of low-energy photon transport.

The effect of the bound electron on the scattered photon's *angular* **distribution appears as a reduction in the total scattering cross section in the forward direction. MCNP4C3 accounts for the electron binding effects on the angular distribution of the scattered photon by modifying the Klein-Nishina differential cross section with a form factor. The electron binding effect on the scattered photon's** *energy* **distribution appears as a broadening of the energy spectrum due to the precollision momentum of the electron. This effect on the energy distribution of the incoherently scattered photon is called photon Doppler broadening. MCNP4C3 does not account for the energy broadening of the scattered photon. MCNP5 includes this photon Doppler broadening physics treatment.**

The purpose of this research note is to give a review of incoherent (Compton) scattering treatment in MCNP5 and document the methods and new data used to include photon Doppler energy broadening in MCNP5. It summarizes internal MCNP-team documentation. A follow-up research note documents the explicit details to the integration of this new physics feature.

Introduction

Incoherent (Compton) scattering is an increasingly important interaction mechanism for low-energy photons scattering down to a few hundred keV. The photon Doppler effect considers the precollision motion of the electron for incoherent scattering and is important for accurately simulating the transport of photons in this low-energy range. The most dramatic effect appears in the pulse height spectra in the prediction of energy distribution in the region near the Compton edge and the associated continuum. This can be seen when comparing Monte Carlo simulated results and experimental results for sources of a few keV. Electron binding effects are important in other areas including X-ray shielding and radiation background calculations involving deep penetration of low-energy photons. The need for accurate simulation of low-energy photon transport is increasing due to the wide use of low-energy photons in medical applications and other fields.

Previous Work

Evidence of the need for photon Doppler energy broadening has been documented very well in the past few years (Namito, 1994 and Lee, 2000). Direct comparison of experimental and calculated pulse height spectra demonstrates the dramatic difference in the Compton region (Namito, 1994 and Sood, 2004). As incident photon energy increases, the effect of the precollision momentum of the electron decreases the effect on the predicted pulse height spectra. This effect becomes increasingly negligible as incident photon energies exceed a few hundred keV.

The modification of the angular distribution has been accounted for by several Monte Carlo transport codes by using an incoherent scattering function multiplying the total cross section. The effect of the incoherent scattering function is to decrease the Klein-Nishina cross section per electron more extremely in the forward direction for low-energy and for high Z, independently. However, the broadening of the scattered photon energy is not treated by many versions of general purpose Monte Carlo transport codes like ITS 3.0, EGS4, and MCNP4C3.

The first inclusion of the photon Doppler broadened energy in a Monte Carlo code that appears in the literature was by Felsteiner, Pattison and Cooper (1974) with the purpose to correct experimental Compton profiles for the effect of multiple scattered photons in their measurement sample. A standard method of implementing photon Doppler broadening was set forth by Namito, Ban, and Hirayama (1994) in an improved version of EGS4. Their paper provides a discussion of the formulas for describing the photon Doppler broadening, incoherent scattering function, and total incoherent cross section of a low-energy photon. The method outlined by Namito et al (1994) is implemented in MCNP5. This note provides some of the details for the equations in the literature usually stated without derivation. This note also indicates some of the software and data quality checks for the new MCNP5 physics feature.

A First-Principles Review of Incoherent Scattering [1]

Incoherent Scattering with an Unbound Electron

In an incoherent (Compton) scatter, a photon collides with an atomic electron. If the electron is considered to be unbound, the conservation of energy equation can be written as:

$$E = E' + E'_e \tag{1}$$

where E and E' are the initial and scattered photon energies and E'_e is the scattered electron energy. The initial and scattered photon momentum are related by:

$$mc\vec{\mathbf{k}} = mc\vec{\mathbf{k}}' + \vec{\mathbf{p}}' \tag{2}$$

[1] These derivations were done to interpret the equations seen in the literature while studying incoherent scattering in graduate school along with other students. (Peplow (1999), Lee (2000))

where $\vec{\mathbf{k}}$ and $\vec{\mathbf{k}'}$ are the initial and scattered photon momentum, respectively, and $\vec{\mathbf{p}'}$ is the scattered electron momentum.

It will be useful to relate the magnitude of the scattered electron's momentum to its scattered energy. The magnitude of the scattered electron's momentum, p, is related to its scattered energy by examining the squares of the relativistic energy and momentum equations:

$$E'_e = \frac{mc^2}{(1-\frac{v^2}{c^2})^{1/2}} \quad (3)$$

$$p' = \frac{mv}{(1-\frac{v^2}{c^2})^{1/2}} \quad (4)$$

to get:

$$p'^2c^2 = E'^2_e + 2mc^2E'_e \quad (5)$$

To understand the literature, it is useful if we define the scattering vector, $\vec{\mathbf{q}}$, as the momentum gained by the photon:

$$\vec{\mathbf{q}} = mc(\vec{\mathbf{k}'} - \vec{\mathbf{k}}) \quad (6)$$

$$\vec{\mathbf{q}} = -\vec{\mathbf{p}}' \quad (7)$$

and examine $\vec{\mathbf{q}}^{\mathbf{2}}$, the dot product of $\vec{\mathbf{q}}$:

$$\vec{\mathbf{q}}^{\mathbf{2}} = \vec{\mathbf{p}}' \cdot \vec{\mathbf{p}}' \quad (8)$$

$$\| \vec{\mathbf{p}}' \|^2 = (mc)^2(k^2 + k'^2 - 2kk'\cos(\theta)) \quad (9)$$

where k and k' are the magnitude of the initial and scattered photon's momentum, respectively, and θ is the scattered angle of the photon.

If we insert $E'_e = E - E'$ into equation 5:

$$p^2c^2 = (E-E')^2 + 2mc^2(E-E') \quad (10)$$

and substitute $k = E/mc^2$, we get:

$$\frac{p'^2}{(mc)^2} = (k-k')^2 + 2(k-k') \quad (11)$$

We can use this result with eqn.9, to give:

$$(k^2 + k'^2 - 2kk'\cos(\theta)) = (k-k')^2 + 2(k-k') \quad (12)$$

$$\boxed{k' = \frac{k}{1+k(1-\cos(\theta))}} \quad (13)$$

or, in terms of energy:

$$\boxed{E' = \frac{E}{1+\frac{E}{mc^2}(1-\cos(\theta))}} \quad (14)$$

Equations 13 and 14 relate the scattered photon's energy and angle after an incoherent scatter with a free electron and are often seen in many textbooks and papers.

The momentum transfer to the scattered photon can be quantified using the scattering vector (Eqn.6) and the relativistic momentum of the electron (Eqn 5).

$$c^2\vec{\mathbf{q}}^{\mathbf{2}} = (c\vec{\mathbf{p}}')^{\mathbf{2}} \tag{15}$$

$$= (E-E')^2 + 2mc^2(E-E') \tag{16}$$

Using $k = E/mc^2$ and Eqn. 13, we get (after quite a bit of algebraic manipulations):

$$\frac{q}{mc} = 2k\sin\frac{\theta}{2}\frac{\sqrt{1+(k^2+2k)\sin\frac{\theta}{2}}}{1+2k\sin^2\frac{\theta}{2}} \tag{17}$$

which is the same equations that many texts and papers show.

Klein-Nishina Differential Cross Section

The angular differential cross section for an unpolarized photon incoherently (Compton) scattering with a free electron has been described by Klein and Nishina as:

$$\frac{d\sigma_{KN}}{d\Omega} = \frac{r_e^2}{2}\frac{k(1-\cos(\theta))}{(1+k(1-\cos(\theta)))^3}\left[1+\cos^2(\theta)\frac{k^2(1-\cos(\theta))^2}{1+k(1-\cos(\theta))}\right] \tag{18}$$

This has also been expressed as:

$$\boxed{\frac{d\sigma_{KN}}{d\Omega} = \frac{r_e^2}{2}\frac{E'^2}{E}\left[\frac{E}{E'}+\frac{E'}{E}-\sin^2(\theta)\right]} \tag{19}$$

The total cross section can be found by (Hubbell, 1975):

$$\sigma_{KN} = \int_\Omega \frac{d\sigma_{KN}}{d\Omega}(\theta,\phi)\sin(\theta)d\theta d\phi \tag{20}$$

$$\boxed{\sigma_{KN} = 2\pi r_e^2\left[\frac{1+k}{k^2}\left[\frac{2(1+k)}{1+2k}-\frac{\ln(1+2k)}{k}\right]+\frac{\ln(1+2k)}{2k}-\frac{1+3k}{(1+2k)^2}\right]} \tag{21}$$

Given the incident photon energy, E, Eqn.19 is sampled for the exiting angle. Equation 14 is used to determine the scattered photon's energy. The speed of calculating the Klein-Nishina distribution has been studied (Blomquist, 1983). Methods of sampling the Klein-Nishina include approximate inverse methods, rejection algorithms, and direct methods. The Kahn rejection scheme was found to be best at lower energies and the Koblinger direct method was better at higher energies. MCNP makes use of both Kahn's rejection and Koblinger's direct sampling methods when sampling the Klein-Nishina distribution for scattering angle.

MCNP developer's sidenote 1:

Additionally, MCNP (subroutine calcps) uses the Hasting's empirical fit (Koblinger, 1991) to determine the probability of scattering towards a point detector (MCNP4C manual, pg 2-58). This empirical fit should be replaced with the exact equation. When examining this empirical fit, Koblinger's textbook was found to have an error in Eqn. 3.10 for the analytically integrated Klein-Nishina differential cross section. This error has been reported to the authors and confirmed (Koblinger, 2002).

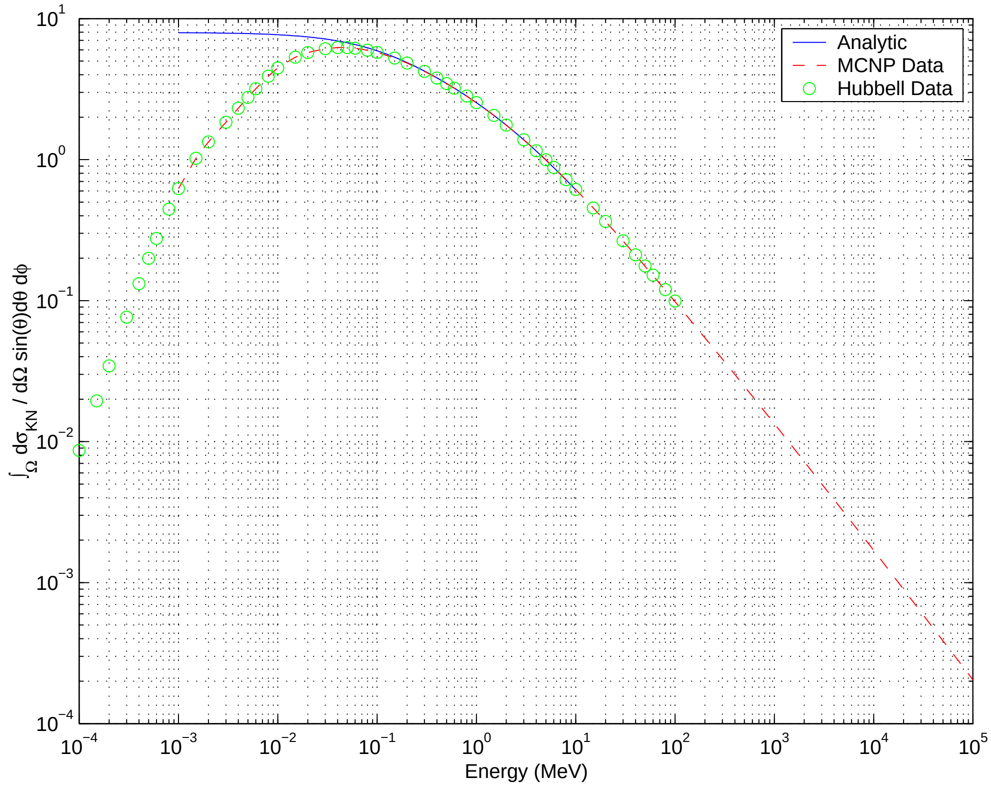

Figure 1: Comparison of Analytically Integrated Klein-Nishina and MCNP Klein-Nishina Data for Z=12

MCNP developer's sidenote 2:

Figure 1 compares the analytic calculation of the integral Klein-Nishina in Eqn. 21 for an unbound electron with the data used by MCNP4C and data published by Hubbell (Table II, Hubbell, 1975). The MCNP4C cross section values are obtained from the MCNP4C cross section plotter using an input deck with the 'simple physics' option and are used in the kinematics of the photon transport. The MCNP4C data (mcplib02) seems to depart from the analytic solution below 100 keV but agrees well with the data published by Hubbell. Figure 1 suggests that the 'simple physics' option in MCNP uses incoherent cross section data that includes the incoherent scatttering function and is contrary to the MCNP4C manual (pg. 2-56, April 2000).

Incoherent Scatter with a Bound Electron

Incoherent Scattering Factors

Incoherent scattering factors, S(x,Z), are used to account for the effects of bound electrons in an atom on the angular distribution of the scattered photon. Values of incoherent scattering factors for various elements are published in tabular form by Hubbell (Hubbell, 1975) as a function of x, the inverse length, and Z. Figure 2 shows an example of S(x,Z) directly from Hubbell's data for Z=12 (Hubbell, 1975).

When a photon undergoes an incoherent scatter with a bound electron in a Monte Carlo simulation, the cosine of the exit angle, θ, is sampled from a modified Klein-Nishina differential cross section:

$$\frac{d\sigma_{inc}}{d\Omega}(\theta,\phi) = \frac{d\sigma_{KN}}{d\Omega}(\theta,\phi)S(x,Z) \qquad (22)$$

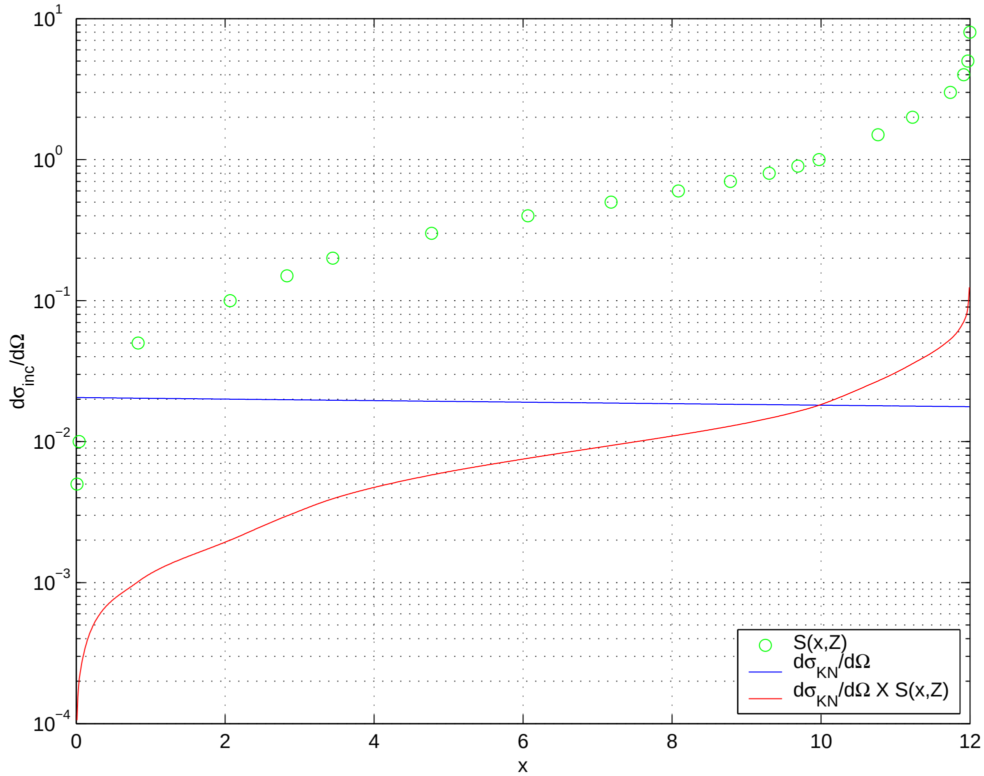

Figure 2: Comparison of Differential Klein-Nishina and Differential Klein-Nishina with Incoherent Scattering Function for Z=12

where S(x,Z) is the incoherent scattering factor. For any Z, S(x,Z) increases from zero until Z at Z=infinity. The parameter, x, is the inverse length.

$$\begin{aligned} x &= \sin(\theta/2)/\lambda \\ &= \kappa\alpha\sqrt{1-\mu} \end{aligned} \tag{23}$$

where κ=10^{-8} mc/(h $\sqrt{2}$) = 29.1445 cm $^{-1}$ and α is the initial photon energy in units of rest mass energy of an electron.

The cosine of the scattering polar angle, μ, is calculated by using either Kahn's rejection method or Koblinger's direct method which samples the Klein-Nishina formula exactly. The final angle is rejected according to the incoherent scattering function, S(x,Z). Figure 2 shows the effect of the incoherent scattering factor on the differential incoherent scattering cross section.

Hartree-Fock Compton Profiles

Bound electrons carry momentum which can add or subtract to the momentum of the scattered photon. The Hartree-Fock Compton profiles, J(p_z), are used to account for the effects of a bound electron on the energy distribution of the scattered photon. These Compton profiles are a collection of orbital and total atom data for 1≤Z≤102 tabulated as a function of the projected precollision momentum of the electron. Values of the Compton profiles for the elements are published in tabular form by Biggs, et al (Biggs, 1975) as a function of p_z. Figure 3 shows J(p_z) from Biggs's data.

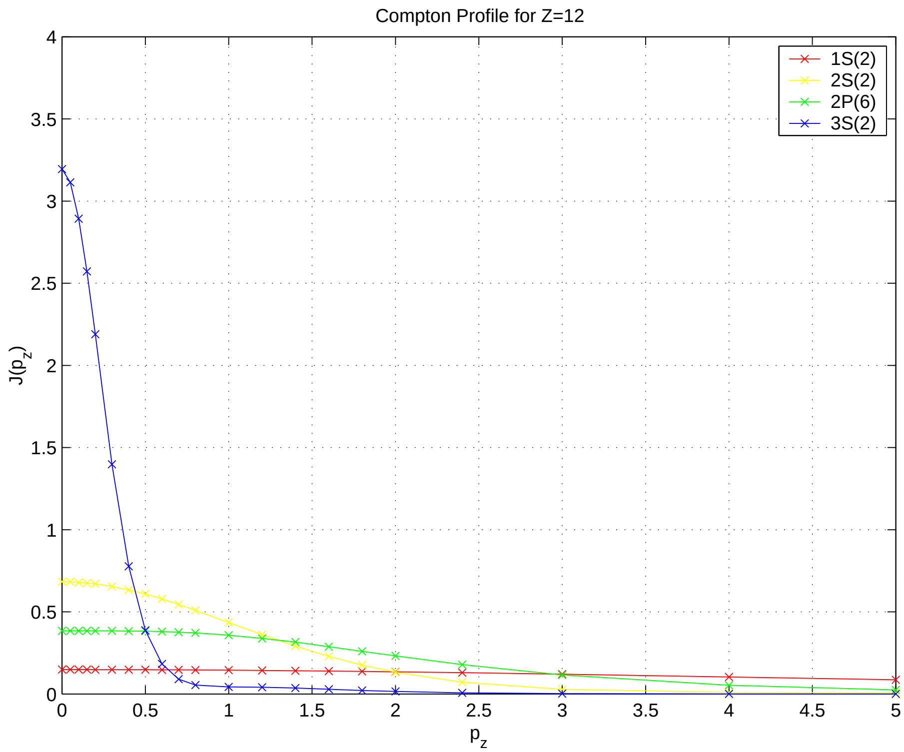

Figure 3: Shellwise Compton profile data for Z=12

It is useful to examine the basic conservation of energy and momentum principles to make use of the Compton profile data and to understand the various equations cited in the literature. The following equations are developed to illustrate the use of the Compton profile data to include photon Doppler energy broadening in MCNP5.

If the electron is considered to be bound, the conservation of energy and momentum equations can be written as:

$$E + E_e = E' + E'_e - E_b \tag{24}$$

$$mc\vec{\mathbf{k}} + \vec{\mathbf{p}} = mc\vec{\mathbf{k'}} + \vec{\mathbf{p'}} \tag{25}$$

where E_b is the binding energy of the orbital electron.

The scattering vector, $\vec{\mathbf{q}}$, is now defined as:

$$\vec{\mathbf{q}} = mc(\vec{\mathbf{k'}} - \vec{\mathbf{k}}) \tag{26}$$

$$\vec{\mathbf{q}} = \vec{\mathbf{p}} - \vec{\mathbf{p}}' \tag{27}$$

As done previously, if we examine $\vec{\mathbf{q}}^{\mathbf{2}}$, we get:

$$(\vec{\mathbf{p}} - \vec{\mathbf{p}}')^{\mathbf{2}} = (mc)^2(k^2 + k'^2 - 2kk' \cos(\theta)) \tag{28}$$

Using the squares of the conservation of energy and relativistic electron momentum, we get a similar result to Eqn. 5:

$$c^2\left[(p')^2 - p^2\right] = (E - E' - E_b)^2 + 2(E - E' - E_b)(mc^2 + E_e) \tag{29}$$

Eqn. 29 is particularly useful when examining p_z, the projection of the electron momentum on the scattering vector defined as $p_z = \vec{\mathbf{p}} \cdot \vec{\mathbf{q}}/q$.

$$\vec{\mathbf{p}}' = \vec{\mathbf{p}} - \vec{\mathbf{q}} \tag{30}$$

$$(p')^2 = p^2 - 2\vec{\mathbf{p}} \cdot \vec{\mathbf{q}} + q^2 \tag{31}$$

$$2\vec{\mathbf{p}} \cdot \vec{\mathbf{q}} = p^2 - (p')^2 + q^2 \tag{32}$$

$$2p_z q = p^2 - (p')^2 + q^2 \tag{33}$$

$$p_z = \frac{1}{2q}\left[p^2 - p'^2 + q^2\right] \tag{34}$$

Using Eqn. 29:

$$p_z = \frac{1}{2qc^2}\left[-(E - E' - E_b)^2 - 2(E - E' - E_b)(mc^2 + E_e) + c^2 q^2\right] \tag{35}$$

$$= \frac{(mc)^2}{2q}\left[-(k - k' - \frac{E_b}{mc^2})^2 - 2(k - k' - \frac{E_b}{mc^2})(1 + \frac{E_e}{mc^2}) + (\vec{\mathbf{k}}' - \vec{\mathbf{k}})^{\mathbf{2}}\right] \tag{36}$$

Inserting Eqn. 13 for k':

$$p_z = \frac{\left[(k' - k)(1 + \frac{E_e - E_b}{mc^2}) - kk'(1 - \cos(\theta)) + (1 + \frac{E_e}{mc^2})(\frac{E_b}{mc^2}) - \frac{1}{2}(\frac{E_b}{mc^2})^2\right]}{\sqrt{k^2 + k'^2 - 2kk'\cos(\theta)}} \tag{37}$$

If E_e and E_b are assumed to be small, this reduces to:

$$\boxed{\frac{p_z}{mc} = \frac{k' - k - kk'(1 - \cos(\theta))}{\sqrt{k^2 + k'^2 - 2kk'\cos(\theta)}}} \tag{38}$$

or, in terms of energy:

$$\boxed{p_z = -137\frac{E - E' - EE'(1 - \cos(\theta))/mc^2}{\sqrt{E^2 + E'^2 - 2EE'\cos(\theta)}}} \tag{39}$$

where p_z is in atomic units of $mc^2/\bar{h}$. Equations 38 and 39 are the familiar forms seen in the literature.

The Hartree-Fock Compton profiles are a collection of orbital and total atom data tabulated as a function of the projected precollision momentum of the electron on the momentum transfer vector of the photon as described by Eqn. 38, where p_z is in atomic units of $mc^2/\bar{h}$. The scattered energy of a Doppler broadened photon can be calculated by selecting an orbital shell, sampling the projected momentum from the Compton profile, and calculating the scattered photon energy. Figure 3 shows the Compton profile for Z=12 for each shell. The Compton profiles are related to the incoherent scattering function, S(x,Z) by:

$$S(x, Z) = \sum_k \int_{-\infty}^{p_z^{max}} J_k(p_z, Z)dp_z \tag{40}$$

where k refers to the particular electron subshell, $J_k(p_z, Z)$ is the Compton profile of the k-th shell for a given element, and p_z^{max} is the maximum momentum transferred and is calculated from Eqn. 39 using $E' = E - E_b$.

Summary

This research note has reviewed the equations and methods required to simulate an incoherent scatter of a photon assuming either a free or bound electron. Analytic equations for the incoherent scattering cross section are provided under the free electron assumption. Comparisons are made to data existing in the MCNP4C data libraries and literature. The comparison implies that the 'simple physics' option in MCNP uses the photon data that implicitly contains the incoherent scattering function. This is contrary to the MCNP4C manual (April 2000).

The effect of the bound electron on the scattered photon's *angular* distribution is taken into account using an incoherent scattering function. The scattering angle is calculated by sampling the Klein-Nishina and rejecting according to the incoherent scattering function. The effect of the bound electron on the scattered photon's *energy* distribution is taken into account using the Hartree-Fock Compton profile. The scattered photon energy is calculated by sampling the projected momentum from the Compton profile data and directly calculating the final energy.

Action items include:

- Change MCNP4C manual documentation (April 2000) page 2-56 from:

  '*...The photoelectric effect is regarded as an absorption (without fluorescence), scattering (Compton) is regarded to be on free electrons (without use of form factors), and the highly forward coherent Thomson scattering is ignored.*'

  to

  '*...The photoelectric effect is regarded as an absorption (without fluorescence). The kinematics of Compton scattering is assumed to be with free electrons (without the use of form factors or Compton profiles). The total scattering cross section, however, includes the incoherent scattering factor regardless of the use of simple or detailed physics. Thus, strict comparisons with codes using only the Klein-Nishina differential cross section are not valid. Highly forward coherent Thomson scattering is ignored.*'

- Change page 3-118, first full paragraph from:

  The simple physics treatment, intended...Compton scattering from free electrons without the use of form factors,...

  to

  The simple physics treatment, intended...Compton scattering,...

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