



# MCS Photon Physics

2017.01.31

Prof. Deokjung Lee

UNIST

## CONTACT

**Ulsan National Institute of Science and Technology**

**Address** 50 UNIST-gil, Ulsu-gun, Ulsan, 44919, Korea  
**Tel.** +82 52 217 0114 **Web.** www.unist.ac.kr



Computational Reactor physics & Experiment lab  
**Tel.** +82 52 217 2940 **Web.** reactorcore.unist.ac.kr

# Purpose of this lecture

- **Teach photon physics**
  - Particle interaction
  - Photon data
  - Theoretical basis of formulas
  
- **Teach state of the art Monte Carlo methods applied to photon physics**
  - Interpolation laws
  - Random sampling techniques
  
- **Provide full understanding of MCS photon-transport subroutines**
  - Implementation choices
  - Validation cases

- 1. Overview of photon transport physics**
- 2. Rayleigh (coherent) scattering**
- 3. Photoelectric effect**
- 4. Pair production**
- 5. Compton (incoherent) scattering**
- 6. Atomic relaxation**
- 7. Thick-Target Bremsstrahlung (TTB)**
- 8. Photon KERMA**
- 9. Verification & Validation**

# 1. Photon transport physics

---

Overview  
9 slides



- **Motivation: complex deep-penetration shielding problems**
  - Photon KERMA / body-equivalent dose
  - Spent nuclear fuel transport/storage casks
  - Reactor shielding
  
- **Implementation in MCS version 0.0.76 (4) (2017, Dec. 12):**
  - Fixed-photon-source simulation only
  - Photon energy simulation domain: 1 keV to 20 MeV
  - For all elements  $1 \leq Z \leq 100$
  
- **Reference document for the whole lecture:**

**Implementing a photon physics model in Serpent2, Toni Kaltiaisenaho, Master thesis, Aalto University, 2016**

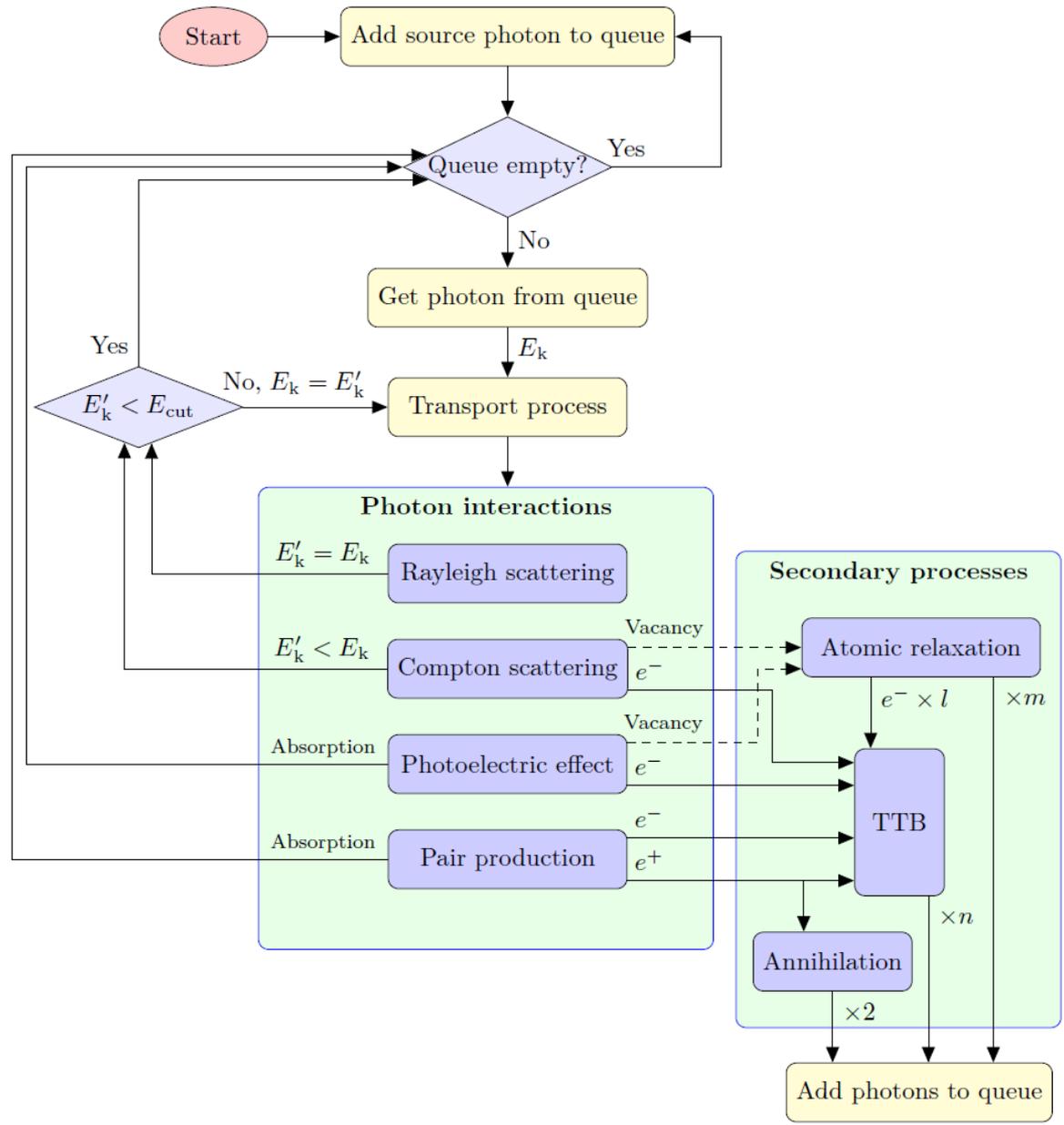
# MCS photon-transport physics module

## Transport kernel

- Rayleigh scattering
- Photoelectric effect
- Pair production
- Compton scattering

## Photon production

- Atomic relaxation (fluorescence / X-ray)
- Electron/positron annihilation
- Thick-Target Bremsstrahlung (TTB)



# Schematics of the main photo-atomic reactions

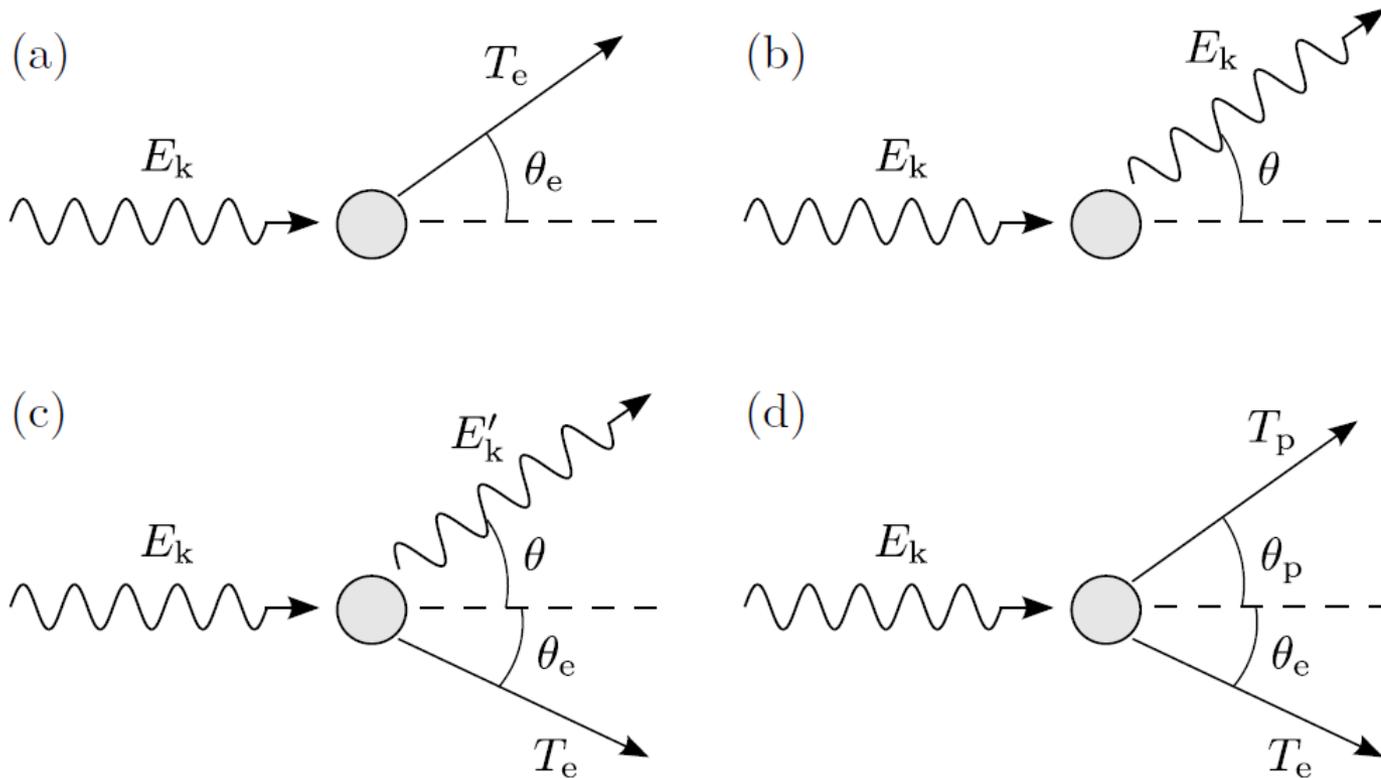
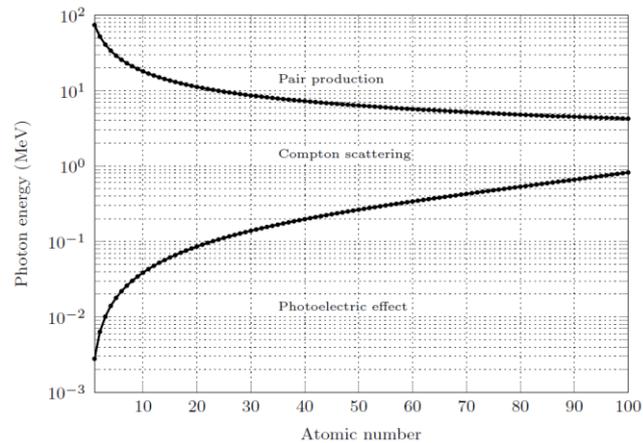
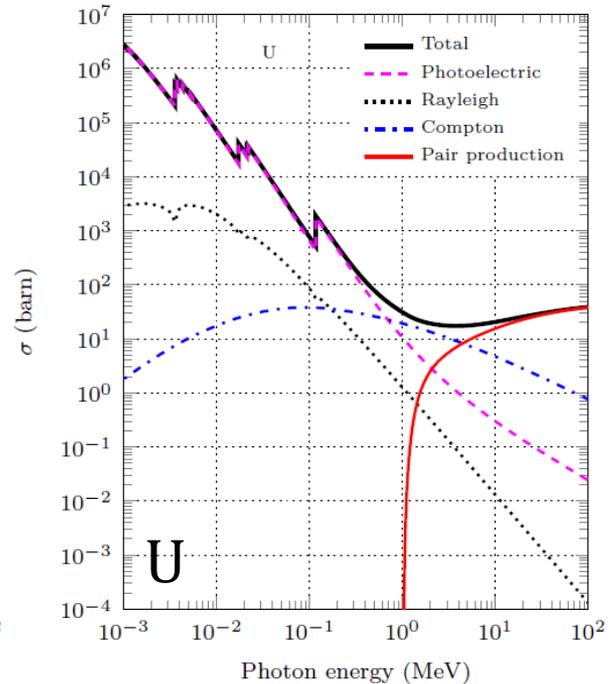
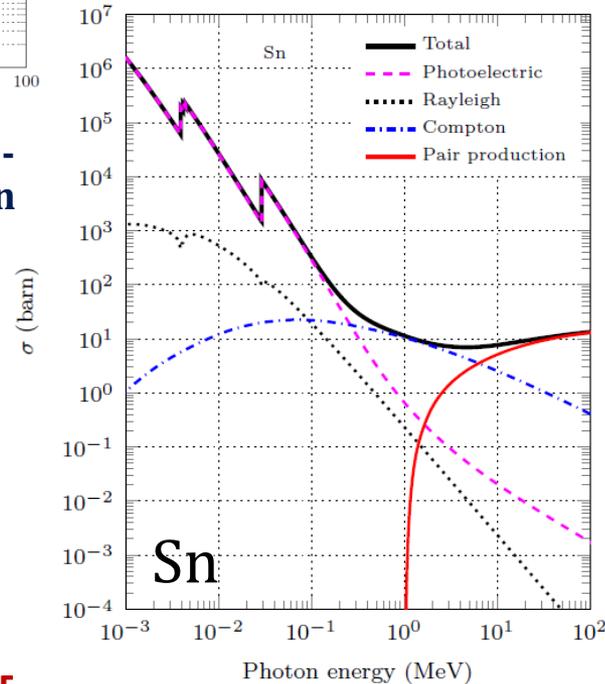
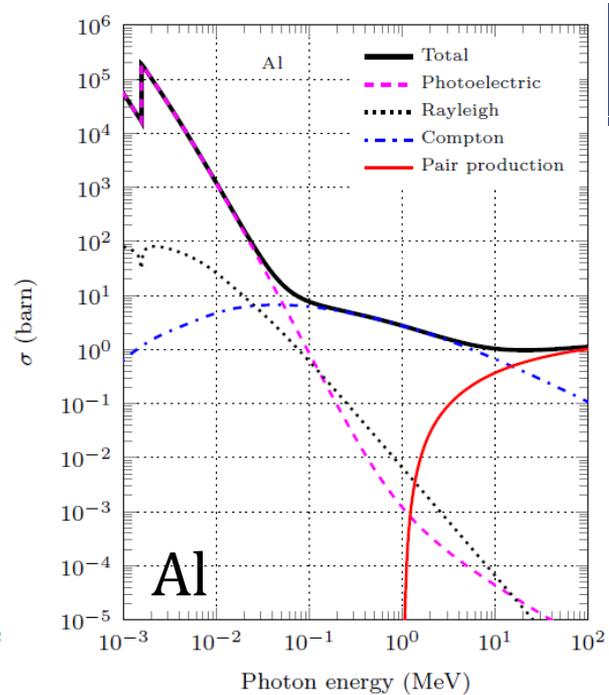
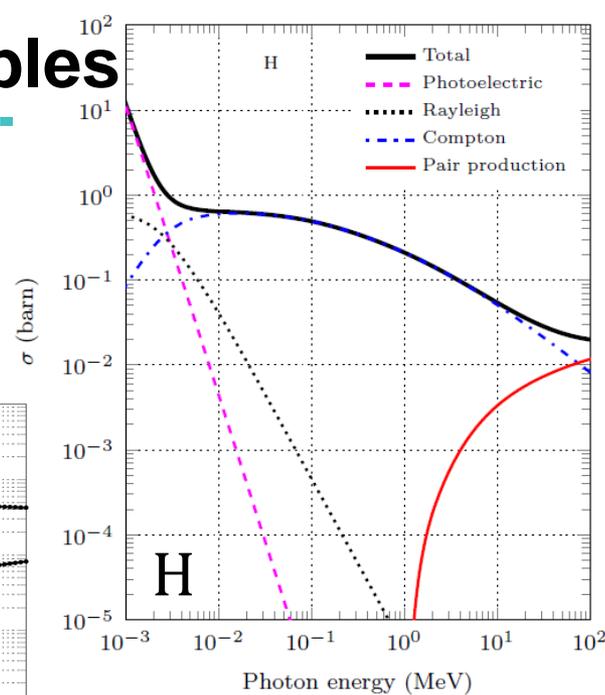


Figure 3.1: Schematics of the four main photon interactions with matter: (a) photoelectric effect, (b) Rayleigh scattering, (c) Compton scattering, and (d) electron-positron pair production. In the figure,  $E_k$  is the energy of the incident photon,  $E'_k$  is the energy of the scattered photon,  $\theta$  is the polar scattering angle of the photon,  $T_e$  and  $T_p$  are the energies of the emitted electron and positron, and  $\theta_e$  and  $\theta_p$  are the polar emission angles of the electron and positron. Note that for Rayleigh scattering  $E'_k$  is equal to  $E_k$ .

# Photon XS examples



**Relative importance of photo-atomic reactions as a function of photon energy and Z**



- **Photon XS from XCOM database**

- <http://www.nist.gov/pml/xcom-photon-cross-sections-database>

- **Neutron XS from ENDF/B-VII.1 (OECD/NEA JANIS4.0)**

Energy	Mean free path (cm)							
	Water		Al27		Fe56		U238	
	neutron	<b>photon</b>	neutron	<b>photon</b>	neutron	<b>photon</b>	neutron	<b>photon</b>
1 keV	0.7	<b>2E-04</b>	12.0	<b>3E-04</b>	1.2	<b>1E-05</b>	2.2	<b>2E-05</b>
10 keV	0.7	<b>0.2</b>	15.8	<b>0.01</b>	2.7	<b>7E-04</b>	3.5	<b>0.001</b>
100 keV	1.0	<b>5.9</b>	3.1	<b>2.1</b>	3.1	<b>0.3</b>	4.0	<b>0.1</b>
1 MeV	1.8	<b>14.2</b>	6.9	<b>5.9</b>	4.2	<b>2.0</b>	6.7	<b>1.5</b>
10 MeV	9.4	<b>45.1</b>	9.5	<b>15.7</b>	3.6	<b>4.1</b>	8.1	<b>2.3</b>
20 MeV	11.5	<b>55.2</b>	9.1	<b>16.8</b>	5.0	<b>3.8</b>	7.7	<b>1.9</b>

- 100 ENDF files (1 for each natural element),
  - $1 \leq Z \leq 100$
  - Photo-atomic XS only depend on Z !
- ENDF/B-VII.1 library processed by NJOY2012:
  - Creation of 100 ACE files
- Each ACE file contains a ESZG block: 5 arrays of size NXS(3)
  - Energy points:  $\ln(E)$ , unit(E) = MeV
  - Photoelectric XS:  $\ln(\sigma)$ , unit( $\sigma$ ) = barn
  - Rayleigh XS:  $\ln(\sigma)$ , unit( $\sigma$ ) = barn
  - Compton XS:  $\ln(\sigma)$ , unit( $\sigma$ ) = barn
  - Pair production XS:  $\ln(\sigma)$ , unit( $\sigma$ ) = barn
- The energy grid is the same for the 4 photo-atomic reactions
- But the energy grid depends on the element:
  - Hydrogen (Z = 1) : NXS(3) = 278 energy points
  - Uranium (Z = 92) : NXS(3) = 1330 energy points
  - Fermium (Z = 100): NXS(3) = 1348 energy points

- In ACE files: logarithms of energy and XS
- MCS reads the ACE files, quantities are stored as logarithms too
- 1 binary search per element:  $E_i \leq E < E_{i+1}$  (Fast! Max(NXS(3)) = 1348)
- Recommended interpolation: linear interpolation of log quantities

$$XS(E) = \exp\left(\frac{\ln(E) - \ln(E_i)}{\ln(E_{i+1}) - \ln(E_i)} [\ln(XS(E_{i+1})) - \ln(XS(E_i))] + \ln(XS(E_i))\right)$$

(Implementation detail: careful with log for pair production! XS = 0 below 1022 keV)

- Total photo-atomic XS = sum of 4 interpolated partials

$$XS_{TOTAL} = XS_{PHOTOELECTRIC} + XS_{RAYLEIGH} + XS_{COMPTON} + XS_{PAIR\_PRODUCTION}$$

⇒ Sampling of distance to collision

⇒ Sampling of photo-atomic reaction

- **100 ACE files “ZZZ000.04p”**
  - Photo-atomic cross-sections ( $1 \leq Z \leq 100$ )
- **cohff.dat**
  - Coherent form factors for Rayleigh scattering ( $1 \leq Z \leq 100$ )
- **ComptonProfiles.dat**
  - Compton profile data for Compton scattering ( $1 \leq Z \leq 100$ )
- **incohsf.dat**
  - Incoherent scattering functions for Compton scattering ( $1 \leq Z \leq 100$ )
- **gsconfig.dat**
  - Atomic configurations of conduction band electrons for bremsstrahlung ( $1 \leq Z \leq 100$ )
- **pdebr.dat**
  - Scaled bremsstrahlung cross-sections ( $1 \leq Z \leq 99$ )
- **relax.dat**
  - Atomic relaxation data (fluorescence X-ray, Auger electrons) ( $1 \leq Z \leq 100$ )
- **xspess.dat**
  - Subshell photoelectric cross-sections ( $1 \leq Z \leq 100$ )
- **xspetot.dat**
  - Total photoelectric cross-sections ( $1 \leq Z \leq 100$ )

# A view at the photon ACE data file format

**NXS(1):** number of elements in XSS

**NXS(2):** **Z**, atomic number

**NXS(3):** **NES**, number of energy points

**NXS(4):** **NFLO**, length of fluorescence data

**NXS(5):** **NSH**, number of electron shells

## **ESZG block:**

NES energy points      ! ln(E)

Compton XS              ! ln( $\sigma$ )

Coherent XS             ! ln( $\sigma$ )

Photoelectric XS        ! ln( $\sigma$ )

Pair production XS      ! ln( $\sigma$ )

Note: the total XS must be calculated as the sum of the 4 partial XS (all the time!)

**JXS(1):** **ESZG**, energy points + XS of 4 main photo-atomic reactions

**JXS(2):** **JINC**, incoherent scattering function

**JXS(3):** **JCOH**, coherent form factors

**JXS(4):** **JFLO**, fluorescence data (edge energies, relative probabilities of ejection from shells, yields, fluorescent energies)

**JXS(5):** **LHNM**, average heating numbers

**JXS(6):** **LNEPS**, number of electrons per shell

**JXS(7):** **LBEPS**, binding energy per shell

**JXS(8):** **LPIPS**, probability of interaction per shell

**JXS(9):** **LSWD**, location of Compton profile data

**JXS(10):** **SWD**, Compton profile data

## 2. Rayleigh scattering

---

Coherent scattering  
5 slides



# Angular differential Rayleigh cross-section

- Incident photon

- Energy  $E_k$

- Outgoing photon

- Polar angle  $\theta \in [0; \pi]$

- One task only: set the polar scattering angle  $\theta$

- Thomson cross-section with free-point charge form factors:

$$\frac{d\sigma_R}{d\Omega} = \frac{r_e^2}{2} (1 + \cos^2 \theta) |f(x, Z)|^2$$

- $\frac{\sigma_R}{d\Omega}$  : differential angular Rayleigh cross-section

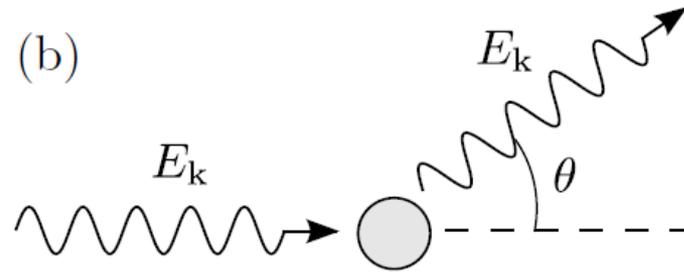
- $r_e$  : classical electron radius

- $x = \sin(\theta/2) \frac{E_k}{hc}$  : the momentum transfer (unit =  $\text{\AA}^{-1}$ )

( $h$  Planck constant,  $c$  speed of light)

- $Z$  : atomic number of target element

- $f$  : atomic form factor (cf. next slide)



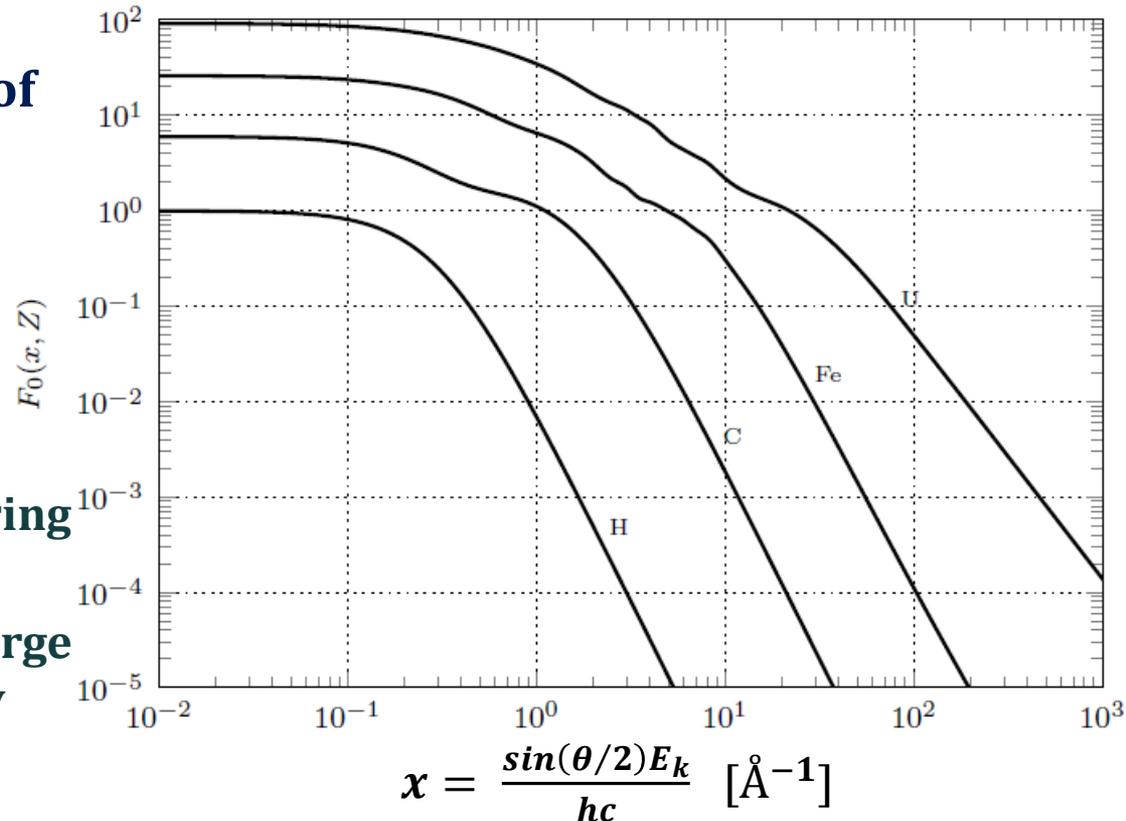
# Non-relativistic atomic form factor (1)

- File available for download on SERPENT2 website: “cohff.dat”
  - Extracted from EPICS2014 library by SERPENT2 developers
  - Form factors for all elements  $1 \leq Z \leq 100$  and  $0 \leq x \leq 10^9 \text{ \AA}^{-1}$
  - Recommended interpolation: linear interpolation on log-log scale

## ▪ Non-relativistic form factors of

- Hydrogen
- Carbon
- Iron
- Uranium

- $\forall Z, f(0, Z) = Z$  : small scattering angles are advantaged
- $x \rightarrow +\infty$  then  $f(x, Z) \rightarrow 0$  : large scattering angles are less likely



# Non-relativistic atomic form factor (2)

- **Coherent form factors treated by NJOY2012 and available in ACE files**
  - Block JCOH at location JXS(3) in XSS block
  - For each element, legacy grid of 55 momentum transfers from  $0 \text{ \AA}^{-1}$  to  $6 \text{ \AA}^{-1}$
- **But! Problem with the NJOY truncation at  $6 \text{ \AA}^{-1}$** 
  - Too many backscattered photons are neglected
  - It is NOT recommended to use the JCOH block from NJOY/ACE [1]
  - This problem might be solved in new ACE format/NJOY releases to come [1]
- **Current solution: read EPICS2014 form factors from an external file**
  - SERPENT2 solution shown in previous slide and adopted for MCS
  - Each element has its own momentum transfer grid (size 90 to 170 depending on element)
  - In all cases, the EPICS2014 grid covers from  $0 \text{ \AA}^{-1}$  to  $10^9 \text{ \AA}^{-1}$

[1] J.S. Hendricks, B.J. Quiter, "MCNP/X form factor upgrade for improved photon transport," Nuclear Technology, 175, pp. 150-161, 2011

# MCS sampling of polar angle $\Theta$ for given $E_k$

- Starting point:  $\frac{d\sigma_R}{d\Omega} = \frac{r_e^2}{2} (1 + \cos^2\theta) |f(x, Z)|^2$        $x = \frac{\sin(\theta/2) E_k}{hc}$
- Max. value of  $x$ :  $x_{max} = \frac{E_k}{hc}$       Trigonometry:  $\cos\theta = 1 - 2 \frac{x^2}{x_{max}^2}$

- Then the differential XS can be rewritten as:  $\frac{d\sigma_R}{d\Omega} = C \cdot \varphi(x^2) \cdot g(x^2)$

$$C = r_e^2 \int_0^{x_{max}^2} |f(x, Z)|^2 \cdot dx^2 \quad \varphi(x^2) = \frac{1}{2} \left( 1 + \left[ 1 - 2 \frac{x^2}{x_{max}^2} \right]^2 \right) \quad g(x^2) = \frac{|f(x, Z)|^2}{\int_0^{x_{max}^2} |f(x, Z)|^2 \cdot dx^2}$$

- C is a constant
- $\varphi$  is a rejection function:  $\forall x^2, \frac{1}{2} \leq \varphi(x^2) \leq 1$
- $g$  is the PDF of  $x^2$  in the interval  $[0; x_{max}^2]$
- Sampling algorithm:
  - 1) Sample  $x^2$  using the PDF  $g$  (cf. next slide)
  - 2) Compute  $\varphi(x^2)$  and get uniform  $0 < r < 1$
  - 3) Accept  $x^2$  if  $r \leq \varphi(x^2)$  else go back to step 1)
  - 4) Compute  $\cos\theta = 1 - 2 \frac{x^2}{x_{max}^2}$

# Sampling algorithm to sample $x^2$ from the PDF $g$ (fixed $E_k$ )

1) Calculate  $x_{max} = \frac{E_k}{hc}$

2) Calculate  $I_{max} = \int_0^{x_{max}^2} |f(x, Z)|^2 \cdot dx^2$

3) Get uniform  $0 < \xi < 1$

4) Solve for  $x^2$  the equation  $\xi = \left( \int_0^{x^2} |f(u, Z)|^2 \cdot du^2 \right) / I_{max}$

▪ Main question: how to compute  $\int_0^{x^2} |f(u, Z)|^2 \cdot du^2$  for  $x^2 \in [0, x_{max}^2]$  ?

▪ MCS formulas:

- cohff.dat contains  $(x_i, f(x_i))$ ,  $i = 1, 2, \dots, N$ , for linear interpolation on log-log scale

- MCS stores  $x_i^2$  ;  $\ln(x_i^2)$  ;  $f(x_i)^2$  ;  $c_i = \frac{\ln f(x_{i+1}) - \ln f(x_i)}{\ln x_{i+1} - \ln x_i}$  ;  $\text{CDF}(x_i^2) = \int_0^{x_i^2} |f(u, Z)|^2 \cdot du^2$

- $\text{CDF}(x_i^2)$  calculated recursively: for  $x^2 \in [x_i^2, x_{i+1}^2]$ ,  $\text{CDF}(x^2) = \text{CDF}(x_i^2) + A(x^2)$

- if  $c_i \neq -1$   $A(x^2) = \frac{x_i^2 \cdot f(x_i)^2}{1+c_i} \left[ \frac{(x^2)^{1+c_i}}{(x_i^2)^{1+c_i}} - 1 \right] \Leftrightarrow x^2 = x_i^2 \left[ (1+c_i) \frac{A(x^2)}{x_i^2 \cdot f(x_i)^2} + 1 \right]^{\frac{1}{1+c_i}}$

- if  $c_i = -1$   $A(x^2) = x_i^2 \cdot f(x_i)^2 \cdot \ln \left( \frac{x^2}{x_i^2} \right) \Leftrightarrow x^2 = x_i^2 \cdot \exp \left( \frac{A(x^2)}{x_i^2 \cdot f(x_i)^2} \right)$

# 3. Photoelectric effect

---

Photon absorption  
9 slides

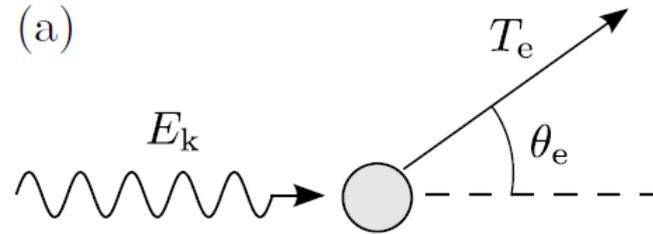


## ▪ Incident photon

- Energy  $E_k$

## ▪ Outgoing electron

- Energy  $T_e$
- Polar angle  $\theta_e \in [0;\pi]$



$$T_e = E_k - W_X$$

$W_X$  is the binding energy of the electron subshell x (x = K, L, M, etc.)

## ▪ Two tasks:

- Set the energy  $T_e$  (=> bremsstrahlung / KERMA)
- Set the angle  $\theta_e$  (=> bremsstrahlung)

## ▪ To sample the energy $T_e$ :

- Binding energy  $W_X$  must be determined
- Electron subshell x must be sampled (=> atomic relaxation)

- Total and subshell photoelectric cross-sections available in ENDF/BVII.1 library (ENDF files)
- Subshell is sampled using partial subshell XS

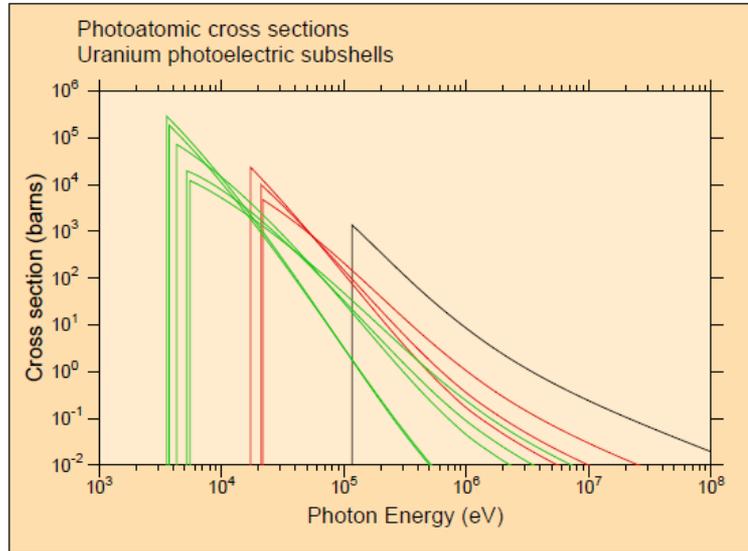
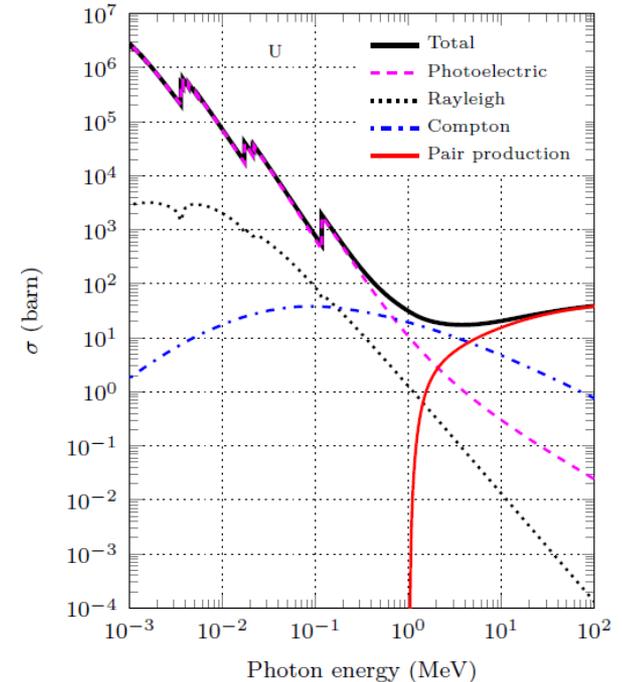


Figure 37: The first nine photoelectric subshell cross sections for uranium from ENDF/B-VII.0. Black is the S subshell ( $1s^{1/2}$ ), red is the L1, L2, and L3 subshells ( $2s^{1/2}$ ,  $2p^{1/2}$ ,  $2p^{3/2}$ ), and green is the M1 through M5 subshells ( $3s^{1/2}$ ,  $3p^{1/2}$ ,  $3p^{3/2}$ ,  $3d^{3/2}$ ,  $3d^{5/2}$ ).



- **But... only the total photoelectric XS is treated by NJOY2012 !**
  - NJOY2012 manual p. 536 “The detailed sub-shell cross section for photo-ionization supported by the most recent version of the ENDF-6 photo-atomic format are not supported in this version of acepho”
  - Subshell cross-sections NOT available in ACE files

# A look at the subshell photoelectric data

- Available in EPICS2014 (ENDLX format) or ENDF/B-VII.1 (ENDF format)
  
- Example: uranium has data (energy grid + XS) for 29 electron subshells
  - K
  - L1-L2-L3
  - M1-M2-M3-M4-M5
  - N1-N2-N3-N4-N5-N6-N7
  - O1-O2-O3-O4-O5-O6-O7
  - P1-P2-P3-P3-P4-P5
  - Q1
  
- 29 different energy grids (one per subshell), different from the energy grid for the total photoelectric XS
  - This would require one binary search per subshell !
  - Energy edge of many subshells below 1 keV

- **ENDF data files directly preprocessed with Matlab scripts**
  - Only electron subshells with edge energy  $> 1$  keV are kept
  - Calculation of a photoelectric unionized energy grid per element
- **Two files available for download on SERPENT2 website: “xspetot.dat” and “xspess.dat”**
  - Extracted from EPICS2014 library by SERPENT2 developers
  - xspetot.dat: cross-sections of total photo-electric effect
  - xspess.dat: cross-sections for each individual subshell
  - For all elements  $Z = 1$  to 100
- **Example: uranium**
  - 1 photoelectric energy grid: 911 energy points
  - 1 total photoelectric XS array (consistent with ACE data): 911 energy points
  - 12 subshells (instead of 29): size of XS array between 469 and 907
  - 1 array of 12 integers: starting index of subshell data on energy grid
  - 1 single binary search necessary to interpolate all the subshell and total XS

# Sampling the subshell: more details

- **Number of subshells per element (edge energy > 1 keV)**
  - 0 for  $Z \leq 10$
  - 1 for  $11 \leq Z \leq 27$
  - 2 for  $Z = 28$  and  $29$
  - 4 for  $30 \leq Z \leq 53$
  - 5 for  $Z = 54$
  - 6 for  $Z = 55$
  - 7 for  $56 \leq Z \leq 59$
  - 8 for  $Z = 60$
  - 9 for  $61 \leq Z \leq 84$
  - 10 for  $85 \leq Z \leq 87$
  - 11 for  $88 \leq Z \leq 91$
  - 12 for  $92 \leq Z \leq 98$
  - 13 for  $Z = 99$  and  $Z = 100$
  
- **Recommended interpolation: linear interpolation of log quantities**
  - XS and energy are stored as logarithms in MCS
  - CDF is build from total and subshell XS, starting with K-shell

- How many subshells with edge energy  $> 1$  keV for the colliding element?
  - If number of subshells = 0 or  $E_k < \min(W)$ , nothing to do:  $T_e = E_k$
- Get uniform  $0 < r < 1$
- CDF = 0
- 1 binary search on the total photoelectric energy grid
- Interpolate total photoelectric XS
- For each subshell (starting from K-shell)
  - If  $E_k < W$  then cycle to next subshell
  - Interpolate subshell photoelectric xs
  - CDF = CDF + (subshell photoelectric xs / total photoelectric xs)
  - If CDF  $> r$  then accept subshell:  $T_e = E_k - W$
- If no subshell accepted ( $r > \text{CDF}$ ):  $T_e = E_k$

## ▪ Relativistic Sauter cross-section

- Formally only valid for K-shell electrons in light elements
- Agreement is good for light elements, deviates for heavy elements
- Still widely applied in Monte Carlo codes (EGS5, Geant4, PENELOPE)

$$\left( \frac{d\sigma_{pe}}{d \cos \theta_e} \right)_{Sauter,R} \propto \frac{\sin^2 \theta_e}{(1 - \beta \cos \theta_e)^4} \left[ 1 + \frac{1}{2} \gamma(\gamma - 1)(\gamma - 2)(1 - \beta \cos \theta_e) \right]$$

- $\beta = \frac{\sqrt{T_e(T_e + 2m_e c^2)}}{T_e + m_e c^2} < 1$ ;  $m_e c^2$  = electron rest mass energy;  $\gamma$  = Lorentz factor
- Low sampling efficiency <50% in Geant4/PENELOPE

## ▪ Non-relativistic Sauter cross-section

- $\gamma \rightarrow 1$ : formally only valid for photoelectrons with  $T_e < 1$  MeV
- Used in SERPENT2 and MCS; sampling efficiency = 67%

$$\left( \frac{d\sigma_{pe}}{d \cos \theta_e} \right)_{Sauter,NR} \propto \frac{\sin^2 \theta_e}{(1 - \beta \cos \theta_e)^4}$$

# Sampling $\theta_e$ from non-relativistic Sauter XS

$$\mu = \cos \theta_e$$

▪ **Starting point**  $\left( \frac{d\sigma_{pe}}{d \cos \theta_e} \right)_{Sauter, NR} \propto f(\theta_e) = \frac{\sin^2 \theta_e}{(1 - \beta \cos \theta_e)^4}$

▪ **Rewriting :**  $f(\mu) = \frac{1 - \mu^2}{(1 - \beta\mu)^4} = C \cdot \varphi(\mu) \cdot g(\mu)$

$$C = \frac{1}{1 - \beta^2} \quad \varphi(\mu) = (1 - \beta^2) \frac{1 - \mu^2}{(1 - \beta\mu)^2} \quad g(\mu) = \frac{1}{(1 - \beta\mu)^2}$$

- $C$  is a constant (for given photoelectron energy  $T_e$ )
- $\varphi$  is a rejection function:  $\forall \mu, 0 \leq \varphi(\mu) \leq 1$
- $g$  is an (unnormalized) PDF of  $\mu$  in the interval  $[-1; 1]$

▪ **Basic sampling algorithm:**

- 1) Sample  $\mu$  using the PDF  $g$
- 2) Compute  $\varphi(\mu)$  and get uniform  $0 < r < 1$
- 3) Accept  $\mu$  if  $\varphi(\mu) \geq r$ , else go back to step 1)

## ▪ Sampling $\mu$ using the PDF $g$ :

- Get uniform  $0 < \xi < 1$  and solve for  $\mu$ :

$$\xi = \frac{CDF(\mu)}{CDF(1)} = \frac{\int_{-1}^{\mu} g(x) dx}{\int_{-1}^1 g(x) dx} = \frac{\int_{-1}^{\mu} (1 - \beta x)^{-2} dx}{\int_{-1}^1 (1 - \beta x)^{-2} dx} \Leftrightarrow \mu = \frac{2\xi + \beta - 1}{2\beta\xi - \beta + 1}$$

- Get uniform  $0 < r < 1$  and check the rejection criterion  $\varphi(\mu) \geq r$ :

$$\varphi(\mu) = (1 - \beta^2) \frac{1 - \mu^2}{(1 - \beta\mu)^2} = (1 - \beta^2) \frac{1 - \left(\frac{2\xi + \beta - 1}{2\beta\xi - \beta + 1}\right)^2}{\left(1 - \beta \frac{2\xi + \beta - 1}{2\beta\xi - \beta + 1}\right)^2} = 4\xi(1 - \xi)$$

## ▪ Optimized sampling algorithm:

- 1) Get uniform  $0 < r < 1$  and uniform  $0 < \xi < 1$

- 2) If  $4\xi(1 - \xi) \geq r$  then calculate  $\mu = \frac{2\xi + \beta - 1}{2\beta\xi - \beta + 1}$  else go back to step 1)

# 4. Pair production

---

Electron/positron pair creation  
7 slides



## ▪ Incident photon

- Energy  $E_k$

## ▪ Outgoing electron

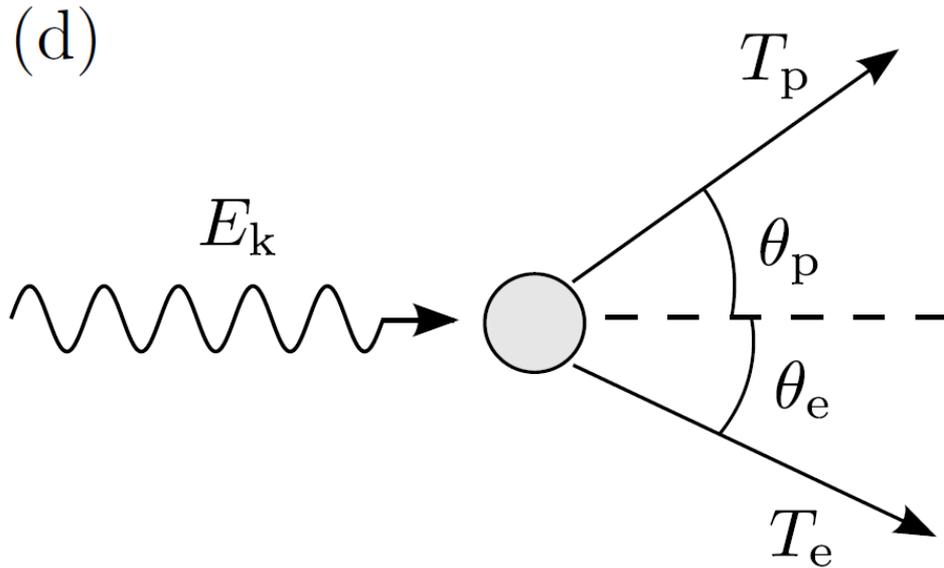
- Energy  $T_e$
- Polar angle  $\theta_e \in [0;\pi]$

## ▪ Outgoing positron

- Energy  $T_p$
- Polar angle  $\theta_p \in [0;\pi]$

## ▪ Three tasks:

- Set the energies  $T_e$  and  $T_p$  (=> bremsstrahlung)
- Set the angles  $\theta_e$  and  $\theta_p$  (=> bremsstrahlung)
- Simulate positron annihilation



- Sampling of the kinetic energy  $T_e$  of electron
- Kinetic energy  $T_p$  of positron deduced by energy conservation
  - Energy conservation:  $E_k = T_e + T_p + 2m_e c^2$
- Notation:
  - Electron reduced energy  $\epsilon = \frac{T_e + m_e c^2}{E_k}$
  - Minimum energy :  $T_e = 0 \Rightarrow \epsilon_{min} = \frac{m_e c^2}{E_k}$
  - Maximum energy :  $T_p = 0 \Rightarrow \epsilon_{max} = \frac{(E_k - 2m_e c^2) + m_e c^2}{E_k} = 1 - \epsilon_{min}$
- Davies-Bethe-Maximon XS for sampling  $\epsilon$  in the range  $[\epsilon_{min}; \epsilon_{max}]$

$$\frac{d\sigma_{pp}}{d\epsilon} = (2\epsilon^2 - 2\epsilon + 1)\Phi_1(\epsilon, E_k, Z) + \frac{2}{3}\epsilon(1 - \epsilon)\Phi_2(\epsilon, E_k, Z)$$

$$\Phi_i(\epsilon, E_k, Z) = S_i(G) - \frac{4}{3}\ln Z - 4f_c(Z) + F_0(\epsilon_{min}, Z)$$

H. Davies, H. A. Bethe, L. C. Maximon, "Theory of Bremsstrahlung and Pair Production. II. Integral Cross Section for Pair Production," *Phys. Rev.*, 93, 788-795 (1954).

- $S_1$  and  $S_2$  are screening functions from Butcher & Messel [1]

$$S_1(G) = \begin{cases} 20.867 - 3.242G + 0.625G^2 & , G \leq 1 \\ 21.12 - 4.184 \ln(G + 0.952) & , G > 1 \end{cases}$$

$$S_2(G) = \begin{cases} 20.209 - 1.930G - 0.086G^2 & , G \leq 1 \\ S_1(G) & , G > 1 \end{cases}$$

$$G = \frac{136}{Z^{1/3}} \frac{\epsilon_{min}}{\epsilon(1 - \epsilon)}$$

- $f_c$  is the Coulomb correction factor from Davies-Bethe-Maximon

$$f_c(a) = a^2 \left[ (1 + a^2)^{-1} + 0.202059 - 0.03693a^2 + 0.00835a^4 - 0.00201a^6 + 0.00049a^8 - 0.00012a^{10} + 0.00003a^{12} \right]$$

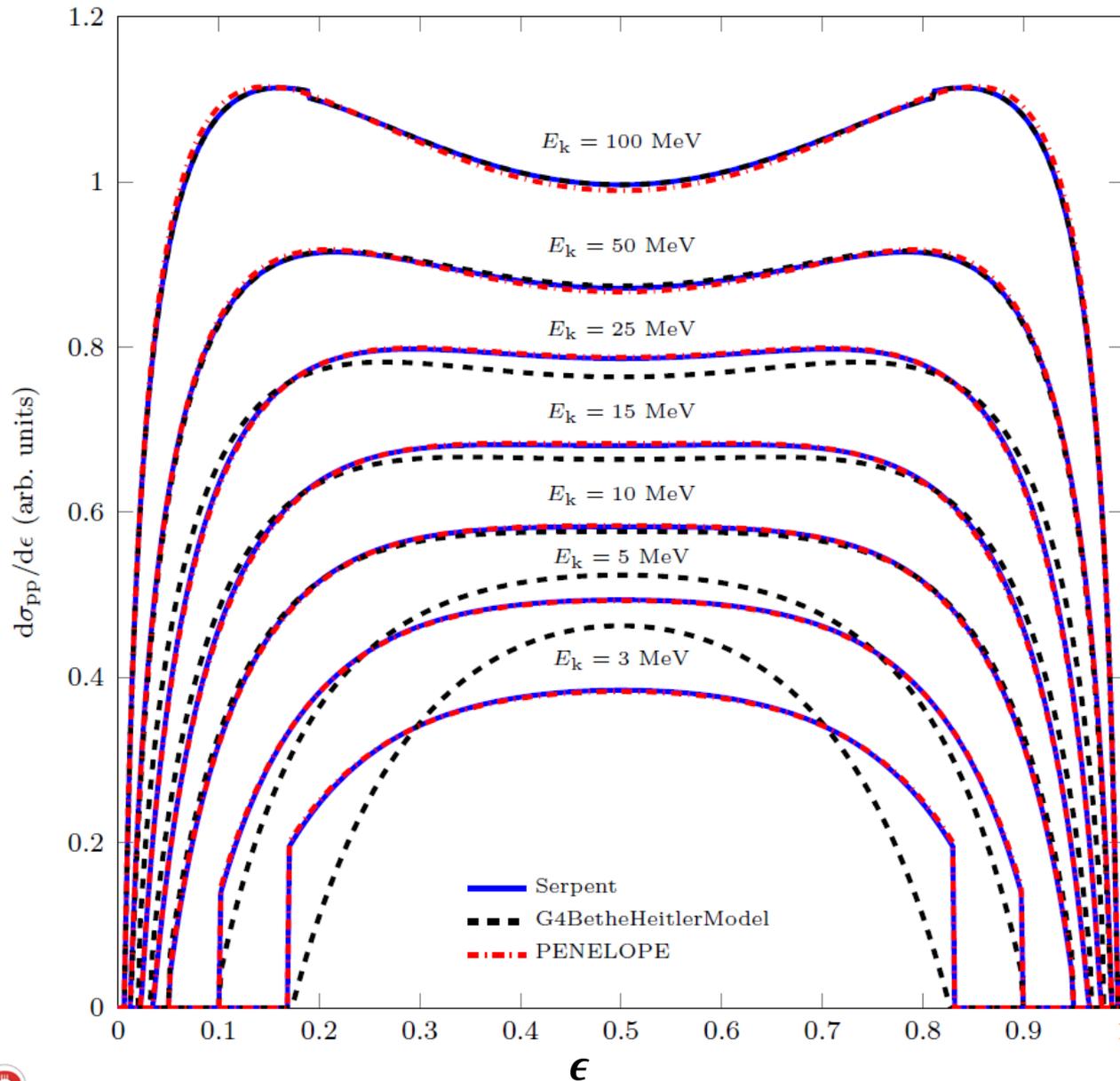
$$a = \alpha Z; \alpha \approx \frac{1}{137} \text{ is the fine-structure constant}$$

- $F_0$  is a correction factor from PENELOPE Monte Carlo code [2]

$$F_0(\epsilon_{min}, Z) = -\left(1.774 + 12.1a - 11.18a^2\right)(2\epsilon_{min})^{1/2} + \left(8.523 + 73.26a - 44.41a^2\right)(2\epsilon_{min}) - \left(13.52 + 121.1a - 96.41a^2\right)(2\epsilon_{min})^{3/2} + \left(8.946 + 62.05a - 63.41a^2\right)(2\epsilon_{min})^2$$

[1]Butcher & Messel, Electron number distribution in electron-photon showers in air and aluminium absorbers, Nuclear Physics, 20, 15-128 (1960)

[2]PENELOPE-2014: A Code System for Monte Carlo Simulation of Electron and Photon Transport, page 76 (typo corrected)



- Domain of interest:  
 $E_k \leq 20 \text{ MeV}$
- PENELOPE reference Monte Carlo code for photon/electron transport
- GEANT4 far away from PENELOPE
- SERPENT2 (=MCS) very close from PENELOPE
- $\frac{d\sigma_{pp}}{d\epsilon}$  very close from uniform distribution for  $E_k \leq 2 \text{ MeV}$

- If  $E_k \leq 2 \text{ MeV}$ :
  - $\epsilon$  sampled uniformly in  $[\epsilon_{min}; \epsilon_{max}]$  with good approximation
- If  $E_k > 2 \text{ MeV}$ :
  - Rejection sampling using the maximum of  $\frac{d\sigma_{pp}}{d\epsilon}$
  - Step 1: sample  $\epsilon_{min} \leq \epsilon_r \leq \epsilon_{max}$  and  $0 < r < 1$  uniformly
  - Step 2: if  $r * \max_{\epsilon} \frac{d\sigma_{pp}}{d\epsilon} \leq \epsilon_r$  then accept  $\epsilon_r$ , else go back to step 1
- $\max_{\epsilon} \frac{d\sigma_{pp}}{d\epsilon}$  is fitted as a function of  $E_k > 2 \text{ MeV}$  and  $Z$ 
  - $\max_{\epsilon} \frac{d\sigma_{pp}}{d\epsilon} = \frac{p_1(Z)E_k^2 + p_2(Z)E_k + p_3(Z)}{E_k^2 + q_1(Z)E_k + q_2(Z)}$
  - Coefficients  $p_1, p_2, p_3, q_1, q_2$  hard-coded in SERPENT2/MCS source code
- Finally:
  - $T_e = \epsilon_r \cdot E_k - m_e c^2$
  - $T_p = E_k - \epsilon_r \cdot E_k - m_e c^2$

## ▪ Leading order of the Sauter-Gluckstern-Hull distribution:

- $\left(\frac{d\sigma_{pp}}{d\cos\theta}\right)_{SGH} \propto \frac{1}{(1-\beta\cos\theta)^2}$  with  $\beta = \frac{\sqrt{T(T+2m_e c^2)}}{T+m_e c^2}$
- Valid for both the electron and the positron
- Used in PENELOPE Monte Carlo code
- $\theta_e$  and  $\theta_p$  sampled independently from each other
- Positron and electron supposed coplanar

## ▪ Sampling of $\mu = \cos\theta$

- Get uniform  $0 < \xi < 1$  and solve for  $\mu$ :

$$\xi = \frac{CDF(\mu)}{CDF(1)} = \frac{\int_{-1}^{\mu} (1-\beta x)^{-2} dx}{\int_{-1}^1 (1-\beta x)^{-2} dx} \Leftrightarrow \mu = \frac{2\xi + \beta - 1}{2\beta\xi - \beta + 1}$$

- **After a pair production:**
  - Positron slowing-down from energy  $T_p$  to thermal energy
  - Positron collision with electron  $\rightarrow$  annihilation particle/antiparticle  
 $\rightarrow$  creation of photons
- **Positron annihilation modelled at rest in MCS/SERPENT2:**
  - Positron at thermal energy, supposed equal to 0
  - 2 collinear photons produced, emitted in opposite direction
  - Direction sampled isotropically
  - Photon energy =  $m_e c^2$
- **For the future, positron annihilation modelled in flight:**
  - Annihilation happens before the positron thermalizes
  - Initial momentum of positron non negligible  $\rightarrow$  more complicated distribution of angles/energies for the two resulting photons
  - In-flight annihilation probably requires full charged-particle transport

# 5. Compton (incoherent) scattering

---

The most complicated photo-atomic interaction  
20 slides



# Compton scattering in Monte Carlo codes

## ▪ Incident photon

- Energy  $E_k$

## ▪ Scattered photon

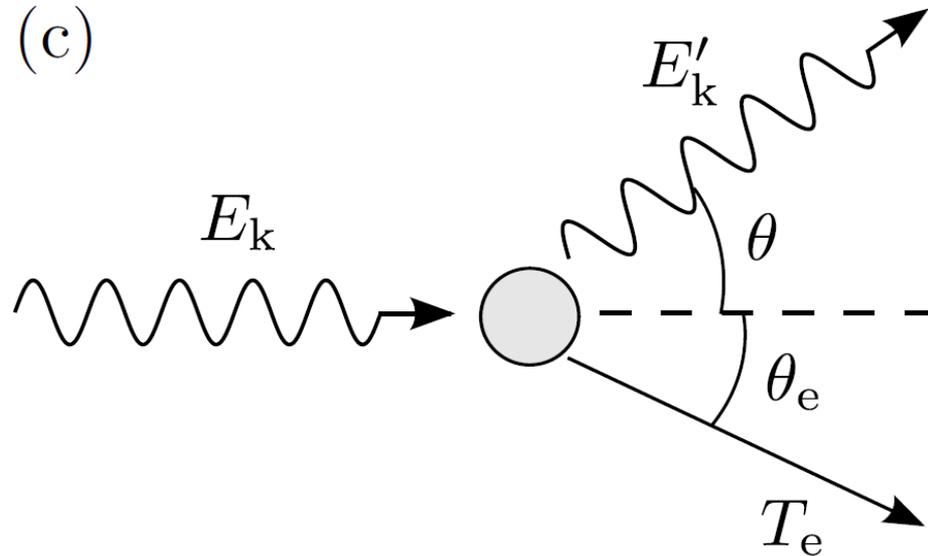
- Energy  $E'_k$
- Polar angle  $\theta \in [0;\pi]$

## ▪ Outgoing electron

- Energy  $T_e$
- Polar angle  $\theta_e \in [0;\pi]$

## ▪ To-do list:

- Set the directions of the scattered photon and of the electron
- Set the electron subshell
- Set the energies  $E'_k$  and  $T_e$



# Free electron at rest problem

## Notation

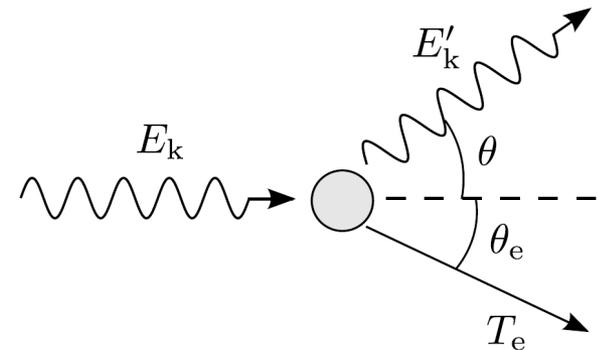
- $\|\vec{p}_k\| = \frac{E_k}{c}$  and  $\|\vec{p}'_k\| = \frac{E'_k}{c}$  momentum of incident and scattered photon
- $\vec{p}_e$  and  $\vec{p}'_e$  momentum of electron before and after scattering

## Total energy / momentum conservation

- $E_k + m_e c^2 = E'_k + (m_e c^2 + T_e)$
- $\vec{p}_k + \vec{p}_e = \vec{p}'_k + \vec{p}'_e$

- Free electron at rest  $\Rightarrow \vec{p}_e = \mathbf{0} \Rightarrow \vec{p}'_e = \vec{p}_k - \vec{p}'_k$   

$$\Rightarrow p_e'^2 = \left(\frac{E_k}{c}\right)^2 + \left(\frac{E'_k}{c}\right)^2 - 2\frac{E_k E'_k}{c^2} \cos \theta$$



## Relativistic electron energy equation:

- $(m_e c^2 + T_e)^2 = p_e'^2 c^2 + m_e^2 c^4$   

$$\Rightarrow (E_k - E'_k + m_e c^2)^2 = E_k^2 + E_k'^2 - 2E_k E'_k \cos \theta + m_e^2 c^4$$

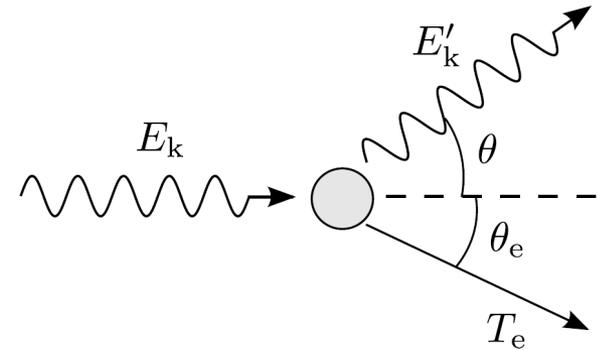
$$\Rightarrow E'_k = \frac{E_k}{1 + \frac{E_k}{m_e c^2} (1 - \cos \theta)} \equiv E_c$$

## ■ Notation

- $\|\vec{p}_k\| = \frac{E_k}{c}$  and  $\|\vec{p}'_k\| = \frac{E'_k}{c}$  momentum of incident and scattered photon
- $\vec{p}_e$  and  $\vec{p}'_e$  momentum of electron before and after scattering
- $E_e$  and  $E'_e$  electron energy before and after scattering
- $E_{b,i} > 0$  binding energy of electron subshell i

## ■ Momentum transfer vector $\vec{q}$

$$\cdot \hbar\vec{q} = \vec{p}_k - \vec{p}'_k \Rightarrow \|\vec{q}\| = \frac{1}{\hbar c} \sqrt{E_k^2 + E'_k{}^2 - 2E_k E'_k \cos \theta}$$



## ■ Total energy / momentum conservation

- $E_k + E_e = E'_k + E'_e + E_{b,i}$
- $\vec{p}_k + \vec{p}_e = \vec{p}'_k + \vec{p}'_e \Rightarrow \hbar\vec{q} = \vec{p}_k - \vec{p}'_k = \vec{p}'_e - \vec{p}_e$

## ■ Relativistic electron energy equations

- $E_e^2 = p_e^2 c^2 + m_e^2 c^4 \Rightarrow p_e^2 = \frac{E_e^2}{c^2} - m_e^2 c^2$
- $E'_e{}^2 = p_e'^2 c^2 + m_e^2 c^4 \Rightarrow p_e'^2 = \frac{E_e'^2}{c^2} - m_e^2 c^2$

## ■ Projection $p_z$ of initial electron momentum on vector $-\vec{q}$

$$\cdot p_z = -\frac{\vec{p}_e \cdot \vec{q}}{\|\vec{q}\|} = -\frac{\vec{p}_e \cdot (\vec{p}'_e - \vec{p}_e)}{\hbar \|\vec{q}\|} = \frac{p_e^2 - \vec{p}_e \cdot \vec{p}'_e}{\hbar \|\vec{q}\|}$$

# Bound electron problem (2) resolution $p_z = f(E'_k)$

- $(\vec{p}'_e - \vec{p}_e)^2 = (\vec{p}_k - \vec{p}'_k)^2 \Rightarrow p_e^2 + p_e'^2 - 2\vec{p}'_e \cdot \vec{p}_e = \hbar^2 \|\vec{q}\|^2$
- $p_z = \frac{p_e^2 - \vec{p}'_e \cdot \vec{p}_e}{\hbar \|\vec{q}\|} = \frac{1}{\hbar \|\vec{q}\|} \left( \frac{E_e^2}{c^2} - \cancel{m_e^2 c^2} + \frac{1}{2} \hbar^2 \|\vec{q}\|^2 - \frac{1}{2} \left( \frac{E_e^2}{c^2} - \cancel{m_e^2 c^2} \right) - \frac{1}{2} \left( \frac{E_e'^2}{c^2} - \cancel{m_e^2 c^2} \right) \right)$
- $p_z = \frac{1}{\hbar \|\vec{q}\|} \left( \frac{1}{2} \hbar^2 \|\vec{q}\|^2 + \frac{1}{2} \frac{E_e^2}{c^2} - \frac{1}{2} \frac{E_e'^2}{c^2} \right) = \frac{1}{2\hbar \|\vec{q}\| c^2} \left( E_k^2 + E_k'^2 - 2E_k E_k' \cos \theta + E_e^2 - E_e'^2 \right)$
- $E_k + E_e = E'_k + E'_e + E_{b,i} \Rightarrow E_e'^2 = (E_k + E_e - E'_k - E_{b,i})^2$

## ▪ Relativistic Impulse approximation

- $E_{b,i} \approx 0 \quad \rightarrow E_e'^2 = (E_k - E'_k + m_e c^2)^2$
- $E_e = m_e c^2 \quad = E_k^2 + E_k'^2 + m_e^2 c^4 - 2E_k E'_k + 2(E_k - E'_k) m_e c^2$

## ▪ Replacing $E_e'^2$ in $p_z$ yields

$$p_z = \frac{E_k E'_k (1 - \cos \theta) - m_e c^2 (E_k - E'_k)}{c \sqrt{E_k^2 + E_k'^2 - 2E_k E'_k \cos \theta}}$$

- If  $p_z = 0$  then  $E'_k = E_C =$  energy of scattered photon in free-electron case

- 1) Solve the free electron at rest problem: rejection sampling of the polar angle  $\theta$  and energy  $E_c$  of the scattered photon
  - a. Sample  $\theta$  (and  $E_c$ ) from Klein-Nishina distribution
  - b. Accept  $\theta$  using the incoherent scattering function test or go to 1) a.
- 2) Solve the bound electron problem: rejection sampling of the energy  $E'_k$  of the scattered photon
  - a. Sampling the electron subshell  $x$  of binding energy  $W_x$  with rejection method using electron number CDF and Compton profiles
  - b. Sample the initial electron momentum  $p_z$  using the Compton profile of the electron subshell  $x$
  - c. Solve the energy  $E'_k$  for the sampled initial electron momentum  $p_z$
  - d. Sample random  $0 < r < 1$
  - e. If  $\frac{E'_k}{(E_k - W_x)} \leq r$  then accept  $E'_k$  else go to 2) a.
- 3) Set electron energy  $T_e$  and polar angle  $\theta_e$ 
  - $T_e = E_k - E'_k - W_x$
  - Direction of the electron taken equal to the momentum transfer vector
- 4) Finally:
  - Simulate bremsstrahlung
  - Simulate fluorescence in subshell  $x$

# 1) a. Klein-Nishina distribution

- **Free-electron diff. angular cross-section of Compton scattering**

$$\left(\frac{d\sigma_{Co}}{d\Omega}\right)_{KN} = \frac{r_e^2}{2} \left(\frac{E_C}{E_k}\right)^2 \left(\frac{E_C}{E_k} + \frac{E_k}{E_C} - \sin^2\theta\right)$$

- $r_e$  is the classical electron radius
- $E'_k = E_C$  for Compton scattering on free (unbound) electrons
- **Recommended  $\theta$  sampling method [1]**
  - $E_k > 1.4$  MeV : probability mixing (PMIX) method of Koblinger [2]
  - $E_k \leq 1.4$  MeV : rejection step (RSTEP) method of Matthews [1]
- **$\theta$  sampling method implemented in MCS**
  - $E_k > 1.4$  MeV : PMIX method of Koblinger
  - $E_k \leq 1.4$  MeV : rejection inverse square (RIS) method of Matthews
- **For  $E_k \leq 1.4$  MeV, RIS method is the second-fastest sampling method right after RSTEP method [1]**

[1] Matthews K, "Random Sampling from the Klein-Nishina distribution," Nucl. Sci. Eng., 173, 207-221 (2013)

[2] Koblinger L, Lux I, Monte Carlo Particle Transport Methods: Neutron and Photon Calculations, p. 9, p. 67, CRC Press (1991)

TABLE II  
Ratios of Speeds

Method	Ratio of Method Speed to Speed of Kahn’s Method		
	Random in [0.2,2.73]	Decreasing by Scatters: 2.731 to 0.001	Various, Repeated 0.003 to 2.723
Step with pretest	1.65	1.78	1.80
Step without pretest	1.61	1.75	1.57
Inverse square	1.10	1.37	1.16
Kahn	1	1	1

## VI. RECOMMENDATIONS

Step sampling with rejection, including the pretest, is the overall best choice for  $0 \leq \alpha \leq 1 + \sqrt{3}$ . It is, overall,  $\sim 75\%$  faster than Kahn’s method, with acceptance efficiency of 90% to 98% and only two random numbers used per trial. We did not test it above that range, because the needed resolution in  $\alpha$  increases as  $\alpha$  increases, and there is no obvious upper bound for  $\alpha$ . Therefore, we recommend the combination of step sampling with rejection and pretest for  $\alpha \leq 1 + \sqrt{3}$  and Koblinger’s method for  $\alpha > 1 + \sqrt{3}$ .

For applications in which minimal memory usage is more important than speed, the inverse square method provides the best speed without tables and is a simple algorithm. It is faster and more parsimonious than Kahn’s method while being of comparable efficiency. For  $\alpha \leq 1 + \sqrt{3}$ , inverse square rejection is recommended as a general replacement for Kahn’s method, with Koblinger’s method used for  $\alpha > 1 + \sqrt{3}$ , for such applications.

[1] Matthews K, “Random Sampling from the Klein-Nishina distribution: efficiency, parsimony, and speed,” Nucl. Sci. Eng., 173, 207-221 (2013)

# 1) a. PMIX method of Koblinger (1/2)

$$\left(\frac{d\sigma_{Co}}{d\Omega}\right)_{KN} = \frac{r_e^2}{2} \left(\frac{E_C}{E_k}\right)^2 \left(\frac{E_C}{E_k} + \frac{E_k}{E_C} - \sin^2\theta\right) = \frac{r_e^2}{2} \frac{1}{x^2} \left(\frac{1}{x} + x + \mu^2 - 1\right)$$

## ■ Notations:

- $\alpha_0 = \frac{E_k}{m_e c^2}$ ;  $\mu = \cos\theta$ ; **PMIX samples the variable**  $x = \frac{E_k}{E_C}$

## ■ Using the expression of $E_C$ (free electron solution):

- $E_C = \frac{E_k}{1 + \frac{E_k}{m_e c^2}(1 - \cos\theta)} \Rightarrow x = 1 + \alpha_0(1 - \mu) \Rightarrow \mu = \frac{\alpha_0 - x + 1}{\alpha_0}$

- $\mu \in [-1; 1] \Rightarrow x \in [1; 1 + 2\alpha_0]$

- $\left(\frac{d\sigma_{Co}}{d\Omega}\right)_{KN} \propto \frac{1}{x^2} \left(\frac{1}{x} + x + \left(\frac{\alpha_0 - x + 1}{\alpha_0}\right)^2 - 1\right) = \frac{1}{x^3} + \frac{2\alpha_0 + 1}{\alpha_0^2 x^2} + \frac{1 - \frac{2(\alpha_0 + 1)}{\alpha_0^2}}{x} + \frac{1}{\alpha_0^2}$   
 $= P_3(x) + P_2(x) + P_1(x) + P_0(x)$

## ■ PMIX can only be applied if $\forall i \forall x \in [1; 1 + 2\alpha_0] P_i(x) \geq 0$

- $P_1(x) \geq 0 \Leftrightarrow \alpha_0 \geq 1 + \sqrt{3} \Leftrightarrow E_k \geq (1 + \sqrt{3})m_e c^2 \approx 1.396 \text{ MeV}$

# 1) a. PMIX method of Koblinger (2/2)

## ■ Notation

$$\left(\frac{d\sigma_{c0}}{d\Omega}\right)_{KN} \propto \frac{1}{x^3} + \frac{2\alpha_0+1}{\alpha_0^2 x^2} + \frac{1-\frac{2(\alpha_0+1)}{\alpha_0^2}}{x} + \frac{1}{\alpha_0^2} = P_3(x) + P_2(x) + P_1(x) + P_0(x)$$

$$x \in [1; \delta]; \delta = 1 + 2\alpha_0; \gamma = 1 - 1/\delta^2; \alpha_0 \geq 1 + \sqrt{3}$$

■ Define  $I_i = \int_1^\delta P_i(x) dx$ ;  $I = \sum_0^3 I_i$ ;  $CDF_i(x) = (\int_1^x P_i(x) dx) / I_i$

## ■ PMIX sampling algorithm of $x$ variable:

- Get uniform  $0 < r < 1$  and find index  $j$  so that  $\sum_0^{j-1} I_i < I \cdot r \leq \sum_0^j I_i$
- Get uniform  $0 < \xi < 1$  and solve for  $x$  the equation  $\xi = CDF_j(x)$
- Compute  $\mu = \frac{\alpha_0 - x + 1}{\alpha_0}$  and  $E_C = \frac{E_k}{x}$

## ■ Solutions:

- $I_0 = I_2 = 2/\alpha_0$ ;  $I_1 = (1 - (1 + \delta)/\alpha_0^2) \cdot \ln \delta$ ;  $I_3 = \gamma/2$
- $j = 0$ :  $x = 1 + 2\alpha_0 \xi$
- $j = 1$ :  $x = \delta^\xi$
- $j = 2$ :  $x = \frac{\delta}{1 + 2\alpha_0 \xi}$
- $j = 3$ :  $x = \frac{1}{\sqrt{1 - \gamma \xi}}$

# 1) a. RIS method of Matthews

$$\left(\frac{d\sigma_{Co}}{d\Omega}\right)_{KN} = \frac{r_e^2}{2} \frac{1}{x^2} \left(\frac{1}{x} + x + \mu^2 - 1\right) = \frac{r_e^2}{2} \frac{1}{[1 + \alpha_0(1 - \mu)]^2} \left(\frac{1}{1 + \alpha_0(1 - \mu)} + \alpha_0(1 - \mu) + \mu^2\right)$$

▪ **Reminder**  $E_C = \frac{E_k}{1 + \frac{E_k}{m_e c^2}(1 - \cos \theta)} \Rightarrow x = 1 + \alpha_0(1 - \mu)$

▪ **Rejection sampling method of  $\mu = \cos \theta$  for  $\alpha_0 \leq 1 + \sqrt{3}$**

- Inverse square function  $S(\mu) = \frac{r_e^2}{2} \frac{16 + \alpha_0}{2[2 + \alpha_0(1 - \mu)]^2} \geq \left(\frac{d\sigma_{Co}}{d\Omega}\right)_{KN} \forall \alpha_0 \in [0; 1 + \sqrt{3}] \forall \mu \in [-1; 1]$
- **Step 1: get uniform  $0 < \xi < 1$  and solve for  $\mu_\xi$ :**

$$\xi = \frac{CDF(\mu_\xi)}{CDF(1)} = \frac{\int_{-1}^{\mu_\xi} S(x) dx}{\int_{-1}^1 S(x) dx} \Leftrightarrow \mu_\xi = 1 - \frac{2\xi}{1 + \alpha_0(1 - \xi)}$$

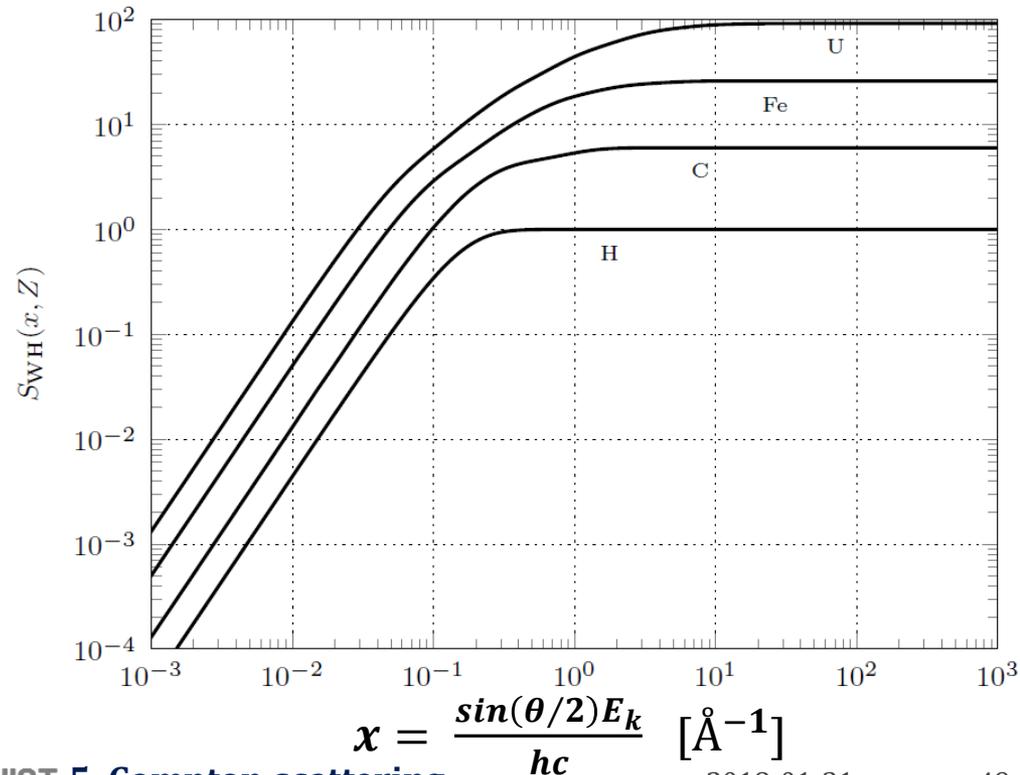
- **Step 2: get uniform  $0 < r < 1$**

- **Step 3: If  $r \leq \frac{\left(\frac{d\sigma_{Co}}{d\Omega}\right)_{KN}(\mu_\xi)}{S(\mu_\xi)}$  then accept  $\mu_\xi$ , else go back to step 1**

# 1) b. Total diff. angular XS for Compton scattering

$$\left(\frac{d\sigma_{co}}{d\Omega}\right)_{ISF} = \left(\frac{d\sigma_{co}}{d\Omega}\right)_{KN} \times S_{WH}(x, Z)$$

- MCS differential angular cross-section (DCS) for Compton scattering
- $S_{WH}(x, Z)$  =Waller-Hartree Incoherent Scattering (WH-ISF)
  - ISF accounts for the fact that the electron is not free, but bound to an atom
  - Function of momentum transfer  $x$  and atomic number  $Z$
- Plot of WH-ISF data for
  - Hydrogen
  - Carbon
  - Iron
  - Uranium
- $\forall Z, S_{WH}(0, Z) = 0$  : DCS suppressed at low energies and in the forward direction
- $x \rightarrow +\infty$  then  $S_{WH}(x, Z) \rightarrow Z$  : large scattering angles are more likely



# Incoherent scattering function (ISF)

- Incoherent scattering function treated by NJOY2012 and available in ACE files
  - Block JINC at location JXS(2) in XSS block
  - For each element, legacy grid of 21 momentum transfers from  $0 \text{ \AA}^{-1}$  to  $8 \text{ \AA}^{-1}$
- **But! Problem with the NJOY truncation at  $8 \text{ \AA}^{-1}$** 
  - The truncation of high  $x$  tail leads to physical errors in photon energy spectrum
  - It is NOT recommended to use the JINC block from NJOY/ACE [1]
  - Similar problem as the coherent form factors shown previously
  - This problem might be solved in new ACE format/NJOY releases to come [1]
- **Current solution: get ISF from EPICS2014 / ENDF/B-VII library**
  - Each element has its own momentum transfer grid (size 94 to 174 depending on element)
  - In all cases, the EPICS2014 grid covers from  $0 \text{ \AA}^{-1}$  to  $10^9 \text{ \AA}^{-1}$

[1] J.S. Hendricks, B.J. Quiter, "MCNP/X form factor upgrade for improved photon transport," Nuclear Technology, 175, pp. 150-161, 2011

# 1) b. Sampling of polar scattering angle $\theta$

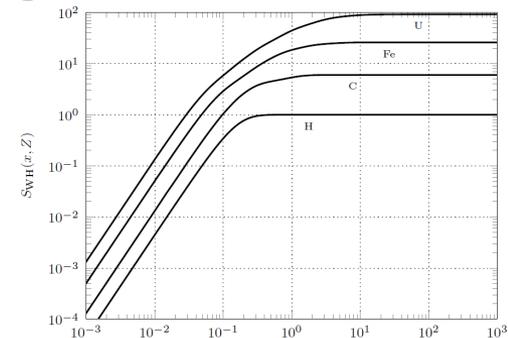
- File available for download on SERPENT2 website: “incohsf.dat”
  - WH-ISF data extracted from EPICS2014 library by SERPENT2 developers
  - For all elements  $1 \leq Z \leq 100$  and  $0 \leq x \leq 10^9 \text{ \AA}^{-1}$
  - Recommended interpolation: linear interpolation on log-log scale

- WH-ISF is used as rejection function

- WH-ISF monotonically increasing:  $\forall Z, x \uparrow \Rightarrow S_{WH}(x, Z) \uparrow$

- Sampling algorithm of  $\mu = \cos \theta$

- $x_{max} = \max_{0 \leq \theta \leq 2\pi} \frac{\sin(\theta/2)E_k}{hc} = \frac{E_k}{hc}$
- $\mu = 1 - 2 \frac{x^2}{x_{max}^2}$  (slide 18)  $\Rightarrow x = x_{max} \sqrt{\frac{1-\mu}{2}}$
- Step 1: sample  $\mu_r = \cos \theta$  from Klein-Nishina distribution
- Step 2: compute  $x_r = \frac{E_k}{hc} \frac{\sqrt{1-\mu_r}}{\sqrt{2}}$  and sample  $0 < r < 1$  uniformly
- Step 3: accept  $\theta_r$  if  $r \leq \frac{S_{WH}(x_r, Z)}{S_{WH}(x_{max}, Z)}$ , otherwise go back to step 1



$$x = \frac{\sin(\theta/2)E_k}{hc} \quad [\text{\AA}^{-1}]$$

## 2) Sampling of the scattered photon energy $E'_k$

- Double differential Compton cross-section of electron momentum  $p_z$  and of polar angle  $\theta$

$$\left( \frac{d^2 \sigma_{Co}}{dp_z d\Omega} \right)_{KN} = \frac{r_e^2 E_C}{2 E_k} \left( \frac{E_C}{E_k} + \frac{E_k}{E_C} - \sin^2 \theta \right) \frac{E'_k}{E_k} \sum_i N_i \cdot H(E_k - E_{b,i}) \cdot J_i(p_z)$$

- Sum on the subshells  $i = 1, 2, \dots$  of the atom
- Subshell  $i$  of binding energy  $E_{b,i}$  contains  $N_i$  electrons
- $J_i$  is the Compton profile of subshell  $i$
- $H$  Heaviside function :  $H(x) = 0$  for  $x < 0$  and  $H(x) = 1$  for  $x \geq 0$
- For fixed  $E_k$  and  $\theta$ , purple part is a constant
- Overview of  $E'_k$  sampling algorithm
  - Step 1: sample a subshell  $jr$  from  $\sum_i N_i \cdot H(E_k - E_{b,i}) \cdot J_i(p_z)$
  - Step 2: sample  $p_{z,r}$  from Compton profile  $J_{jr}$
  - Step 3: compute  $E'_{k,r}$  corresponding to sampled  $p_{z,r}$  value
  - Step 4: sample  $0 < r < 1$  uniformly
  - Step 5: if  $r < \frac{E'_{k,r}}{E_k - E_{b,jr}}$  accept  $E'_{k,r}$  else go back to step 1

# Definition of Compton profiles $J_i$

- Probability distributions of electron momentum  $p_z$  for each electron subshell

- Properties of Compton profiles

- Normalization:  $\int_{-\infty}^{+\infty} J_i(p_z) dp_z = 1$
- Symmetry:  $J_i(-p_z) = J_i(p_z)$
- Maximum  $\forall p_z \quad J_i(0) \geq J_i(p_z)$

- Momentum  $p_z$  is sampled in the range  $[p_{z,min}; p_{z,max,i}]$

(reminder slide 42:  $p_z = \frac{E_k E'_k (1 - \cos \theta) - m_e c^2 (E_k - E'_k)}{c \sqrt{E_k^2 + E'_k{}^2 - 2 E_k E'_k \cos \theta}}$ )

- $E'_k = 0 \rightarrow p_{z,min} = -m_e c \approx -137 \alpha m_e c$  ( $\alpha =$  fine structure constant)
- $E'_k = E_k - E_{b,i} \rightarrow p_{z,max,i} = \frac{E_k (E_k - E_{b,i}) (1 - \cos \theta) - m_e c^2 E_{b,i}}{c \sqrt{2 E_k (E_k - E_{b,i}) (1 - \cos \theta) + E_{b,i}{}^2}}$

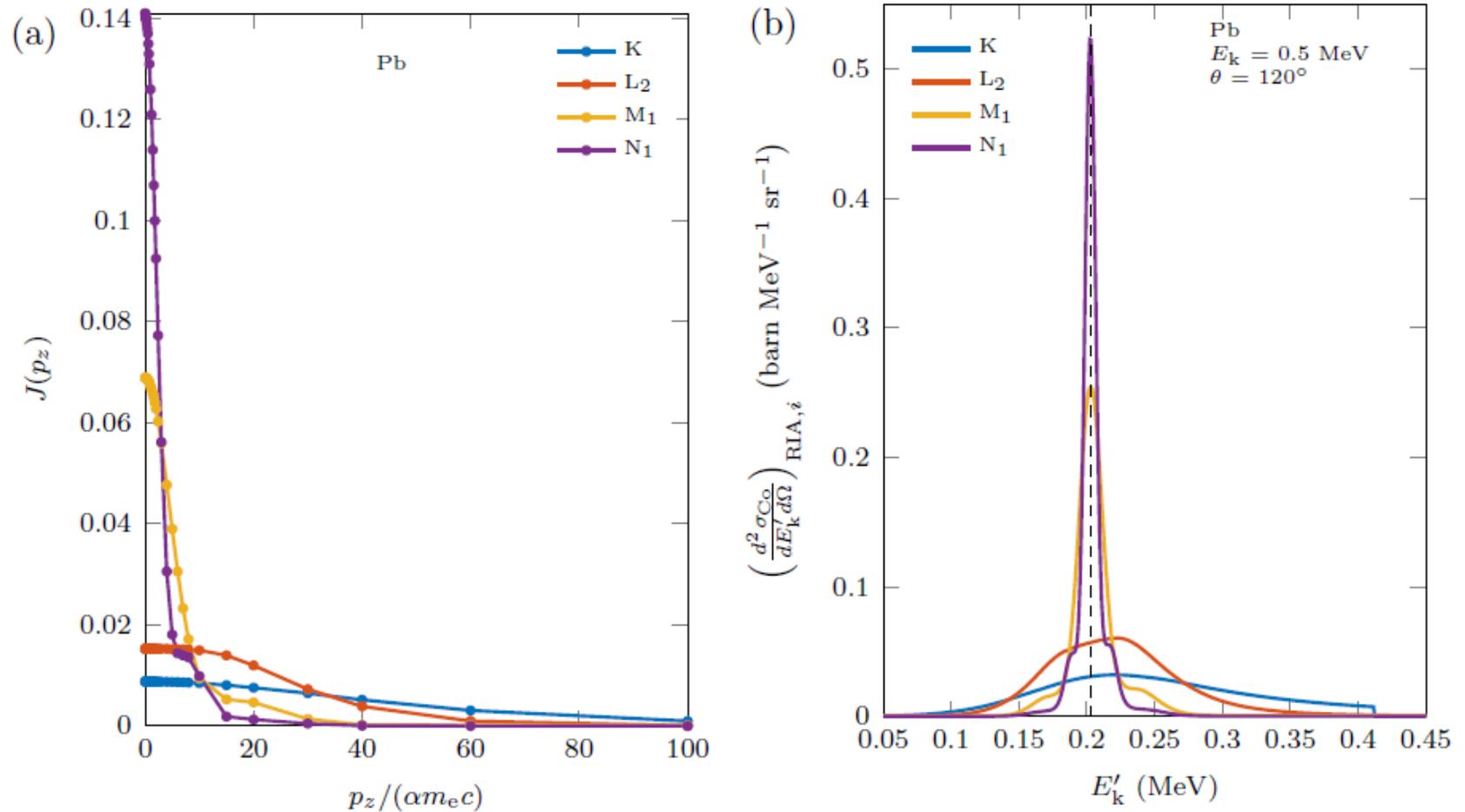


Figure 3.13: (a) Hartree-Fock Compton profiles for K-, L<sub>2</sub>-, M<sub>1</sub>-, and N<sub>1</sub>-shell electrons of lead [54], and (b) the corresponding DDCS according to Eq. (3.58) for the scattering of 0.5 MeV photons into 120°. The dashed black line in (b) presents the free electron scattering energy  $E_C$  given by Eq. (3.43).

## ■ Biggs Compton [1] profile data in file “ComptonProfiles.dat”

- Provides EPICS2014 electron number  $N_i$  and binding energy  $E_{b,i}$  values

- Provides  $J_i(p_z)$  at values

$$\frac{p_z}{\alpha m_e c} = \{0; 0.05; 0.1; 0.15; 0.2; 0.3; 0.4; 0.5; 0.6; 0.7; 0.8; 1; 1.2; 1.4; 1.6; 1.8; 2; 2.4; 3; 4; 5; 6; 7; 8; 10; 15; 20; 30; 40; 60; 100\}$$

- Range [0:100] not enough to cover range  $[p_{z,min}; p_{z,max,i}] \rightarrow$  extrapolation

## ■ MCS pre-processing scheme (=SERPENT2)

- $J_i(p_z)$  points added by log-lin interpolation at values

$$\frac{p_z}{\alpha m_e c} = \{12; 17; 25; 35; 45; 50; 55; 65; 70; 80; 90\}$$

- $J_i(p_z)$  points added by log-lin extrapolation with last 2 Biggs values (60 & 100)

$$\frac{p_z}{\alpha m_e c} = \{110; 120; 130; 1/\alpha\}$$

- Resulting profiles are normalized so that  $\forall i \int_{-\infty}^{+\infty} J_i(p_z) dp_z = 1$

## ■ MCS calculation of $J_i(p_z)$ (=SERPENT2)

- For  $|p_z|/\alpha m_e c \leq 1/\alpha$ : direct linear interpolation

- For  $|p_z|/\alpha m_e c > 1/\alpha$ : log-lin extrapolation with last 2 Biggs values (60 & 100)

[1] Biggs F et al. Hartree-Fock Compton profiles for the elements. At Data Nucl Data Tables. 1975 16(3): 201-309.

## 2) a. b. Subshell sampling method and $p_z$ sampling

- **Reminder : Compton DDCS of electron momentum  $p_z$  & polar angle  $\theta$**

$$\left( \frac{d^2 \sigma_{Co}}{dp_z d\Omega} \right)_{KN} = \frac{r_e^2 E_C}{2 E_k} \left( \frac{E_C}{E_k} + \frac{E_k}{E_C} - \sin^2 \theta \right) \frac{E'_k}{E_k} \sum_i N_i \cdot H(E_k - E_{b,i}) \cdot J_i(p_z)$$

- **DDCS integration  $\rightarrow$  probability of subshell  $j$**

$$P(j) = \frac{N_j \cdot H(E_k - E_{b,j}) \cdot \int_{p_{z,min}}^{p_{z,max,j}} J_j(p_z) dp_z}{\sum_i N_i \cdot H(E_k - E_{b,i}) \cdot \int_{p_{z,min}}^{p_{z,max,i}} J_i(p_z) dp_z}$$

- **Approximation: rejection method to avoid computing all the integrals**

- **Step 1: sample subshell  $jr$  according to probability  $P(j) = \frac{N_j \cdot H(E_k - E_{b,j})}{\sum_i N_i \cdot H(E_k - E_{b,i})}$**

- **Step 2: sample  $0 < r < 1$  uniformly and compute  $\int_{p_{z,min}}^{p_{z,max,jr}} J_{jr}(p_z) dp_z$**

- **Step 3: accept  $jr$  if  $r \leq \int_{p_{z,min}}^{p_{z,max,jr}} J_{jr}(p_z) dp_z$ , else go back to step 1**

- **Momentum  $p_z$  is then sampled using  $J_{jr}(p_z)$  as PDF in the range  $[p_{z,min}; p_{z,max,jr}]$**

## 2) c. Solve $E'_k = f(p_z)$

- $\widetilde{p}_z = c \cdot p_z = \frac{E_k E'_k (1 - \cos \theta) - m_e c^2 (E_k - E'_k)}{\sqrt{E_k^2 + E_k'^2 - 2 E_k E'_k \cos \theta}} \Rightarrow 0 = A E_k'^2 + 2 E_k B E'_k + E_k^2 C$  with
  - $A = \widetilde{p}_z^2 - [m_e c^2 + E_k (1 - \cos \theta)]^2$ ;
  - $B = -\{\widetilde{p}_z^2 \cos \theta - m_e c^2 [m_e c^2 + E_k (1 - \cos \theta)]\}$
  - $C = \widetilde{p}_z^2 - m_e^2 c^4$
- **Solutions of second-order polynomial:**  $E'_k = E_k \frac{-B \pm \sqrt{B^2 - AC}}{A}$
- **How to determine sign + or -?**
  - Both solutions are physical: the correct sign depends on the sign of  $\widetilde{p}_z$
  - If  $E'_k = 0$  then  $\widetilde{p}_z = -m_e c^2$  so  $\widetilde{p}_z = -m_e c^2 \Rightarrow E'_k = 0$  and  $\widetilde{p}_z = m_e c^2 \Rightarrow E'_k > 0$
- **Assuming  $|p_z| = m_e c^2$  then  $C = 0$  and  $E'_k = E_k \frac{-B \pm \sqrt{B^2}}{A}$** 
  - The sign + must be chosen if  $\widetilde{p}_z < 0$
  - The sign - must be chosen if  $\widetilde{p}_z > 0$
- **If  $\widetilde{p}_z = 0$  (free-electron case) then**
  - $\sqrt{B^2 - AC} = 0$
  - $E'_k = E_k \frac{-B}{A} = \frac{E_k}{1 + \frac{E_k}{m_e c^2} (1 - \cos \theta)} = E_C$

### 3) How to set the electron energy $T_e$ and direction $\vec{v}_e$

- Kinetic energy  $T_e$  of electron obtained by energy conservation

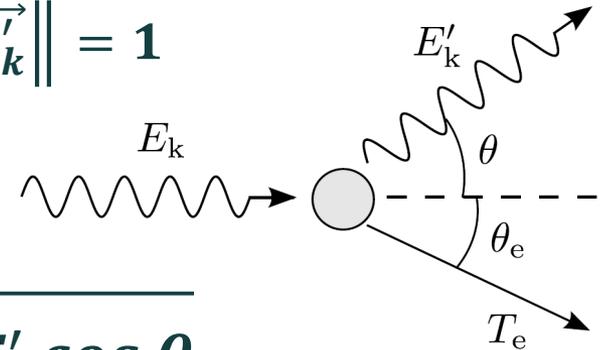
$$T_e = E_k - E'_k - E_{b,i}$$

- Approximation: electron direction = direction of free-electron case  
= direction of momentum transfer vector  $\vec{q}$

- $\vec{p}_k = \frac{E_k}{c} \vec{u}_k$  momentum of incident photon with  $\|\vec{u}_k\| = 1$

- $\vec{p}'_k = \frac{E'_k}{c} \vec{u}'_k$  momentum of scattered photon  $\|\vec{u}'_k\| = 1$

- $\|\vec{u}_k\| \cdot \|\vec{u}'_k\| = \cos \theta$



- Momentum transfer vector  $\vec{q}$

- $\hbar \vec{q} = \vec{p}_k - \vec{p}'_k \Rightarrow \|\vec{q}\| = \frac{1}{\hbar c} \sqrt{E_k^2 + E'_k{}^2 - 2E_k E'_k \cos \theta}$

- Electron direction vector  $\vec{v}_e$

$$\vec{v}_e = \frac{\vec{q}}{\|\vec{q}\|} = \frac{E_k \vec{u}_k - E'_k \vec{u}'_k}{\sqrt{E_k^2 + E'_k{}^2 - 2E_k E'_k \cos \theta}}$$

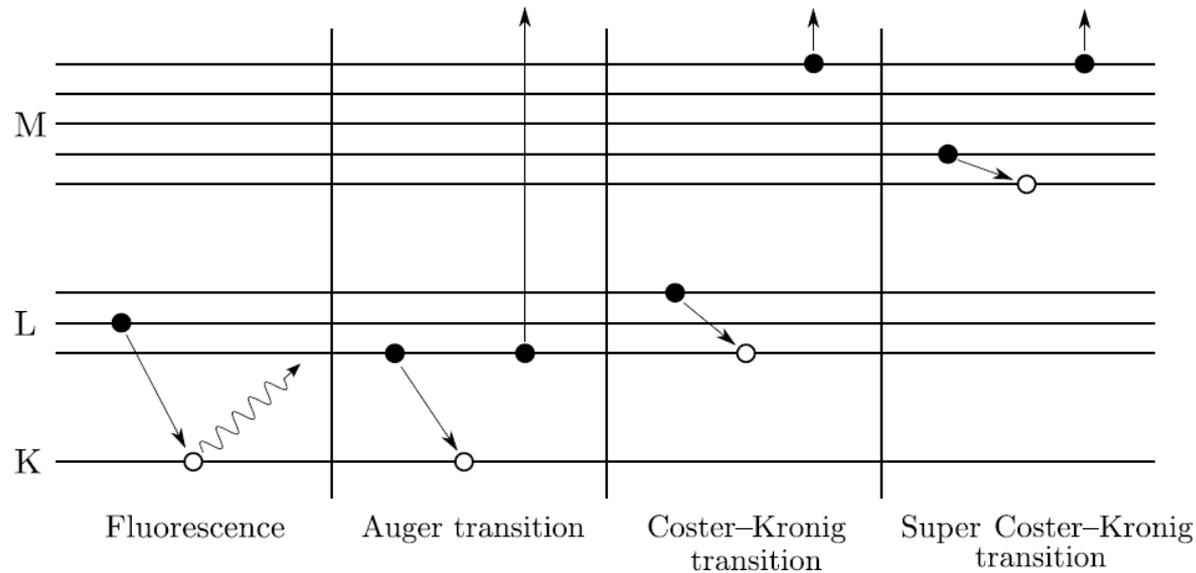
# 6. Atomic relaxation

---

Production of fluorescence / X-ray photons  
4 slides



- **Electron vacancies physically created in electron clouds by**
  - Photoelectric effect
  - Compton scattering
  - **Electron/positron interaction (not simulated in MCS)**



## ▪ 2 kinds of transition

- Radiative: X-ray photon emission and **one** new vacancy is created
- Non-radiative : electron emission and **two** new vacancies are created

## NJOY 2012 manual page 515

The fluorescence part is not coded yet. This section will be completed when the new fluorescence methods have been developed and installed in MCNP. In the meantime, ambitious users may be able to meld the new cross sections computed by the methods discussed in this section with the fluorescence data from the current MCNP library.

## NJOY 2012 manual page 537

The calculation of fluorescence data for photoelectric absorption is not complete in this version. A message to the user is provided.

- **Atomic relaxation data NOT treated by NJOY2012**
  - But available in ENDF/B.VII (ENDF) and EPICS2014 (ENDLX) library
  - Also available in some “manually-melded” ACE files of MCNP6 library
  - ENDF data post-processed by SERPENT2 team → “relax.dat” file added to MCS photon library

## Simple example: aluminium (Z = 13) electronic structure

subshell	1 K	2 L1	3 L2	4 L3	5 M1	6 M2	7 M3
label	1s(1) <sup>2</sup>	2s(1) <sup>2</sup>	2p(1) <sup>2</sup>	2p(3) <sup>4</sup>	3s(1) <sup>2</sup>	3p(1) <sup>0.33</sup>	3p(1) <sup>0.67</sup>
(EBI) Binding Energy (eV)	1549.9	119.05	81.2	80.73	10.16	4.88	4.87

```

Element 13
NSS 1
SUBI 1
NTR 22
EBI 1.549900E+03
ELN 2
 3  0  1.468700E+03  1.236990E-02
 4  0  1.469170E+03  2.455280E-02
 6  0  1.545020E+03  7.558540E-05
 7  0  1.545030E+03  1.500390E-04
 2  2  1.311800E+03  7.839440E-02
 2  3  1.349650E+03  8.321800E-02
 2  4  1.350120E+03  1.627250E-01
 2  5  1.420690E+03  1.358840E-02
 2  6  1.425970E+03  8.967940E-04
 2  7  1.425980E+03  1.764850E-03
 3  3  1.387500E+03  1.429200E-02
 3  4  1.387970E+03  3.669420E-01
 3  5  1.458540E+03  6.492940E-03
 3  6  1.463820E+03  3.013180E-04
 3  7  1.463830E+03  3.658830E-03
 4  4  1.388440E+03  2.092260E-01
 4  5  1.459010E+03  1.270630E-02
 4  6  1.464290E+03  3.651890E-03
 4  7  1.464300E+03  4.204210E-03
 5  5  1.529580E+03  5.811390E-04
 5  6  1.534860E+03  7.174400E-05
 5  7  1.534870E+03  1.363110E-04
    
```

- NSS** : only 1 subshell with EBI > 1000 eV cutoff
  - SUBI**: index of primary subshell where a vacancy is located. For aluminium, only one subshell SUBI = 1 → K-subshell vacancy
  - NTR**: 22 possible transitions for a vacancy in subshell SUBI
  - EBI** binding energy / **ELN** number of electrons of subshell SUBI
- 22 lines** : “**SUBJ SUBK  $E_{tr}$   $PDF_{tr}$** ”
  - SUBJ** = index of secondary subshell providing an electron which fills the primary vacancy
  - SUBK** = 0 : radiative transition → X-ray photon emission
  - SUBK** > 0 : non-radiative emission → electron emission from subshell with index SUBK
  - Transition energy  $E_{tr} = \text{EBI}(\text{SUBI}) - \text{EBI}(\text{SUBJ}) - \text{EBI}(\text{SUBK})$
  - $E_{tr}$  = energy of emitted particle;  $\text{EBI}(\text{SUBK}=0) = 0$
  - $PDF_{tr}$  : transition probability:  $\sum_{tr=1}^{tr=NTR} PDF_{tr} = 1$

- Generate a normalized CDF :  $CDF_{tr} = \sum_{t=1}^{t=tr} PDF_t$
- Create vacancy queue with initial Compton/photoelectric-induced vacancy
- Atomic relaxation algorithm
  1. Take one vacancy in primary subshell SUBI from the vacancy queue.
  2. If EBI(SUBI) > 1 keV, simulate relaxation, otherwise discard vacancy and go back to 1.
  3. Sample transition according to CDF. If secondary subshell SUBJ or tertiary subshell SUBK > 0 of sampled transition is already empty (ELN is finite!), repeat this step
  4. If  $E_{tr} > 1$  keV, add particle to queue: a photon if SUBK = 0, an electron if SUBK > 0
  5. Sample particle direction isotropically
  6. Add 1 vacancy in secondary subshell SUBJ to vacancy queue
  7. If SUBK > 0, also add 1 vacancy in tertiary subshell SUBK to vacancy queue
  8. Go back to 1. until no vacancies are left in the queue
- Implementation detail: binding energies / electron numbers (EBI/ELN) of relax.dat file
  - Must be consistent with (EBI/ELN) of ComptonProfiles.dat
  - Must be consistent with photo-atomic cross-section peaks
  - Otherwise energy conservation violation and complications for future KERMA calculations
  - MCS choice: EPICS2014 (EBI/EN) values adopted for both relax.dat and ComptonProfiles.dat

# 7. Thick-Target Bremsstrahlung (TTB)

---

Production of photons by charged particles  
12 slides



- Energetic electrons/positrons (short  $e^-/e^+$ ) are created by
  - Photoelectric effect
  - Compton scattering
  - Pair production
  - Atomic relaxation
- During slowing-down,  $e^-/e^+$  lose energy by emitting “bremsstrahlung” photons
  - Neglecting bremsstrahlung photons lead to underestimation of photon flux
- Full  $e^-/e^+$  transport more complicated than neutron/photon transport, so **TTB (Thick-Target Bremsstrahlung)** approximation
  - $e^-/e^+$  slowing-down on site ; actual displacement neglected
  - bremsstrahlung photons emitted on site, where  $e^-/e^+$  are created
  - bremsstrahlung (daughter) photon inherit the direction of mother  $e^-/e^+$
  - bremsstrahlung photons produced according to Continuous Slowing-Down Approximation (CSDA)
- Our goal: sample the yield and energy of bremsstrahlung photons emitted by  $e^-/e^+$  of energy  $T_e$

# Bremsstrahlung yield $Y_n(T_e, E_{cut})$

- Average number  $Y_n(T_e, E_{cut})$  of bremsstrahlung photons with energy higher than  $E_{cut}$  emitted by a charged particle slowing down from energy  $T_e$  to  $E_{cut}$

$$Y_n(T_e, E_{cut}) = \int_{T'=E_{cut}}^{T'=T_e} \frac{\lambda_{br}^{-1}(T', E_{cut})}{S_{tot}(T')} dT'$$

- For MCS,  $E_{cut} = 1$  keV
- Knowledge of  $Y_n(T_e, E_{cut}) \rightarrow$  knowledge of bremsstrahlung photon yields and spectra
  - YIELD: assuming  $T_1 > T_2 > E_{cut}$  then the number of bremsstrahlung photons with energy higher than  $E_{cut}$  emitted by a charged particle slowing down from energy  $T_1$  to  $T_2$  is

$$Y_n(T_1, E_{cut}) - Y_n(T_2, E_{cut})$$

- SPECTRUM: assuming  $T_e > E_1 > E_2 > E_{cut}$  then the number of bremsstrahlung photons with energy between  $E_1$  and  $E_2$  is

$$Y_n(T_e, E_2) - Y_n(T_e, E_1)$$

# Inverse bremsstrahlung mean free path $\lambda_{br}^{-1}(T', E_{cut})$

$$\lambda_{br}^{-1}(T_e, E_{cut}) = \frac{1}{\beta^2} \sum_{j=1}^P Z_j^2 \cdot C_j \int_{\kappa = \kappa_{cut}}^{\kappa = 1} \frac{1}{\kappa} \chi(Z_j, T_e, \kappa) d\kappa$$

- $\beta = \frac{v}{c} = \frac{\sqrt{T_e(T_e + 2m_e c^2)}}{T_e + m_e c^2}$ ; reduced electron energy  $\kappa = \frac{E_k}{T_e}$
  
- For a material M with n elements  $j = 1, \dots, P$ 
  - $Z_j$  atomic number of element j
  - $C_j$  number density of element j ( $\#/cm^3$ )
  
- $\chi(Z_j, T_e, \kappa)$  is the **scaled bremsstrahlung cross-section** of element j
  - NOT available in ACE files and in ENDF/B-VII files, NOT treated by NJOY
  - PENELOPE 2014 database: 99 files “pdebr01.p08” → “pdebr99.p08” for Z = 1-99
  - PENELOPE 2014 file processed by SERPENT2 team → “pdebr.dat” file added to MCS photon library

## Content of “pdebr.dat” file

- Tabulated values of  $\chi(Z_j, T_e, \kappa)$  for  $Z = 1-99$  for 57 electron energies  $T_e = 1 \text{ keV}$  to  $10 \text{ GeV}$  and 32  $\kappa$  values from  $\kappa = 10^{-12}$  to 1
- Recommended interpolation: cubic spline log-log interpolation [1] (= solving a tridiagonal matrix system using Thomas algorithm [2])

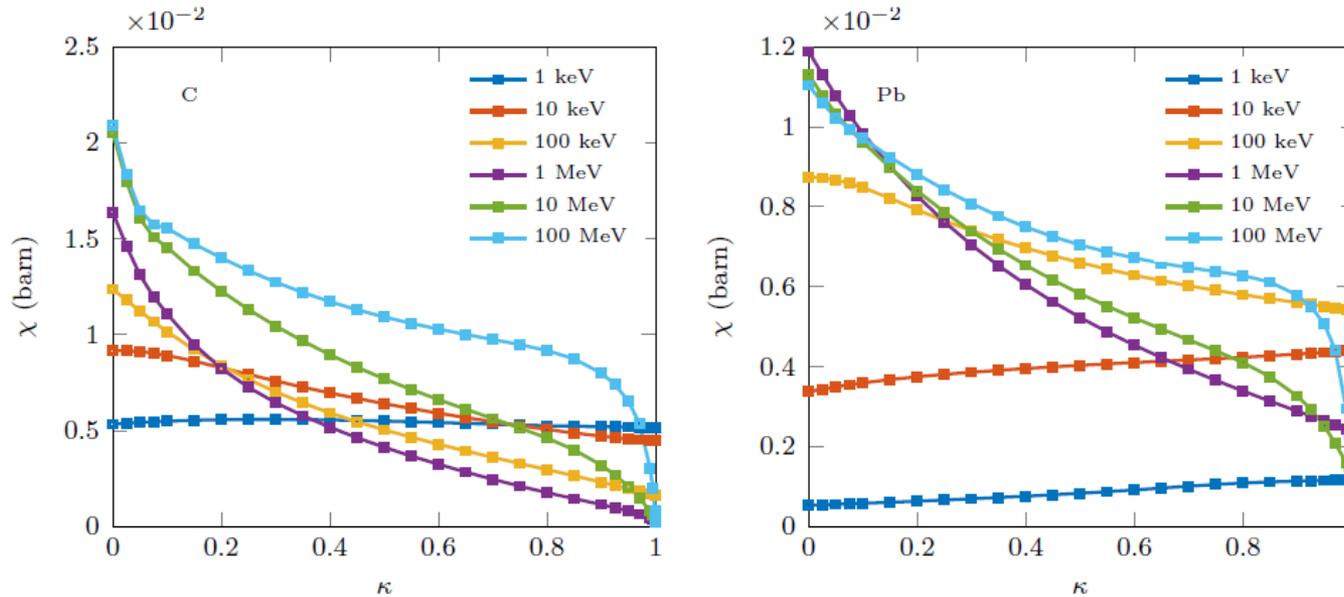


Figure 5.1: Scaled bremsstrahlung DCS as a function of the variable  $\kappa = E_{\kappa}/T$  in carbon and lead for different electron kinetic energies

[1] Wikiversity, article “Cubic Spline Interpolation”

[2] Wikipedia, article “Tridiagonal Matrix Algorithm”

# Total stopping power $S_{tot}$

- $T_e$  kinetic energy of electron/positron
- Total stopping power  $S_{tot}$ 
  - Average energy loss per unit length (all energy losses totaled)

$$S_{tot}(T_e) = S_{col}(T_e) + S_{rad}(T_e) \text{ [MeV/cm]}$$

- Collision stopping power  $S_{col}$ 
  - Energy loss by collision
  - Coulomb interactions with atoms and electron clouds (ionization, excitation)
- Radiative stopping power  $S_{rad}$ 
  - Energy loss by radiative emission (bremsstrahlung photon emission)
- Online calculation tool: ESTAR database [1]

[1] National Institute of Standards and Technology, "ESTAR: Stopping Powers and Ranges for Electrons," <http://physics.nist.gov/PhysRefData/Star/Text/ESTAR.html>

$$S_{rad}(T_e) = \frac{T_e}{\beta^2} \sum_{j=1}^P R(Z_j, T_e) \cdot Z_j^2 \cdot C_j \int_{\kappa=0}^{\kappa=1} \chi(Z_j, T_e, \kappa) d\kappa$$

- For electrons  $R(Z_j, T_e) = 1$
- For positrons  $R(Z_j, T_e) = 1 - \exp[-1.2359 * 10^{-1}t + 6.1274 * 10^{-2}t^2 - 3.1516 * 10^{-2}t^3 + 7.7446 * 10^{-3}t^4 - 1.0595 * 10^{-3}t^5 + 7.0568 * 10^{-5}t^6 - 1.8080 * 10^{-6}t^7]$
- $R(Z_j, T_e)$  is the positron correction factor used by PENELOPE 2014
- $t = \ln\left(1 + \frac{10^6}{Z_j^2} \frac{T_e}{m_e c^2}\right)$
- Reduced electron energy  $\kappa = \frac{E_k}{T_e}$
- $\beta = \frac{v}{c} = \frac{\sqrt{T_e(T_e + 2m_e c^2)}}{T_e + m_e c^2}$ ;

$$\frac{1}{\rho} S_{col}(T_e) = \frac{2\pi r_e^2 m_e c^2}{\beta^2} N_{el} \left[ 2 \ln \frac{T_e}{I_{MEE}} + \ln \left( 1 + \frac{\tau}{2} \right) + F(\tau) - \delta(\beta, I_{MEE}) \right]$$

- For electrons  $F(\tau) = (1 - \beta^2) \left[ 1 + \frac{\tau^2}{8} - (2\tau + 1) \cdot \ln(2) \right]$
- For positrons  $F(\tau) = 2 \cdot \ln(2) - \left( \frac{\beta^2}{12} \right) \left[ 23 + \frac{14}{\tau+2} + \frac{10}{(\tau+2)^2} + \frac{4}{(\tau+2)^3} \right]$
- Description of all the variables

- $\beta = \frac{v}{c} = \frac{\sqrt{T_e(T_e + 2m_e c^2)}}{T_e + m_e c^2}$

- $r_e$  classical electron radius ( $\approx 2.8179 \times 10^{-13}$  cm)

- $m_e c^2$  electron rest mass ( $\approx 0.511$  MeV) and  $\tau = \frac{T_e}{m_e c^2}$

- $N_{el}$  electron gram density [# of electrons/gram]

- $\rho$  material density [g/cm<sup>3</sup>]

- $I_{MEE}$  is the **Mean Excitation Energy** of the material [MeV]

- $\delta(\beta, I_{MEE})$  is the **density-effect correction** [unitless]

# Calculation of Mean Excitation Energy $I_{MEE}$

- For a material M with n elements  $j = 1, \dots, P$

- $Z_j$  atomic number of element j
- $C_j$  number density of element j [ $\#/cm^3$ ]
- $I_j$  “potential” of element j [MeV]

$$I_{MEE} = \exp \left[ \frac{\sum_{j=1}^P C_j \cdot Z_j \cdot \ln(I_j)}{\sum_{i=1}^P C_j \cdot Z_j} \right]$$

- Potential  $I_j$  depends

- on material phase (gaseous or condensed)
- on material composition (single element or chemical compound)

- Example: oxygen  $Z = 8$

- Mono-element, gaseous phase: potential = 95 eV (pure  $O_2$  gas)
- Compound, gaseous phase : potential = 105 eV (steam water)
- Mono-element, condensed state : potential = 97 eV
- Compound, condensed state: potential = 106 eV (uranium dioxide)

- Tabulated  $I_j$  values from MCNP6 adopted for MCS

- From subroutine “get\_excitation\_MeV” in file excitation\_energies.f90
- Good agreement with  $I_{MEE}$  from ESTAR database

- MCS density cut-off  $\rho_{cut} = 0.03 \text{ g/cm}^3$

- If  $\rho < \rho_{cut}$ , material phase is set to gaseous
- If  $\rho \geq \rho_{cut}$ , material phase is set to condensed
- User can override this choice using “is\_gas” tag in MCS input

# Examples of Mean Excitation Energy $I_{MEE}$ (eV)

	MATERIAL	ESTAR (reference value)	STARCODES (Matlab, reverse engineering)	PENELOPE 2014 (directly from code)	MCNP6	MCS (inspired from MCNP6)
1	lithium 0.534 g/cm <sup>3</sup>	40.00	40.00	40.00	40.00	40.00
2	carbon 2 g/cm <sup>3</sup>	81.00	78.00	81.00	78.00	78.00
3	oxygen	95.00	95.00	95.00	95.00	95.00
4	chlorine	174.00	159.29	174.00	159.29	159.29
5	iron	286.00	286.00	286.00	286.00	286.00
6	bromine	343.00	357.00	343.00	357.00	357.00
7	uranium	890.00	890.00	890.00	890.00	890.00
8	plutonium	921.00	921.00	921.00	921.00	921.00
9	uranium oxide	720.60	720.62	638.91	720.62	720.62
10	plutonium oxide	746.50	746.52	661.86	746.52	746.52
11	uranium dicarbide	752.00	752.04	674.97	752.04	752.04
12	water, liquid	75.00	75.32	69.00	75.32	75.32
13	water, vapor	71.60	70.16	69.00	70.16	70.16
14	dry air	85.70	86.20	85.67	86.20	86.20
15	muscle	74.30	74.68	69.56	74.68	74.68
16	barium fluoride	375.90	375.94	344.94	375.94	375.94
17	dichlorobenzene	106.50	108.15	106.48	108.15	108.15
18	lithium carbonate	87.90	87.93	80.09	87.93	87.93

# Density-effect correction $\delta(T_e, I_{MEE})$ [1]

- We consider a medium M (notation from previous slides)

- Electron number density  $n = \sum_{j=1}^P C_j \cdot Z_j$  [# of electron/m<sup>3</sup>]

- Plasma oscillation energy  $I_{POE} = \frac{h}{2\pi} \sqrt{\frac{n \cdot e^2}{m_e \cdot \epsilon_0}}$

( $h$  Planck constant;  $\epsilon_0$  vacuum permittivity;  $e$  elementary charge;  $m_e$  electron rest mass)

- Element j has  $P_j$  electron subshells, numbered  $k = 1, \dots, S = \sum_{j=1}^P P_j$

- Electron from subshells  $k = 1, \dots, R$  are NOT conduction band electrons

- Electron from subshells  $k = R+1, \dots, S$  are conduction band electrons

- Binding energy of subshell k is  $EB_k$

- Number of electrons in subshell k is  $N_k$ . By definition  $\forall j \sum_{k=1}^{P_j} N_k = Z_j$

- Resistivity/conductivity

- M is **electrical insulator** if gaseous state OR at least one element without a conduction band electron (MCS data file “gsconfig.dat”)

- Otherwise M is **electrical conductor**

- MCS user can override this choice using “is\_conductor” tag in MCS input

[1] M. Sternheimer, S. M. Seltzer, and M. J. Berger, "Density effect for the ionization loss of charged particles in various substances," Phys. Rev. B, 26, 6067-6076 (1982)

# Calculation of density-effect correction $\delta(T_e, I_{MEE})$ (1)

$$\delta(\beta) = -L^2(1 - \beta^2) + \sum_{k=1}^S f_k \cdot \ln \left[ \frac{l_k^2 + L^2}{l_k^2} \right]$$

- **Special case: in insulators, for  $\beta < \beta_0$  then  $\delta(\beta) = 0$ .**

The threshold  $\beta_0$  is given by

$$\frac{1}{\beta_0^2} - 1 = \sum_{k=1}^S \frac{f_k}{\mu_k^2}$$

- **For conduction band electrons in conductor materials,  $l_k^2 = f_k$**
- **Otherwise  $l_k^2 = \mu_k^2 + \frac{2}{3}f_k$**
- **For subshell k in element j,  $f_k = \frac{N_k \cdot C_j}{n}$  (by definition  $\sum_{k=1}^S f_k = 1$ )**
- **L is solution of equation  $\frac{1}{\beta^2} - 1 = \sum_{k=1}^S \frac{f_j}{\mu_k^2 + L^2}$**
- **For conduction band electrons in conductor materials,  $\mu_k = 0$**
- **Otherwise  $\mu_k = \omega \frac{EB_k}{I_{POE}}$**

- For a conductor,  $\omega$  is solution of equation

$$\ln I_{MEE} = \sum_{k=1}^R f_k \cdot \ln \left[ \sqrt{(EB_k \cdot \omega)^2 + \frac{2}{3} f_k I_{POE}^2} \right] + \sum_{k=R+1}^S f_k \cdot \ln [I_{POE} \sqrt{f_k}]$$

- For an insulator,  $\omega$  is solution of equation

$$\ln I_{MEE} = \sum_{k=1}^S f_k \cdot \ln \left[ \sqrt{(EB_k \cdot \omega)^2 + \frac{2}{3} f_k I_{POE}^2} \right]$$

# 8. Photon KERMA

---

Kinetic Energy Relaxed per MAss  
3 slides



- Kinetic Energy Relaxed per MAss

$$KERMA = \frac{\textit{transferred energy}}{\textit{mass}}$$

- Unit(KERMA) = gray = joule/kg
- Neutron KERMA / photon KERMA
- Transferred energy
  - Kinetic energy of charged particles created / released in matter after uncharged particle interaction
- Collision photon KERMA
  - Fraction of the transferred energy not re-emitted as photons (by bremsstrahlung / annihilation) divided by mass

# What MCS tallies in KERMA calculation

- **Kinetic energy of electron / positron not re-emitted as photons by bremsstrahlung / annihilation**
  - Electrons from Compton / photoelectric / pair production
  - Positrons from pair production
  - Electrons from atomic relaxation
- **Energy of electrons and photons below 1 keV cutoff**
  - Bremsstrahlung photons
  - Fluorescence photons
  - Auger electrons
- **Final MCS tally unit = MeV**
  - Must be divided by mass by the user to yield collision photon KERMA

- **KERMA from 20 MeV photon source in infinite lead medium**
  - Energy deposited per source photon = 20 MeV because infinite medium
  - Mode P calculation with & without bremsstrahlung (TTB)
  - 1 million photon histories; tally  $\pm$  absolute standard deviation (in MeV)

	MCS	MCNP6.1		
	KERMA detector	+F6 tally	F6:P tally	*F8:P tally
TTB off	$20.0000 \pm 3.10^{-9}$	$19.9891 \pm 2.10^{-2}$	$19.9891 \pm 2.10^{-2}$	$20.0000 \pm 0$
TTB on	$20.0000 \pm 0$	$20.4299 \pm 2.10^{-2}$	$20.4299 \pm 2.10^{-2}$	$20.0000 \pm 0$

- **+F6 and F6 give tallies > 20 MeV per particle source !!**
- **Double counting of +F6 and F6 with bremsstrahlung on**
  - Kinetic energy of created electrons is tallied
  - AND energy deposited by bremsstrahlung photons from those electrons
- **Problem is solved when bremsstrahlung is turned off**
- **MCS KERMA detector similar to MCNP6 \*F8:P tally in mode P**

# 9. Verification & Validation

---

Code/code and code/experiment comparison  
2 slides



- **Comparison to MCNP6.1 and SERPENT2.1.29**
- **A: multigroup photon flux spectrum benchmark**
  - Comparison of ~500-group photon flux in infinite medium
  - Isotropic mono-kinetic point photon source
  - Medium compositions: H / O / H<sub>2</sub>O / Fe / Ag / Nd / UO<sub>2</sub> / U
  - Source energies: 100 keV / 1 MeV / 10 MeV / 20 MeV
- **B: energy-space photon flux distribution benchmark**
  - Comparison of spatial distribution of photon flux in a cylinder
  - Upward-oriented mono-kinetic point photon source
  - Medium compositions: H<sub>2</sub>O / Pb
  - Source energies: 100 keV / 1 MeV / 10 MeV / 20 MeV
- **C: shielding problems**
  - KN-12 spent nuclear fuel transport cask
- **Cf test of MCS v0.0.76(4) / 2017.12.12 in**

Lemaire M et al. "Verification of photon-transport capability of UNIST Monte Carlo code MCS", submitted to Annals of Nuclear Energy

- **Implementation of deep-penetration shielding problems features**
  - Coupled neutron/photon calculations
  - Variance reduction techniques
  
- **Extension of verification/validation database**
  - New cases to cover photon flux / KERMA / dose calculations
  - SINBAD experimental shielding benchmark problems

**UNIST CORE**