An overview of basic concepts and formulas in simulations of the Compton scattering

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Introduction

This conference will be a celebration of a double-scattering formula:

$$\frac{\mathrm{d}^4\sigma_{12}}{\mathrm{d}^2\Omega_1\mathrm{d}^2\Omega_2} = \frac{r_0^4}{16}\left[F(\theta_1)F(\theta_2) - G(\theta_1)G(\theta_2)\cos 2(\phi_1 - \phi_2)\right]$$

It is a differential cross section for the **Compton scattering of two entangled photons from a two-photon electron-positron annihilation**. In that:

$$F(\theta_i) = \frac{2 + (1-\cos\theta_i)^3}{(2-\cos\theta_i)^3} \quad \text{and} \quad G(\theta_i) = \frac{\sin^2\theta_i}{(2-\cos\theta_i)^2}$$

The relevant process qualifiers to be kept in mind are:

(1) the scattering of **two** photons

(2) photons are **entangled** (most importantly, in polarization)

(3) photons originate from a **two-photon** annihilation

(4) annihilation is that of **electron and positron**

Introduction

First published in:

- M.H.L. Pryce, J.C. Ward, *Angular correlation effects with annihilation radiation*, Nature **160**, 435 (1947),

now famous formula for a double-scattering cross section has been regularly quoted in later publications. It applies *exclusively* to photons from the **electron-positron** annihilation (initial photon energy $E_0 = m_e c^2$).

A more general formula for entangled annihilation photons of any initial energy was soon after provided in:

- H.S. Snyder, S. Pasternack, J. Hornbostel, *Angular Correlation of Scattered Annihilation Radiation*, Physical Review C **73**, 440 (1948):

$$\frac{\mathrm{d}^4\sigma_{12}}{\mathrm{d}^2\Omega_1 \mathrm{d}^2\Omega_2} = \frac{r_0^4}{16}\frac{E_1^2}{E_0^2}\frac{E_2^2}{E_0^2}\times \left[\varepsilon_1\varepsilon_2 - \varepsilon_1 \sin^2\theta_2 - \varepsilon_2 \sin^2\theta_1 + 2\sin^2\theta_1 \sin^2\theta_2 \sin^2(\phi_1-\phi_2)\right]$$

with E_0 as initial photons energy, E_1 and E_2 as scattered photon energies, and $\varepsilon_i = E_i/E_0 + E_0/E_i$.

Single-photon scattering: polarized Klein-Nishina

Considering a scattering of each photon separately (independently from the other photon) gives rise to the **uncorrelated** double-scattering process. In a context of *entangled* annihilation-photons, an experimental evidence for the photon entanglement and its effect upon subsequent scattering can be found in the observed **deviations** from the uncorrelated scattering. Therefore, the uncorrelated scattering must be perfectly characterized.

A starting point is the Klein-Nishina cross section for a single photon with a **particular polarization**:

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}^2\Omega} = \frac{r_0^2}{4}\frac{E_\theta^2}{E_0^2}\left(\frac{E_0}{E_\theta} + \frac{E_\theta}{E_0} + 2\cos 2\Theta\right)$$

with Θ as an angle between polarization vectors before and after the scattering: $\Theta = \sphericalangle\left(\vec{\varepsilon}_0, \vec{\varepsilon}\right)$ [not the same as a scattering angle θ from a solid angle element $\mathrm{d}^2\Omega = \sin\theta \mathrm{d}\theta \mathrm{d}\phi$].

Single-photon scattering: polarized Klein-Nishina

A scattering geometry was analyzed in detail in:

- G.O. Depaola, *New Monte Carlo method for Compton and Rayleigh scattering by polarized gamma rays*, Nuclear Instruments and Methods A **512**, 619 (2003).

finding a geometric relation: $\boldsymbol{\cos^2\Theta = (1-\sin^2\theta\cos^2\phi)\cos^2\beta}$.

Let $\vec{\varepsilon}_0$ and $\vec{k}_0$ be a polarization and a direction of an *initial* photon.
Let $\vec{\varepsilon}$ and $\vec{k}$ be a polarization and a direction of a *scattered* photon.

Aside from $\boldsymbol{\Theta = \sphericalangle(\vec{\varepsilon},\vec{\varepsilon}_0)}$, the relevant angles are:

- scattering angle θ between the two photons: $\boldsymbol{\theta = \sphericalangle(\vec{k},\vec{k}_0)}$
- azimuthal scattering angle ϕ (around $\vec{k}_0$) relative to a direction of initial polarization $\vec{\varepsilon}_0$: $\boldsymbol{\phi = \sphericalangle\left[\vec{k}_0\times(\vec{k}\times\vec{k}_0),\vec{\varepsilon}_0\right]}$
- angle β of a polarization $\vec{\varepsilon}$, relative to a plane spanned by $\vec{\varepsilon}_0$ and $\vec{k}$ (i.e. around $\vec{k}$, relative to a semi-axis in a general direction of $\vec{\varepsilon}_0$): $\boldsymbol{\beta = \sphericalangle\left[\vec{k}\times(\vec{\varepsilon}_0\times\vec{k}),\vec{\varepsilon}\right]}$

(See Depaola reference for geometric sketches.)

Single-photon scattering: polarized Klein-Nishina

Using a previous relation:

$$\cos^2\Theta = (1-\sin^2\theta\cos^2\phi)\cos^2\beta$$

a polarized scattering cross section:

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}^2\Omega} = \frac{r_0^2}{4}\frac{E_\theta^2}{E_0^2}\left(\frac{E_0}{E_\theta}+\frac{E_\theta}{E_0}+2\cos 2\Theta\right)$$

may be expressed as:

$$\boxed{\frac{\mathrm{d}^2\sigma}{\mathrm{d}^2\Omega} = \frac{r_0^2}{4}\frac{E_\theta^2}{E_0^2}\left(\frac{E_0}{E_\theta}+\frac{E_\theta}{E_0}-2+4(1-\sin^2\theta\cos^2\phi)\cos^2\beta\right)}$$

Notice!

Scattering cross section (i.e. the nature of a process) is fully determined by a change of polarization (Θ)! The expanded formula is just a way of expressing this dependence via more convenient geometric parameters. Also, not all values of Θ are compatible with a given scattering angle θ:

$$\boldsymbol{\cos^2\Theta \leq 1-\sin^2\theta \quad \Rightarrow \quad \theta \leq \Theta \leq \pi-\theta}$$

Single-photon scattering: various Klein-Nishinas

Derived, process-specific cross sections

For photons of **specific polarization** (ϕ and β for scattered photon both known from initial photon), a scattering cross section is:

$$\frac{\mathrm{d}^2\sigma^{(\theta\phi\beta)}}{\mathrm{d}^2\Omega} = \frac{r_0^2}{4}\frac{E_\theta^2}{E_0^2}\left(\frac{E_0}{E_\theta} + \frac{E_\theta}{E_0} - 2 + 4(1 - \sin^2\theta\cos^2\phi)\cos^2\beta\right)$$

For photons of **specific initial** but **unspecified final** polarization, a "polarized-in, unpolarized-out" cross section is obtained by summing over the two possible polarization-basis states ($\beta = 0$ and $\frac{\pi}{2}$):

$$\frac{\mathrm{d}^2\sigma^{(\theta\phi)}}{\mathrm{d}^2\Omega} = \frac{r_0^2}{2}\frac{E_\theta^2}{E_0^2}\left(\frac{E_0}{E_\theta} + \frac{E_\theta}{E_0} - 2\sin^2\theta\cos^2\phi\right)$$

With **both polarizations unspecified**, a polarization-uncorrelated cross section is obtained by averaging over all possible initial polarizations (ϕ):

$$\frac{\mathrm{d}^2\sigma^{(\theta)}}{\mathrm{d}^2\Omega} = \frac{r_0^2}{2}\frac{E_\theta^2}{E_0^2}\left(\frac{E_0}{E_\theta} + \frac{E_\theta}{E_0} - \sin^2\theta\right)$$

which is a Klein-Nishina formula most regularly encountered in literature.

Simulating a single-photon scattering

In general, a probability for Compton scattering to occur in a material is:

$$P = \left(1 - e^{-n\Sigma_\mathrm{tot}}\right)\frac{\sigma_\mathrm{Comp}}{\Sigma_\mathrm{tot}}$$

with Σ_tot as a total cross section for *any* photon interaction, and σ_Comp as a total (integrated) cross section for Compton scattering:

$$\sigma_\mathrm{Comp} = \int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\frac{\mathrm{d}^2\sigma^{(\theta)}}{\mathrm{d}^2\Omega}\sin\theta\mathrm{d}\theta\mathrm{d}\phi$$

n is an areal density of targets, i.e. a number of electrons per unit area. In case of a thin material ($n\Sigma_\mathrm{tot} \ll 1$) P may be approximated as:

$$P \approx n\sigma_\mathrm{Comp}$$

From this point we focus exclusively on the electron-positron annihilation photons, so that:

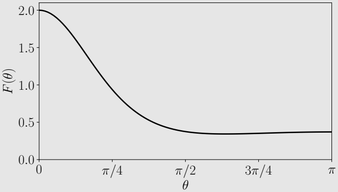
$$\frac{E_\theta}{E_0} = \frac{1}{2-\cos\theta}$$

Hence:

$$\frac{\mathrm{d}^2\sigma^{(\theta)}}{\mathrm{d}^2\Omega} = \frac{r_0^2}{2}\frac{2+(1-\cos\theta)^3}{(2-\cos\theta)^3} = \frac{r_0^2}{2}F(\theta)$$

and:

$$\sigma_\mathrm{Comp} = r_0^2\pi\left(\tfrac{40}{9} - 3\ln 3\right) \approx 3.6\, r_0^2$$



Simulating a single-photon scattering

(1) Sampling a reaction probability

- calculate a reaction probability P
- uniformly generate a random number $r \in [0, 1]$
- if $r \leq P$, scattering occurs

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(2) Sampling a scattering θ

Repeat until θ accepted:

- uniformly generate $\cos\theta \in [-1, 1]$
- use a part of $\mathrm{d}^2\sigma^{(\theta)}/\mathrm{d}^2\Omega$:
$$p(\theta) = F(\theta)$$
  such that $p_{\max} = 2$
- uniformly generate a random number $r \in [0, p_{\max}]$
- if $r \leq p(\theta)$, accept θ

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- uniformly generate a random number $r \in [0, p_{\max}]$
- if $r \leq p(\theta)$, accept θ

(3) Sampling a scattering ϕ

Having θ, repeat until ϕ accepted:

- uniformly generate $\phi \in [0, 2\pi]$
- use a part of $\mathrm{d}^2\sigma^{(\theta\phi)}/\mathrm{d}^2\Omega$:

$$p(\phi) = F(\theta) - G(\theta)\cos 2\phi$$

  such that $p_{\max} = F(\theta) + G(\theta)$
- uniformly generate a random number $r \in [0, p_{\max}]$
- if $r \leq p(\phi)$, accept ϕ

*Reminder:

$$G(\theta) = \frac{\sin^2\theta}{(2-\cos\theta)^2}$$

Simulating a single-photon scattering

(4) Sampling a polarization β

Having θ and ϕ, repeat until β accepted:

- uniformly generate $\beta \in [0, 2\pi]$; use a part of $\mathrm{d}^2\sigma^{(\theta\phi\beta)}/\mathrm{d}^2\Omega$:

$$p(\beta) = \frac{1}{(2-\cos\theta)^2}\left[\frac{1}{2-\cos\theta} - \cos\theta + 4(1-\sin^2\theta\cos^2\phi)\cos^2\beta\right]$$

  such that $p_{\max} = F(\theta) + G(\theta)(1 - 4\cos^2\phi) + 2(2-\cos\theta)^{-2}$
- uniformly generate a random number $r \in [0, p_{\max}]$; if $r \leq p(\beta)$, accept β

Simulating a single-photon scattering

(4) Sampling a polarization β

Having θ and ϕ, repeat until β accepted:

- uniformly generate $\beta \in [0, 2\pi]$; use a part of $\mathrm{d}^2\sigma^{(\theta\phi\beta)}/\mathrm{d}^2\Omega$:

$$p(\beta) = \frac{1}{(2-\cos\theta)^2}\left[\frac{1}{2-\cos\theta} - \cos\theta + 4(1 - \sin^2\theta\cos^2\phi)\cos^2\beta\right]$$

  such that $p_{\max} = F(\theta) + G(\theta)(1 - 4\cos^2\phi) + 2(2-\cos\theta)^{-2}$

- uniformly generate a random number $r \in [0, p_{\max}]$; if $r \le p(\beta)$, accept β

(2–4) Alternative procedure: sampling θ, ϕ, β at once

Repeat until a whole triple θ, ϕ, β accepted:

- uniformly generate $\cos\theta \in [-1, 1]$, $\phi \in [0, 2\pi]$, $\beta \in [0, 2\pi]$
- use a part of $\mathrm{d}^2\sigma^{(\theta\phi\beta)}/\mathrm{d}^2\Omega$ as above, considering it as a distribution $p(\theta, \phi, \beta)$ of three independent parameters, so that $p_{\max} = 4$
- uniformly generate a random number $r \in [0, p_{\max}]$
- if $r \le p(\theta, \phi, \beta)$, accept θ, ϕ, β

Simulating a correlated double-photon scattering

In simulating a correlated scattering of entangled annihilation photons, each photon (by itself) follows a regular Klein-Nishina statistics. However, their joint scattering cross section is correlated:

$$\frac{\mathrm{d}^4\sigma_{12}}{\mathrm{d}^2\Omega_1 \mathrm{d}^2\Omega_2} = \frac{r_0^4}{16}\big[F(\theta_1)F(\theta_2) - G(\theta_1)G(\theta_2)\cos 2(\phi_1 - \phi_2)\big]$$

Simulating correlated scattering

- if a double-photon scattering has already been decided, one could sample four parameters $\theta_1, \theta_2, \phi_1, \phi_2$ at once, applying a rejection sampling to:

$$p(\theta_1, \theta_2, \phi_1, \phi_2) = F(\theta_1)F(\theta_2) - G(\theta_1)G(\theta_2)\cos 2(\phi_1 - \phi_2)$$

- alternatively (or in case of following one photon at a time), one could first sample parameters θ_1, ϕ_1 for one photon, and then apply a rejection sampling to the other photon, wherein already-sampled θ_1, ϕ_1 are to be treated as *fixed-parameters* for the other photon's distribution $p(\theta_2, \phi_2)$
- post-scattering polarizations β_1, β_2 should be sampled as for single photons

Correlated vs. uncorrelated scattering

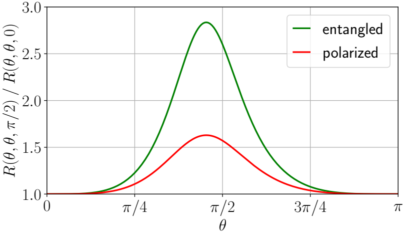
In order to compare the level of azimuthal correlations between different double-photon scattering models, we derive a reduced (and arbitrarily scaled) quantity dependent on the azimuthal difference $\Phi = \phi_2 - \phi_1$:

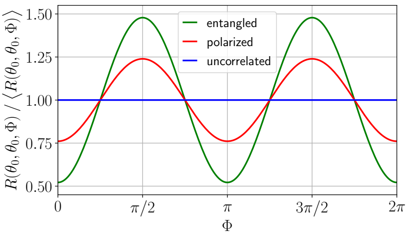
$$R_\mathrm{model}(\theta_1, \theta_2, \Phi) \propto \frac{\mathrm{d}^3\sigma_\mathrm{model}}{\mathrm{d}(\cos\theta_1)\mathrm{d}(\cos\theta_2)\mathrm{d}\Phi}$$

Models

- "entangled" model: from $\mathrm{d}^4\sigma_{12}/\mathrm{d}^2\Omega_1\mathrm{d}^2\Omega_2$ for entangled photons:
$$R_\mathrm{ent}(\theta_1, \theta_2, \Phi) \propto F(\theta_1)F(\theta_2) - G(\theta_1)G(\theta_2)\cos 2\Phi$$
- "polarized" model: from cross section $\mathrm{d}^2\sigma^{(\theta\phi)}/\mathrm{d}^2\Omega$ for polarized but uncorrelated (not entangled) photons:
$$R_\mathrm{pol}(\theta_1, \theta_2, \Phi) \propto 2F(\theta_1)F(\theta_2) - G(\theta_1)G(\theta_2)\cos 2\Phi$$
- "uncorrelated" model: from cross section $\mathrm{d}^2\sigma^{(\theta)}/\mathrm{d}^2\Omega$ for uncorrelated photons of unknown polarization:
$$R_\mathrm{unc}(\theta_1, \theta_2, \Phi) \propto F(\theta_1)F(\theta_2)$$

Correlated vs. uncorrelated scattering





For entangled and polarized models a level of azimuthal modulations varies with θ_1, θ_2 (uncorrelated model stays flat in Φ). It can be expressed as:

$$M_{\mathrm{model}}(\theta_1,\theta_2) = \frac{R_{\mathrm{model}}(\theta_1,\theta_2,\pi/2)}{R_{\mathrm{model}}(\theta_1,\theta_2,0)}$$

For both models it reaches a maximum for $\theta_1 = \theta_2 = \theta_0$, at $\theta_0 \approx 81.7°$:

$$M_{\mathrm{ent}}(\theta_0,\theta_0) \approx 2.836$$
$$M_{\mathrm{pol}}(\theta_0,\theta_0) \approx 1.629$$

One can also observe an azimuthal variation amplitude for each model:

$$A_{\mathrm{model}}(\theta_1,\theta_2) = \frac{R_{\mathrm{model}}(\theta_1,\theta_2,\pi/2)}{\langle R_{\mathrm{model}}(\theta_1,\theta_2,\Phi)\rangle}$$

Maxima for relevant models are:

$$A_{\mathrm{ent}}(\theta_0,\theta_0) \approx 1.479$$
$$A_{\mathrm{pol}}(\theta_0,\theta_0) \approx 1.239$$

A ratio of two models' amplitudes also has a maximum at θ_0:

$$A_{\mathrm{ent}}(\theta_0,\theta_0)/A_{\mathrm{pol}}(\theta_0,\theta_0) \approx 1.193$$

Thank you for your attention!