High Energy Cross Sections by Monte Carlo Quadrature

Thomson Scattering in Electrodynamics

Jackson, Classical Electrodynamics, Section 14.8 Thomson Scattering of Radiation studied in PHY 514 Spring 2012

Jackson Figures 14.17 and 14.18: Differential scattering cross section of unpolarized radiation by a point charged particle initially at rest in the laboratory. The solid curve is the classical Thomson result. The dashed curves are the quantum-mechanical results for a spinless particle, with the numbers giving the values of $\bar{\hbar}\omega/mc^2$. For $\bar{\hbar}\omega/mc^2 = 0.25$, 1.0 the dotted curves show the results for spin $\frac{1}{2}$ point particles (electrons).
The differential scattering cross section is defined by

\[
\frac{d\sigma}{d\Omega} = \frac{\text{Energy radiated/unit time/unit solid angle}}{\text{Incident energy flux/unit area/second}}
\]

\[
= \frac{\text{Number of photons detected/unit time/unit solid angle}}{\text{Number of photons incident/unit area/unit time}}
\]

The differential cross section for a monochromatic plane wave with wavevector \( \mathbf{k}_0 = k \mathbf{e}_z \) and polarization \( \mathbf{\varepsilon}_0 \) incident on a free particle of charge \( e \) and mass \( m \) is

\[
\frac{d\sigma}{d\Omega} = \left( \frac{e^2}{mc^2} \right)^2 |\mathbf{\varepsilon}^* \cdot \mathbf{\varepsilon}_0|^2
\]

where \( \mathbf{k} = k \mathbf{n} \), \( \mathbf{\varepsilon} \) are the wavevector and polarization of the outgoing wave. The polarization vectors

\[
\mathbf{\varepsilon}_1 = \cos \theta (\mathbf{e}_x \cos \phi + \mathbf{e}_y \sin \phi) - \mathbf{e}_z \sin \theta,
\]

\[
\mathbf{\varepsilon}_2 = -\mathbf{e}_x \sin \phi + \mathbf{e}_y \cos \phi
\]

represent polarization in and perpendicular to the scattering plane defined by the initial and final wavevectors \( \mathbf{k}_0, \mathbf{n} \). For plane polarized incident radiation and summing over final polarizations

\[
\sum_{\mathbf{\varepsilon}_{1,2}} |\mathbf{\varepsilon}^* \cdot \mathbf{\varepsilon}_0|^2 = \begin{cases} 
\cos^2 \theta \cos^2 \phi + \sin^2 \phi & \text{for } \mathbf{\varepsilon}_0 = \mathbf{e}_x \\
\cos^2 \theta \sin^2 \phi + \cos^2 \phi & \text{for } \mathbf{\varepsilon}_0 = \mathbf{e}_y
\end{cases}
\]

which give the unpolarized differential and total cross sections

\[
\frac{d\sigma}{d\Omega} = \frac{1}{2} \left( \frac{e^2}{mc^2} \right)^2 (1 + \cos^2 \theta), \quad \sigma_T = \frac{8\pi}{3} \left( \frac{e^2}{mc^2} \right)^2.
\]
The Compton Scattering Cross Sections

The Tompson cross sections are valid only at low frequencies $\hbar \omega / c$ when the momentum of the incident photon is much smaller than $mc$. In this limit the charged particle remains at rest and the energy of the photon does not change.

When $\hbar k \geq mc$, the charged particle will recoil and the photon will change in magnitude and direction, giving rise to Compton scattering. The Compton formula for the change in frequency of the photon is

$$\frac{\omega}{\omega'} = 1 + \frac{\hbar \omega}{mc^2} (1 - \cos \theta)$$

where $\theta$ is scattering angle in the rest frame of the particle before the collision.

To derive this result, let $k_\mu$, $k'_\mu$ be the 4-momenta of the photon before and after the scattering, and $p_\mu, p'_\mu$ the initial and final 4-momenta of the target particle. In the rest frame of the target particle (laboratory frame)

$$p^\mu = (mc, 0, 0, 0), \quad k^\mu = (1, 0, 0, 1) \frac{\hbar \omega}{c}, \quad k'^\mu = (1, \sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) \frac{\hbar \omega'}{c}$$

Using conservation of 4-momentum

$$p' \cdot p' = m^2 c^2 = (p + k - k') \cdot (p' + k' - k) = p^2 + 2p \cdot (k - k') + (k - k')^2$$

$$= m^2 c^2 + 2m\hbar (\omega - \omega') - 2\hbar^2 \omega \omega' (1 - \cos \theta)$$

The cross section is

$$\frac{d\sigma}{d\Omega} = \left( \frac{e^2}{mc^2} \right)^2 \left( \frac{\omega'}{\omega} \right)^2 |\mathbf{\varepsilon}^* \cdot \mathbf{\varepsilon}_0|^2.$$
Compton derived these formulas simply by using relativistic kinematics and conservation of energy and momentum. They are valid for scattering of a photon from a spinless charged particle.

**The Klein-Nishina Formula in Quantum Electrodynamics**

The quantum field theory which describes the interaction of charged electrons and positrons with photons is Quantum electrodynamics or QED.

Relativistic quantum field theory predicts that virtual electron-positron pairs will modify scattering cross section. In QED, these corrections are computed as a perturbation series in the the Fine-structure constant \( \alpha = \frac{e^2}{\hbar c} \approx \frac{1}{137.036} \).

The cross section for Compton scattering in to lowest order in \( \alpha \) is determined by the two Feynman diagrams from Section 5.5 of *Peskin and Schroeder*

![Feynman diagrams for Compton scattering](image)

The probability amplitude for the process is given in Eq. (5.74)

\[
 i\mathcal{M} = -ie^{2}\epsilon^*_\mu(k')\epsilon_\nu(k)\bar{u}(p') \left[ \frac{\gamma^\mu k\gamma^\nu + 2\gamma^\mu p^\nu}{2p \cdot k} + \frac{-\gamma^\nu k\gamma^\mu + 2\gamma^\nu p^\mu}{-2p \cdot k'} \right] u(p),
\]

where \( u(p) \) is a 4-component positive energy spinor wavefunction solution of the Dirac equation and
\( \gamma^\mu \) are Dirac gamma matrices. This amplitude defines the scattering of a photon from an electron for arbitrary photon polarizations and electron spin. To compare with the Compton cross section for spinless particles, the amplitude must be squared to obtain the scattering probability, which is then averaged over the two initial spin states of the electron and summed over the two final spin states. This is a straightforward calculation done in detail in Peskin and Schroeder. The final result in the rest frame of the initial electron is (Jackson footnote on page 697)

\[
\frac{d\sigma}{d\Omega} = \left( \frac{e^2}{mc^2} \right)^2 \left( \frac{\omega'}{\omega} \right)^2 \left[ |\epsilon^* \cdot \epsilon_0|^2 + \frac{(\omega - \omega')^2}{4\omega\omega'} \{ 1 + (\epsilon^* \times \epsilon) \cdot (\epsilon_0 \times \epsilon^*_0) \} \right].
\]

The second dot product can be simplified

\[
(\epsilon^* \times \epsilon) \cdot (\epsilon_0 \times \epsilon^*_0) = (\epsilon^* \cdot \epsilon_0)(\epsilon \cdot \epsilon^*_0) - (\epsilon^* \cdot \epsilon^*_0)(\epsilon \cdot \epsilon_0) = |\epsilon^* \cdot \epsilon_0|^2 - |\epsilon \cdot \epsilon_0|^2
\]

It vanishes for pure linear or circular polarization but can contribute for elliptical polarization.

This is the Klein-Nishina formula for Compton scattering.

**Numerical Evaluation of the Klein-Nishina Formula**

To compare this theoretical prediction with experimental measurements in the laboratory frame we need to express the result in Barns. The Classical electron radius is defined to be

\[
r_e = \frac{e^2}{mc^2} = 2.81794033 \times 10^{-13} \text{ cm}, \quad r_e^2 = 0.07940787703 \text{ b} \simeq 79.4 \text{ mb}.
\]
Using $d\Omega = \sin \theta \, d\theta \, d\phi$ the following dimensionless cross sections can be defined:

$$\frac{1}{r_e^2} \sigma_T = \int_{-1}^{+1} d(\cos \theta) \int_0^{2\pi} d\phi \frac{1}{r_e^2} \frac{d\sigma}{d\Omega}$$

$$\frac{1}{r_e^2} \frac{d\sigma}{d\theta} = \sin \theta \int_0^{2\pi} d\phi \frac{1}{r_e^2} \frac{d\sigma}{d\Omega}$$

$$\frac{1}{r_e^2} \frac{d\sigma}{d\Omega} = \left(\frac{\omega'}{\omega}\right)^2 \left[ |\epsilon^* \cdot \epsilon_0|^2 + \frac{(\omega - \omega')^2}{4\omega\omega'} \left(1 + |\epsilon^* \cdot \epsilon_0|^2 - |\epsilon \cdot \epsilon_0|^2\right) \right]$$

### Polarization Vectors

Polarization vectors are defined in Jackson: Figure 7.2 on the left shows the complex electric field vector for linear and Figure 7.3 on the right shows the field for circular polarization. The most general polarization is a linear superposition of two independent linear or helicity eigenstates

$$E(x, t) = (\epsilon_1 E_1 + \epsilon_2 E_2) e^{i k \cdot x - i \omega t}, \quad E(x, t) = (\epsilon_+ E_+ + \epsilon_- E_-) e^{i k \cdot x - i \omega t}, \quad \epsilon_\pm = \frac{1}{\sqrt{2}} (\epsilon_1 \pm i \epsilon_2),$$
where $\varepsilon_+$ represents photons with positive helicity (left-circular polarization in optics) and $\varepsilon_-$ represents negative helicity (right-circular polarization).

**Specifying Initial and Final State Polarization**

The Klein-Nishina formulas given above have been averaged over initial electron spin states and summed over final electron spin states. The photon polarizations $\varepsilon_0, \varepsilon$ can be specified arbitrarily.

The incident photon has wavevector $\hat{k}_0 = e_z$ in the positive direction and is scattered in the direction $\hat{k} = n = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$.

The simplest and physically most meaningful way to specify high energy photon polarizations is to use the helicity basis. The incident polarization is specified by two complex numbers $(E_{0+}, E_{0-})$ and the scattered state polarization by $(E_+, E_-)$. Linear polarizations are more natural at lower frequencies.

To evaluate the scalar products of the polarization vectors note that the unit vectors perpendicular and parallel to the scattering plane are

$$
\varepsilon_2 = \frac{\hat{n} \times \hat{k}_0}{|\hat{n} \times \hat{k}_0|} = (-\sin \phi, \cos \phi, 0), \quad \varepsilon_1 = \frac{\varepsilon_2 \times n}{|\varepsilon_2 \times n|} = (\cos \theta \cos \phi, \cos \theta \sin \phi, -\sin \theta).
$$

The polarization vectors are $\varepsilon_0 = (E_{10}, E_{20}, 0)$ and

$$
\varepsilon = E_1 \varepsilon_1 + E_2 \varepsilon_2 = (E_1 \cos \theta \cos \phi - E_2 \sin \phi, E_1 \cos \theta \sin \phi + E_2 \cos \phi, -E_1 \sin \theta),
$$

which can be expressed in terms photon helicity components

$$
E_1 = \frac{1}{\sqrt{2}}(E_+ + E_-), \quad E_2 = \frac{i}{\sqrt{2}}(E_+ - E_-).
$$
### C++ Code to Evaluate the Cross Sections

```cpp
#include <cmath>
#include <complex>
#include <cstdlib>
#include <iostream>
using namespace std;

const double pi = 4 * atan(1.0);

#include <gsl/gsl_monte.h>
#include <gsl/gsl_monte_vegas.h>

struct Params {
    double omega; // incident photon angular frequency
    double theta; // for differential cross section
    double phi;
    complex<double> ep_10; // x-component of incident photon polarization
    complex<double> ep_20; // y-component
    complex<double> ep_1; // in-plane scattered photon polarization
    complex<double> ep_2; // perpendicular component
};
```
double integrand(
    double theta,
    double phi,
    void *params)
{
    Params *p = (Params*) params;
    double omega = p->omega;
    double omega_prime = omega / (1 + omega * (1 - cos(theta)));

    // normalize polarization vectors
    double n0 = sqrt(norm(p->ep_10) + norm(p->ep_20)),
                n = sqrt(norm(p->ep_1) + norm(p->ep_2));
    complex<double> ep_10 = p->ep_10 / n0, ep_20 = p->ep_20 / n0,
                        ep_1 = p->ep_1 / n, ep_2 = p->ep_2 / n;

    // compute polarization dot products
    complex<double> ep_star_dot_ep0 =
        conj(ep_1 * cos(theta) * cos(phi) - ep_2 * sin(phi)) * ep_10 +
        conj(ep_1 * cos(theta) * sin(phi) + ep_2 * cos(phi)) * ep_20;
    complex<double> ep_dot_ep0 =
        (ep_1 * cos(theta) * cos(phi) - ep_2 * sin(phi)) * ep_10 +
        (ep_1 * cos(theta) * sin(phi) + ep_2 * cos(phi)) * ep_20;
return pow(omega_prime / omega, 2.0) * 
(norm(ep_star_dot_ep0) + pow(omega - omega_prime, 2.0) / 
(4 * omega * omega_prime) * (1 + norm(ep_star_dot_ep0) - 
norm(ep_dot_ep0)));

}  

// integrand in form expected by VEGAS 
double g(double *k, size_t dim, void *params) 
{
    double theta = k[0], phi = k[1];
    return integrand(theta, phi, params);
}

int main()
{
    cout << " Relativistic Compton Scattering Cross Sections using VEGAS\n";

    const gsl_rng_type *T;
    gsl_rng *r;
    gsl_rng_env_setup();
    T = gsl_rng_default;
    r = gsl_rng_alloc(T);

    double xl[2] = { 0.0, 0.0 };  // min (theta, phi)
double xu[2] = { pi, 2*pi };  // max (theta, phi)

struct Params params;
params.omega = 0.0025;  // incident angular frequency
params.ep_10 = 1;   // incident polarization in x direction
params.ep_20 = 0;
params.ep_1 = 1;  // outgoing in scattering plane
params.ep_2 = 0;

size_t dim = 2;  // 2-D quadrature
gsl_monte_vegas_state *s = gsl_monte_vegas_alloc(dim);

gsl_monte_function G = { &g, dim, &params };

int calls = 500000;  // number of function evaluations
double res, err;  // result and error

cout << " omega = " << params.omega << endl;

gsl_monte_vegas_integrate(&G, xl, xu, dim, calls/5, r, s, &res, &err);
cout << " VEGAS warmup: sigma_tot = " << res << " +/- " << err << endl;

do {
    gsl_monte_vegas_integrate(&G, xl, xu, dim, calls, r, s, &res, &err);
}
cout << " sigma_tot= " << res << " +/- " << err
    << " chisq/dof = " << gsl_monte_vegas_chisq(s) << endl;
} while (abs(gsl_monte_vegas_chisq(s) - 1.0) > 0.5);

gsl_rng_free(r);
return 0;
}