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Note

Using Physical Insight: The Relativistic Compton Scattering Kernel for Radiative Transfer

I. Introduction

Until recently, physicists have had limited access to supercomputers, and thus an important tool to solve analytically intractable problems. Now, however, with the National Science Foundation Supercomputer Centers, the emergence of vector "mini-supercomputers," massively parallel systems, "MIPS" machines, and a myriad of other computational facilities, today's physicist has a potpourri of devices to simulate complex phenomena. The supercomputer has moved from being the elite, dedicated tool of the cryptologist or nuclear effects scientist, to being accessible to all fields of science. For example, the recent Conference on Grand Challenges to Computational Sciences [1] brought together scientists in areas as diverse as biology, physics, and social engineering to discuss the impact of supercomputers on society.

With all the promise that this field brings, there are dangers associated with computational physics. In experimental physics (where with some experiments, one's life may be endangered) researchers *must* know what they are doing; in theoretical physics (where there is no mortal danger, aside from having a bookshelf fall on them), the same holds true; whereas for computational physics, the old adage "garbage in, garbage out" dictates the direction of research. It is extremely easy to run a "black box" program, and unless the physicist is acutely aware of vital issues (stability and convergence, for example), computer generated answers may have no connection with physical reality. This is a growing concern with the large influx of scientists into computational physics.

It is with this motivation that we present an innovative way of viewing relativistic Compton scattering. In particular, we show that errors of up to 10^4 are possible when "standard" numerical methods are used to solve for the relativistic Compton scattering kernel. The emphasis in this note is on the importance of using physical insight *before* a calculation is made.

II. Background

The Compton scattering kernel (CSK) describes how photons interact with a relativistic nondegenerate gas of free electrons. The CSK is defined to be the quan-

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tum-mechanical Klein–Nishina cross section averaged over a relativistic distribution of electrons. The Klein–Nishina formula for a free electron moving with a velocity $\mathbf{v}$, scattering a photon initially traveling in direction $\hat{\Omega}$ with energy ν (in units of the electron rest energy m_0c^2) to a new direction $\hat{\Omega}'$ and energy ν' is [2]

$$\begin{aligned}\sigma(\gamma \to \gamma', \hat{\Omega} \to \hat{\Omega}', \mathbf{v}) = \frac{r_0^2\sqrt{1-v^2/c^2}}{2\gamma\nu}\Bigg[1 + \left(1 - \frac{(1-\hat{\Omega}\cdot\hat{\Omega}')(1-v^2/c^2)}{(1-\hat{\Omega}\cdot\mathbf{v}/c)(1-\hat{\Omega}'\cdot\mathbf{v}/c)}\right)^2 \\ + \frac{(1-v^2/c^2)(1-\hat{\Omega}\cdot\hat{\Omega}')^2\gamma\gamma'}{(1-\hat{\Omega}\cdot\mathbf{v}/c)(1-\hat{\Omega}'\cdot\mathbf{v}/c)}\Bigg] \\ \times\delta\left(\hat{\Omega}\cdot\hat{\Omega}' - 1 + \frac{1-\hat{\Omega}\cdot\mathbf{v}/c}{\gamma'\sqrt{1-v^2/c^2}} - \frac{1-\hat{\Omega}'\cdot\mathbf{v}/c}{\gamma\sqrt{1-v^2/c^2}}\right),\end{aligned} \tag{1}$$

where $\gamma \equiv h\nu/m_0c^2$, $\gamma' \equiv h\nu'/m_0c^2$, r_0 is the classical electron radius, and the Dirac delta function forces energy-momentum conservation during the scattering process. The relativistic Maxwellian distribution $f(v, T_e)$ for a nondegenerate gas of free electrons at a temperature T_e is

$$f(v, T_e) = \frac{m_0c^2(1-v^2/c^2)^{-5/2}\, e^{-m_0c^2/kT_e\sqrt{1-v^2/c^2}}}{4\pi kT_ec^3K_2(m_0c^2/kT_e)}, \tag{2}$$

where K_2 is the modified Bessen function of the second kind, k is Boltzmann's constant, and c is the speed of light. For an electron density of N_e, the CSK is defined as the average of the Klein–Nishina cross section (1) over the relativistic Maxwellian distribution (2):

$$\begin{aligned}\mathrm{CSK} &\equiv \sigma(\gamma \to \gamma', \hat{\Omega} \to \hat{\Omega}', \mathbf{v}) \\ &= \frac{N_er_0^2}{2\gamma\nu}\int \frac{m_0c^2(1-v^2/c^2)^{-2}\, e^{-m_0c^2/kT_e\sqrt{1-v^2/c^2}}}{4\pi kT_ec^3K_2(m_0c^2/kT_e)} \\ &\quad\times\Bigg[1 + \left(1 - \frac{(1-v^2/c^2)(1-\hat{\Omega}\cdot\hat{\Omega}')}{(1-\hat{\Omega}\cdot\mathbf{v}/c)(1-\hat{\Omega}'\cdot\mathbf{v}/c)}\right)^2 \\ &\quad+ \frac{(1-v^2/c^2)(1-\hat{\Omega}\cdot\hat{\Omega}')^2\gamma\gamma'}{(1-\hat{\Omega}\cdot\mathbf{v}/c)(1-\hat{\Omega}'\cdot\mathbf{v}/c)}\Bigg] \\ &\quad\times\delta\left(\hat{\Omega}\cdot\hat{\Omega}' - 1 + \frac{1-\hat{\Omega}\cdot\mathbf{v}/c}{\gamma'\sqrt{1-v^2/c^2}} - \frac{1-\hat{\Omega}'\cdot\mathbf{v}/c}{\gamma\sqrt{1-v^2/c^2}}\right)d\mathbf{v}.\end{aligned} \tag{3}$$

Using the following substitutions

$$D \equiv 1 - \hat{\Omega}\cdot\mathbf{v}/c, \qquad D' \equiv 1 - \hat{\Omega}'\cdot\mathbf{v}/c, \qquad \lambda \equiv (1-v^2/c^2)^{-1/2}, \qquad \xi \equiv \hat{\Omega}\cdot\hat{\Omega}',$$

we write the CSK in a more tractable form as

$$\sigma(\gamma \to \gamma', \xi, \tau) = \frac{N_e r_0^2}{2\gamma v} \int f(v, T_e) \frac{1}{\lambda} \left[1 + \left(1 - \frac{(1-\xi)}{\lambda^2 DD'} \right)^2 + \frac{(1-\xi)^2 \gamma\gamma'}{\lambda^2 DD'} \right]$$
$$\times \delta\left(\xi - 1 + \lambda \frac{D}{\gamma'} - \lambda \frac{D'}{\gamma} \right) d\mathbf{v}, \tag{4}$$

where $\tau \equiv kT_e/m_0 c^2$.

III. Solution of the CSK

A. *Background*

Figure 1 shows a typical *gedanken* scattering experiment. Consider a coordinate frame such that a free electron is situated at the origin of our coordinate system and

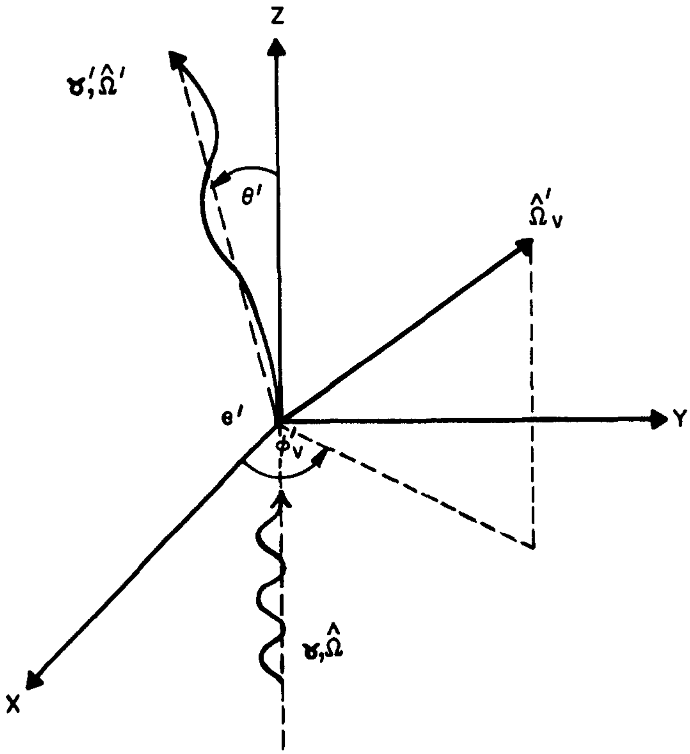

FIG. 1. The traditional method for setting up a coordinate axis for scattering problems takes the incoming photon $(\gamma, \hat{\Omega})$ along the z-axis, scattering to a new photon $(\gamma', \hat{\Omega}')$ confined to the x–z plane. Here γ (γ') denotes the energy and $\hat{\Omega}$ $(\hat{\Omega}')$ denotes the direction of the incoming (scattered) photon, θ' the polar angle of the scattered photon with respect to the z-axis, ϕ'_v the azimuthal angle of the scattered electron with respect to the x-axis, and $\hat{\Omega}'_v$ the direction of the scattered electron.

an incoming photon $(\gamma, \hat{\Omega})$ propagates along the z-axis. After the scattering interaction, we can always choose our coordinate axis such that the outgoing photon $(\gamma', \hat{\Omega}')$ is restricted to the x–z plane.

To solve for (4), we now consider a new frame with coordinate axis parallel to that of the original frame such that the electrons have a velocity $\mathbf{v}$; in this new frame the differential in (4) may be written as $d\mathbf{v} = v^2\, d\hat{\Omega}_v$. Continuing the analogy in Fig. 1, $\hat{\Omega}_v$ is described by θ_v, ϕ_v, and $\hat{\Omega}'$ by θ' and ϕ', where θ is the polar angle with respect to the (old or new) z-axis and ϕ is the azimuthal angle with respect to the (old or new) x-axis. We note $\phi' = 0$, since $\hat{\Omega}'$ lies in the x–z plane and $\cos\theta' = \hat{\Omega}\cdot\hat{\Omega}' = \xi$.

Pomraning has taken advantage of the Dirac delta function in (4) and evaluated the integral over ϕ_v [2]. Here we present the result and refer the reader to Pomraning for the details of this integration:

$$\sigma(\nu \to \nu', \xi) = \frac{N_e c r_0^2}{\nu} \int_0^c dv\, \frac{v}{\lambda^2} f(v) \int_{\mu_v \in A} d\mu_v\, \frac{1}{h(v, \mu_v)} \times \left(1 + \left[1 - \frac{(1-\xi)}{g(v, \mu_v)}\right]^2 + \frac{\gamma\gamma'(1-\xi)^2)}{g(v, \mu_v)}\right), \tag{5}$$

where

$$\mu_v = \cos\theta_v, \qquad g(v, \mu_v) = \lambda\gamma(1 - v\mu_v/c)[\xi - 1 + \lambda(1 - v\mu_v/c)/\gamma'],$$

$$h(v, \mu_v) = \left((1-\mu_v^2)(1-\xi^2) - \left[\frac{c}{v} + \frac{c\gamma}{v\lambda}(1-\xi) - \frac{c\gamma}{v\gamma'}(1 - v\mu_v/c) - \mu_v\xi\right]^2\right)^{1/2},$$

and $A \subset [-1, 1]$ is the subset of those values of μ_v that cause the argument of the Dirac delta function to vanish for some $\phi_v \in [0, \pi]$.

The expression in (5) is quite formidable, and as Pomraning notes [2], "This is as far as it appears profitable to proceed analytically."

Various authors have attacked (5) to numerically evaluate the integrals in the CSK. Among the first was Stone and Nelson [3] who used Gaussian quadratures to generate large tables for use in computer calculations; others [4–6] employed perturbative methods including computing Legendre moments and making the Fokker–Planck approximation (valid for photon energies and electron temperatures $\ll$ electron rest energy).

There are certainly regions where these approximations are valid; however, there lies a danger in trying to extend the limits of these regions: incorrect answers result. For example, when photon energies exceed the electron rest energy, the Fokker–Plank approximation is invalid. Thus, one would like to reduce (5) so that the solutions are not so senstitive to variations in the parameters.

There lies a major problem with this: after many years of study, it appears that others [2–6] have reduced (5) as far as it will go. If there is a less formidable representation of the CSK, then rather than attempting to reduce (5), it may be more productive to return to the basic assumptions behind the choice of coordinate frame. This will allow us to gain fresh insight into the solution of the CSK and perhaps come up with a simpler, more physical representation. It is in this spirit then that we return to our original *gedanken* experiment.

B. *The Photon Momentum Transfer*

Feynman [7] viewed one aspect of the scattering process as the absorption and subsequent emission of a photon (denoted in Fig. 2 by its momentum $\mathbf{q}$) by a free electron ($\mathbf{p}$). During this process, a virtual electron consisting of the electron and absorbed photon is created with momentum $\mathbf{p}+\mathbf{q}$. The scattered electron and photon have momentums $\mathbf{p}'$ and $\mathbf{q}'$, respectively. For this interaction the photon momentum transfer is defined as

$$\hat{n} \equiv \frac{\mathbf{q}'-\mathbf{q}}{\sqrt{q^2+q'^2-2qq'\xi}} = \frac{\gamma'\hat{\Omega}'-\gamma\hat{\Omega}}{\sqrt{\gamma^2+\gamma'^2-2\gamma\gamma'\xi}}. \tag{6}$$

If this is an accurate representation of the scattering process, then one might imagine that the symmetries involved in scattering are ingrained in the photon momentum transfer. If this is indeed so, then the coordinate system used to solve (4) should reflect that basic attribute of the process.

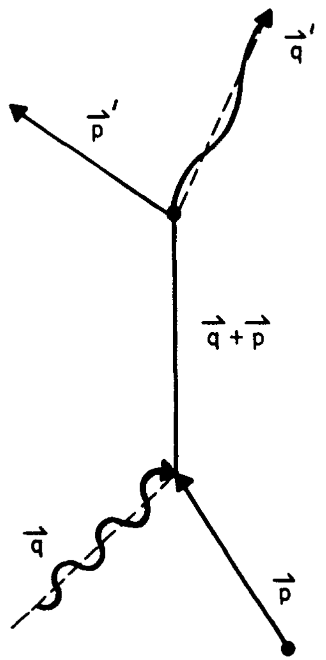

FIG. 2. One of Feynman's representations of the scattering process shows the creation of a "quasi-particle" $\mathbf{q}+\mathbf{p}$ carrying the energy and momentum of the incoming photon $\mathbf{q}$ and electron $\mathbf{p}$. The scattered entities are denoted by primes.

In other words, taking the z-axis of integration along the *photon momentum transfer*, rather than trying to force an artificial coordinate axis upon the system, is "nature's way" of reducing the symmetries. This is shown in Fig. 3—the azimuthal and polar angles define the symmetries in this coordinate system and are not contingent upon the initial selection of a coordinate axis as in Fig. 1.

If one approaches (4) in this manner, performing the integration about the angles is straightforward. We refer the readers to the literature [8, 9] for the details and simply present the result

$$\frac{\sigma(\gamma \to \gamma', \xi, \tau)}{\Sigma_0} = \Psi + \int_0^\infty e^{-\rho/\tau} \left[\left(\Lambda_+ - \frac{\rho + \rho_+}{\tau(1-\xi)} \right) R_+^{-1/2} + \left(-\Lambda_- + \frac{\rho + \rho_-}{\tau(1-\xi)} \right) R_-^{-1/2} \right] d\rho, \tag{7}$$

where

$$\rho_\pm \equiv \pm \left(\frac{\gamma + \gamma'}{2} \right) + \left[\left(1 + \frac{\gamma\gamma'(1-\xi)}{2} \right) \left(1 + \frac{(\gamma - \gamma')^2}{2\gamma\gamma'(1-\xi)} \right) \right]^{1/2}, \tag{7a}$$

$$\Lambda_\pm \equiv -\gamma\gamma' + \frac{2}{1-\xi} + \frac{2}{\gamma\gamma'(1-\xi)^2} - \left(\frac{\pm 1}{\tau} \right) \left(\frac{1}{\gamma} + \frac{1}{\gamma'} \right) \frac{1}{(1-\xi)^2}, \tag{7b}$$

$$\Sigma_0 \equiv \frac{N_e r_0^2}{4\gamma\nu\tau K_2(\tau^{-1})} e^{-\lambda_-/\tau}, \qquad \lambda_+ = \frac{\gamma' - \gamma}{2} + \left(\left[1 + \gamma\gamma' \frac{1-\gamma}{2} \right] \left[1 + \frac{(\gamma - \gamma')^2}{2\gamma\gamma'(1-\xi)} \right] \right)^{1/2}, \tag{7c}$$

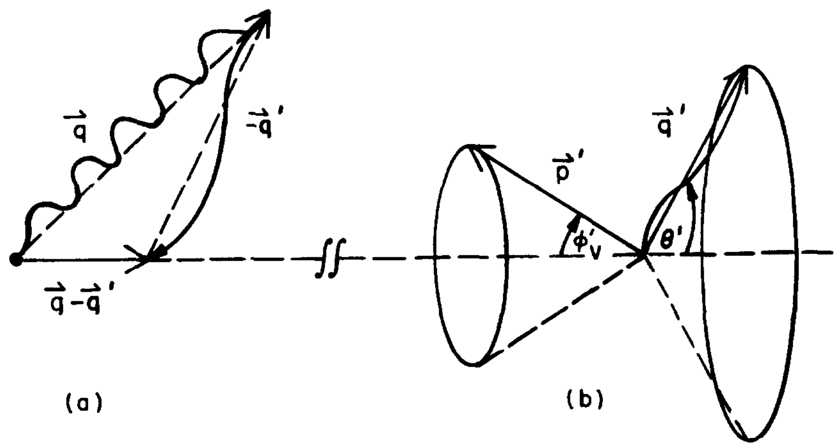

FIG. 3. The direction of the *photon momentum transfer* is $\mathbf{n} \equiv \mathbf{q}' - \mathbf{q}$. Part (a) shows $-\mathbf{n}$ (using $\mathbf{q}$ and $\mathbf{q}'$ from Fig. 2) for ease in visualization. Part (b) depicts the angular symmetries of the scattered photon an electron around the photon momentum transfer. It is this symmetry that reduces the scattering integral to a simple expression.

$$R_{\pm} \equiv (\rho + \rho_{\pm})^2 + \omega^2, \qquad \omega^2 \equiv \frac{1+\xi}{1-\xi}, \qquad \alpha_{\pm} \equiv (\rho_{\pm}^2 + \omega^2)^{-1/2}, \tag{7d}$$

$$\Psi \equiv \frac{2\tau\gamma\gamma'}{q} + \frac{1}{(1-\xi)^2}\left(\frac{1}{\gamma} + \frac{1}{\gamma'}\right)(\alpha_+ + \alpha_-) + \frac{(\rho_+\alpha_+ - \rho_-\alpha_-)}{1-\xi}. \tag{7e}$$

Conclusions

The integral in (7) cannot be reduced further; however, there are several methods available to the readers to quickly compute the CSK [8, 9], based upon a power series expansion, an asymptotic series, and a rational approximation. These algorithms have been realized in a FORTRAN code available from the authors. In addition, others [10] have refined these algorithms by removing the singularity in (7) and will soon present their work in the literature.

Turning now to some attributes of (7), we note that detailed balance is satisfied; e.g.,

$$\gamma^2 \sigma(\gamma \to \gamma', \xi, \tau)\, e^{-\gamma/\tau} = \gamma'^2 \sigma(\gamma' \to \gamma, \xi, \tau)\, e^{-\gamma'/\tau} \tag{8}$$

which is essential so that the CSK is symmetric in γ and γ'. We also note that the intrinsic features of the CSK are contained in Σ_0, with everything else in the CSK varying smoothly.

The exponential factor in Σ_0 has a simple physical explanation. The smallest electron energy for which photon scattering is possible for a given γ, γ', and ξ is $\lambda_+ m_0 c^2$; an electron of probability $e^{-\lambda_+/\tau}$ or lower must therefore be sampled for this scattering to occur. Thus, it is highly inaccurate to expand the ξ dependence of σ in Legendre polynomials because one can choose physically relevant values of γ, γ', and τ for which $e^{-\lambda_+/\tau}$ changes many orders of magnitude with arbitrarily small variations in ξ.

In addition, numerical solutions to (5) that use weighting functions to evaluate the double integrals do not catch this rapid change in Σ_0. We have performed a random comparison of the Stone–Nelson tables using 10^5 points and have found the Stone–Nelson cross sections may be 10 to 100,000 times too large. We attribute this to the rapidly fluctuating exponential in Σ_0.

In conclusion, the solution of the CSK provides an example of how a seemingly intractable problem may be reduced using physical insight. Examining basic symmetries in nature and taking advantage of those symmetries may shed light on otherwise pertinacious problems.

Computers are an invaluable tool for the physicist—in fact the motivation for our work came from the need to implement Compton scattering in the discrete ray method radiation transport subroutines used at the Lawrence Livermore National Laboratory; however, we submit that computational physicists are charged with ensuring they not adopt a "if it compiles, publish" attitude, and instead spend time examining the physical basis behind the phenomenon.

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