KOLMOGOROV EQUATION SOLUTION: MULTIPLE SCATTERING EXPANSION AND PHOTON STATISTICS EVOLUTION MODELING

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Abstract: We consider a formulation of the Cauchy problem for the Kolmogorov equation which corresponds to a localized source of particles to be scattered by a medium with a given scattering amplitude density. The multiple scattering amplitudes are introduced and the corresponding series solution of the equation is constructed. We investigate the integral representation for the first series terms, its estimations and values of the photon number of finite and point receivers. Application to the LIDAR problem and X-ray beam scattering for orthogonal and inclined to a layer is considered.

Keywords: Kolmogorov equation, Fokker-Plank equation, multiple scattering expansion, photon statistics evolution, single scattering term, X-rays in beryl

1. Introduction

We study the modeling of photon beam propagation through a layer, neglecting the photons phase that excludes such wave phenomena as total reflection [1] or focusing [2]. In such context the propagation of electromagnetic waves, such as X-ray, may be interpreted via two phenomena: absorption and scattering of the corresponding photons. Absorption of electromagnetic radiation is the way in which the energy of a photon is taken up by the matter, typically the electrons of an atom. Thus, the electromagnetic energy is transformed into internal energy of the absorber, for example, thermal energy. Scattering is a process in which moving particles or waves are forced to deviate from a straight trajectory by one or more paths due to localized non-uniformities in the medium through which they pass. Scattering phenomena can be divided into two classes: elastic and non-elastic. In the elastic process the photon energy is conserved while in the non-elastic it is not. Rayleigh scattering is an example of elastic scattering. Non-elastic scattering has very low influence in X-ray propagation, therefore, it will be ignored in this work. The simple model used in this theory to represent the light-matter interaction is a crude assumption that avoids getting inside the actual complexity of the phenomena of light-matter interaction, taking into account elastic scattering and absorption and it has the advantage of leading to relatively simple analytical solutions for photon propagation valid for many real media. The light-matter interaction is characterized by several phenomena that will be neglected in the consideration since they may affect the results of the investigations but could be taken into account by direct development of the theory. Scattering phenomena have been studied in LIDAR (Light Detection and Ranging) problems since the 70s. A LIDAR works similarly to a radar. A laser shots short impulses of light in a certain direction that is scattered by a medium (atmosphere, glass, water, *etc.*). Then, a telescope collects the light that is scattered back and a gauge inside the apparatus measures the intensity of that light. One of the first mathematical descriptions is found in the works of [3]. The backscattering and absorption phenomena are modeled by the linearized Boltzmann equation, that in fact is a version of the Kolmogorov equations [4], the diffusion-term version named as Fokker-Planck (Kolmogorov forward) equations [5]. The derivation on the quantum base is given in [6]. Studies about the backscattering of a pulse emitted to the atmosphere through Monte Carlo simulations have been carried out by [7], [8], and [9]. Double scattering has been studied in the work [10]. More recent work using the Monte Carlo approach has been conducted by [11] who has studied the contribution of multiple scattering in the pulse stretching. A cloudy sky, fog or rain have been considered for the simulations. A problem of mono energetic particles pulse reflection from a half-infinite stratified medium is considered in the conditions of elastic scattering with an absorption account in the article [12]. More recent articles on the LIDAR sounding of atmosphere like [13] reveal interest in the related direct and inverse problems of today [14].

In this article the scattering/absorption phenomena are modeled by the Kolmogorov equation. It is applied to a LIDAR problem and to a mono-energetic X-ray particle pulse propagating in the free space, reaching a layer of a metal and next going through the free space again arriving at a cylindrical detector. We simplify the problem taking the speed of the electromagnetic waves to be constant through air and inside the layer, neglecting the corresponding delay. The theory is based on the multiple scattering series solution of the Kolmogorov equation for the one-particle distribution function [12] see also [15]. Whereas it is the backscattering that is considered in the cited articles, in this work we will focus on the forward or some nonzero angle scattering [16]. The main purpose of this paper is, by means of laboratory experimental data on the differential and total cross section [17], to obtain expressions for the intensity arriving at the detector after one-scattering phenomena [18]. The initial condition will be a point pulse source.

2. Problem formulation

The equation for the probability density $f = f(t',\vec{r},\vec{v})$ has the following form:

$$\frac{1}{c}[\partial_{t'} f + \vec{v}\cdot\nabla f] = -\sigma_{\text{tot}}(z)f - \int \sigma_{\text{scat}}(\cos\gamma,z)f\,d\Omega' \tag{1}$$

where t'-time, $d\Omega' = \sin\theta' d\theta' d\phi'$ – solid scattering angle, σ – bulk differential cross-section of elastic scattering to the angle γ; σ_{tot} – the sum of $\int \sigma_{\text{scat}} d\Omega + \sigma_{\text{abs}}$, scattering and absorption total cross-sections of elastic scattering, and

$$\frac{\vec{v}}{c} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) \tag{2}$$

– velocity components. Equation (1) is derived from the Kolmogorov equation and has been taken from [12]. In spherical coordinates: r,θ,ϕ the scattering angle is expressed as

$$\cos\gamma = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\phi-\phi') \tag{3}$$

where θ' and ϕ' are the angles after the scattering occurs. We suppose that the scattering is elastic, $|\vec{v}|$ does not change while the scattering process occurs. The initial conditions are represented by the distributions

$$f(0,x,y,z) = V\delta(x)\delta(y)\delta(z)\delta(\theta-\theta_0) \tag{4}$$

which means that an initial pulse is emitted from position $(x,y,z) = (0,0,0)$ at a certain direction $\theta = \theta_0$. V represents the number of photons emitted from the source. We will consider the parameter $V = \frac{1}{2\pi}$, so that the function f can be interpreted as a density probability function.

It means that we build a solution for the probability density as a weak limit (when $t' \to 0$) to δ-function at $t' > 0$. The distribution $\delta(\theta-\theta_0)$ is chosen as

$$\big(\delta(\theta-\theta_0), \psi(\theta,\phi)\big) = \int_0^{2\pi} \psi(\theta_0,\phi)d\phi \tag{5}$$

The definition of the action of function f on function ψ in x,y,z coordinates from the Shwartz space is standard.

3. Solution for the modeling equation

3.1. Solution for 0 angle initial pulse

Let us start with a simple example of zero initial angle $\theta_0 = 0$. Denote $t = ct'$ and c the speed of light in air. This makes a unit of space and a unit of time equivalent. A solution is searched as an multiple scattering expansion

$$f = f_0 + f_1 + f_2 + \dots \tag{6}$$

We are interested in single scattering, *i.e.*, the approximation $f = f_0 + f_1$ For f_0 we choose

$$Lf_0 = \frac{\partial f_0}{\partial t} + \sin\theta\cos\phi\frac{\partial f_0}{\partial x} + \sin\theta\sin\phi\frac{\partial f_0}{\partial y} + \cos\theta\frac{\partial f_0}{\partial z} = -\sigma_{\text{tot}}(z)f_0 \tag{7}$$

and the initial condition

$$f_0(0,x,y,z)=V\delta(x)\delta(y)\delta(z)\delta(\theta) \tag{8}$$

To find the equation for f_1 from (1) we write

$$Lf_0+Lf_1=-\sigma_{\mathrm{tot}}(z)(f_0+f_1)-\int\sigma_{\mathrm{scat}}(\cos\gamma,z)(f_0+f_1)d\Omega' \tag{9}$$

We know from (7) $Lf_0=-\sigma_{\mathrm{tot}}(z)f_0$, then

$$Lf_1=-\sigma_{\mathrm{tot}}(z)f_1-\int\sigma_{\mathrm{scat}}(\cos\gamma,z)f_0\,d\Omega' \tag{10}$$

with the initial condition

$$f_1|_{t=0}=0 \tag{11}$$

Let us change the variables in (7) to solve the equation:

$$x'=x-t\sin\theta\cos\phi \tag{12a}$$

$$y'=y-t\sin\theta\sin\phi \tag{12b}$$

$$z'=z-t\cos\theta \tag{12c}$$

$$t'=t \tag{12d}$$

Therefore:

$$\begin{aligned}
\frac{\partial}{\partial x}&=\frac{\partial x'}{\partial x}\frac{\partial}{\partial x'}=\frac{\partial}{\partial x'}\\
\frac{\partial}{\partial y}&=\frac{\partial y'}{\partial y}\frac{\partial}{\partial y'}=\frac{\partial}{\partial y'}\\
\frac{\partial}{\partial z}&=\frac{\partial z'}{\partial z}\frac{\partial}{\partial z'}=\frac{\partial}{\partial z'}\\
\frac{\partial}{\partial t}&=\frac{\partial x'}{\partial t}\frac{\partial}{\partial x'}+\frac{\partial y'}{\partial t}\frac{\partial}{\partial y'}+\frac{\partial z'}{\partial t}\frac{\partial}{\partial z'}+\frac{\partial t'}{\partial t}\frac{\partial}{\partial t'}=\\
&=-\sin\theta\cos\phi\frac{\partial}{\partial x'}-\sin\theta\sin\phi\frac{\partial}{\partial y'}-\cos\theta\frac{\partial}{\partial z'}+\frac{\partial}{\partial t'}
\end{aligned} \tag{13}$$

Equation (7) is transformed to

$$\begin{gathered}
\frac{\partial f_0}{\partial t'}=-\sigma_{\mathrm{tot}}(z'+t'\cos\theta)f_0\\
f_0=K(x',y',z')\exp\left[-\int_0^{t'}\sigma_{\mathrm{tot}}(z'+\tau\cos\theta)d\tau\right]
\end{gathered} \tag{14}$$

Going back to the old variables:

$$\begin{aligned}
f_0=&K(x-t\sin\theta\cos\phi,y-t\sin\theta\sin\phi,z-t\cos\theta)\cdot\\
&\cdot\exp\left[-\int_0^{t}\sigma_{\mathrm{tot}}(z-t\cos\theta+\tau\cos\theta)d\tau\right]
\end{aligned} \tag{15}$$

Let us remark a useful fact

$$\exp\left[-\int_0^{t}\sigma_{\mathrm{tot}}\big(z-(t-\tau)\cos\theta\big)d\tau\right]=\exp\left[-\int_0^{t}\sigma_{\mathrm{tot}}(z-\tau\cos\theta)d\tau\right] \tag{16}$$

Denote function E via

$$E(t,z,\theta)=\exp\left[-\int_0^t \sigma_{\rm tot}(z-\tau\cos\theta)d\tau\right] \tag{17}$$

Using the initial condition (4) with $V=\frac{1}{2\pi}$, the expression for f_0 is:

$$\begin{aligned} f_0 =& \frac{1}{2\pi}\delta(x-t\sin\theta\cos\phi)\delta(y-t\sin\theta\sin\phi)\delta(z-t\cos\theta)\delta(\theta)\cdot \\ &\cdot\exp\left[-\int_0^t \sigma_{\rm tot}\big(z-(t-\tau)\cos\theta\big)d\tau\right] \end{aligned} \tag{18}$$

which, taking in account that the expression will not vanish only if $\theta=0$, simplifies as:

$$f_0=\frac{1}{2\pi}\delta(x)\delta(y)\delta(z-t)\delta(\theta)\exp\left[-\int_0^t \sigma_{\rm tot}\big(z-(t-\tau)\big)d\tau\right]. \tag{19}$$

$$f_0=\frac{1}{2\pi}\delta(x)\delta(y)\delta(z-t)\delta(\theta)E(t,z,0). \tag{20}$$

This expression would be slightly different if the change of the speed of light in different media were taken in account. Now, once we know f_0, we have to solve equation (10). We use the same change of variables (12) to transform equation (10) into

$$\begin{aligned} f_1\exp\left(\int_0^{t'}\sigma_{\rm tot}(z'+\tau_2\cos\theta)d\tau_2\right) =& -\int_0^{t'}\exp\left(\int_0^{\tau}\sigma_{\rm tot}(z'+\tau_2\cos\theta)d\tau_2\right)\cdot \\ &\cdot\int\sigma_{\rm scat}(\cos\gamma,z'+\tau\cos\theta)f_0(\tau,x',y',z',\theta)d\Omega' d\tau + C_1 \end{aligned} \tag{21}$$

From the initial conditions we conclude that $C_1=0$

$$\begin{aligned} f_1 =& V\int_0^{t'}\exp\left(-\int_{\tau}^{t'}\sigma_{\rm tot}(z'+\tau_2\cos\theta)d\tau_2\right)\cdot \\ &\cdot\int\sigma_{\rm scat}(\cos\theta',z'+\tau\cos\theta)E(\tau,z'+\tau\cos\theta,0)\cdot \\ &\cdot\delta(x'+\tau\sin\theta\cos\phi)\delta(y'+\tau\sin\theta\sin\phi)\delta(z'+\tau\cos\theta-\tau)\delta(\theta')d\Omega' d\tau \end{aligned} \tag{22}$$

Transformation to the original variables, taking into account (5)

$$\begin{aligned} f_1 =& 2\pi\int_0^t\exp\left(-\int_{\tau}^{t}\sigma_{\rm tot}(z-(t-\tau_2)\cos\theta)d\tau_2\right)\cdot \\ &\cdot E(\tau,z-(t-\tau)\cos\theta,0)\sigma_{\rm scat}(\cos\theta,z-(t-\tau)\cos\theta)\cdot \\ &\cdot V\delta(x-(t-\tau)\sin\theta\cos\phi)\delta(y-(t-\tau)\sin\theta\sin\phi)\delta(z-(t-\tau)\cos\theta-\tau)d\tau \end{aligned} \tag{23}$$

after simplification

$$\begin{aligned} f_1 =& \int_0^t E(\tau,z,\theta)\cdot \\ &\cdot E(t-\tau,z-\tau\cos\theta,0)\sigma_{\rm scat}(\cos\theta,z-\tau\cos\theta)\cdot \\ &\cdot V\delta(x-\tau\sin\theta\cos\phi)\delta(y-\tau\sin\theta\sin\phi)\delta\big(z-\tau\cos\theta-(t-\tau)\big)d\tau \end{aligned} \tag{24}$$

Integrations by θ,ϕ,τ are understood as integrations of the distribution by these parameters. For example, by definition (38) f_1 acts on function ψ from the Schwartz space as

$$\begin{aligned}\big(f_1(t,x,y,z,\theta,\phi),\psi(x,y,z)\big) = \int_0^t & E(\tau,\tau\cos\theta+t-\tau,\theta)\cdot \\ & \cdot E(t-\tau,t-\tau,0)\sigma(\cos\theta,t-\tau)\cdot \\ & \cdot \psi(\tau\sin\theta\cos\phi,\tau\sin\theta\sin\phi,\tau\cos\theta+t-\tau)d\tau\end{aligned} \tag{25}$$

The function ψ will be used to determine the position, size and configuration of the receiver.

3.2. Initial condition for non-zero angle initial pulse

In the problem formulation we considered a pulse emitted from the source in direction $\theta=0$. We will also discuss the problem with an initial condition for different small angles of an initial direction of $\theta=\theta_0$ of the pulse:

$$f(0,x,y,z) = V\delta(x)\delta(y)\delta(z)\delta(\theta-\theta_0) \tag{26}$$

3.3. Solution for non-zero angle initial pulse

Proceeding the same way as before we get a solution of f_0 with the initial condition

$$f(0,x,y,z) = V\delta(x)\delta(y)\delta(z)\delta(\theta-\theta_0) \tag{27}$$

We take the general solution for probability – normalized f_0

$$\begin{aligned}f_0 = & \frac{1}{2\pi}\delta(x-t\sin\theta\cos\phi)\delta(y-t\sin\theta\sin\phi)\delta(z-t\cos\theta)\delta(\theta-\theta_0)\cdot \\ & \cdot\exp\left[-\int_0^t \sigma_{\mathrm{tot}}\big(z-(t-\tau)\cos\theta\big)d\tau\right]\end{aligned} \tag{28}$$

Which, taking in account (17) and that the expression will not vanish only if $\theta=\theta_0$, simplifies to:

$$f_0 = \frac{1}{2\pi}\delta(x-t\sin\theta_0\cos\phi)\delta(y-t\sin\theta_0\sin\phi)\delta(z-t\cos\theta_0)\delta(\theta-\theta_0)E(t,z,\theta_0) \tag{29}$$

or, going back to $\theta_0=0$, yields

$$f_0 = \frac{1}{2\pi}\delta(x)\delta(y)\delta(z-t)\delta(\theta)E(t,z,0) \tag{30}$$

The equation for f_1 in transformed variables (12)

$$\begin{aligned}f_{1t'} = & -\sigma_{\mathrm{tot}}(z'+t'\cos\theta)f_1 - \int\sigma_{\mathrm{scat}}(\cos\gamma,z'+t'\cos\theta)\cdot \\ & \cdot f_0(t',x'+t'\sin\theta\cos\phi,y'+t'\sin\theta\sin\phi,z'+t'\cos\theta,\theta)d\Omega'\end{aligned} \tag{31}$$

with the initial condition

$$f_1\big|_{t=0} = 0 \tag{32}$$

Integrating yields

$$f_1 \exp\left(\int_0^{t'} \sigma_{\mathrm{tot}}(z'+\tau'\cos\theta)d\tau'\right) = -\int_0^{t'} \exp\left(\int_0^{\tau} \sigma_{\mathrm{tot}}(z'+\tau'\cos\theta)d\tau'\right)\cdot \\ \cdot \int \sigma_{\mathrm{scat}}(\cos\gamma, z'+\tau\cos\theta)\cdot \\ \cdot f_0(\tau, x'+\tau\sin\theta\cos\phi, y'+\tau\sin\theta\sin\phi, z'+\tau\cos\theta,\theta)d\Omega'\,d\tau \tag{33}$$

Solution f_1 for these initial conditions with the original variables is

$$f_1 = -E(t,z,\theta)\int_0^t \exp\left(\int_{t-\tau}^{t} \sigma_{\mathrm{tot}}(z-\tau''\cos\theta)d\tau''\right)\cdot \\ \cdot \int \sigma_{\mathrm{scat}}(\cos\gamma, z-(t-\tau)\cos\theta)\cdot \\ \cdot f_0(\tau, x+(t-\tau)\sin\theta\cos\phi, y'+(t-\tau)\sin\theta\sin\phi, z-(t-\tau)\cos\theta,\theta)d\Omega'\,d\tau \tag{34}$$

Changing the variables of integration $t-\tau=\tau'$ and omitting the primes

$$f_1 = -\int_0^t E(\tau,z,\theta)\cdot \\ \cdot \int \sigma_{\mathrm{scat}}(\cos\theta\cos\theta'+\sin\theta\sin\theta'\cos(\phi-\phi'), z-\tau\cos\theta)\cdot \\ \cdot f_0(t-\tau, x-\tau\sin\theta\cos\phi, y-\tau\sin\theta\sin\phi, z-\tau\cos\theta,\theta)d\Omega'\,d\tau \tag{35}$$

Plugging the point pulse (29) yields

$$f_1 = -\frac{1}{2\pi}\int_0^t E(\tau,z,\theta)E(t-\tau,z-\tau\cos\theta,\theta)\cdot \\ \cdot \int \sigma_{\mathrm{scat}}(\cos\theta\cos\theta'+\sin\theta\sin\theta'\cos(\phi-\phi'), z-\tau\cos\theta)\cdot \\ \cdot \frac{1}{2\pi}\delta(x-\tau\sin\theta\cos\phi)\delta(y-\tau\sin\theta\sin\phi)\delta(z-\tau\cos\theta)\delta(\theta-\theta_0)d\Omega'\,d\tau \tag{36}$$

or, taking into account independence of the indicatrix σ_{scat} on ϕ' and the $\delta(\theta-\theta_0)$ definition

$$f_1 = -\int_0^t E(\tau,z,\theta_0)E(t-\tau,z-\tau\cos\theta_0,\theta_0)\cdot \\ \cdot \int_0^{\pi} \sigma_{\mathrm{scat}}(\cos\theta_0\cos\theta', z-\tau\cos\theta_0)\cdot \\ \cdot \delta(x-\tau\sin\theta_0\cos\phi)\delta(y-\tau\sin\theta_0\sin\phi)\delta(z-\tau\cos\theta_0)\delta(\theta-\theta_0)\sin\theta'\,d\theta'\,d\tau \tag{37}$$

The distribution action for the cylindrical symmetry is evaluated as

$$(f_1,\psi) = -\int_0^t E(\tau,z,\theta_0)E(t-\tau,z-\tau\cos\theta_0,\theta_0)\cdot \\ \cdot \int_0^{\pi} \sigma_{\mathrm{scat}}(\cos\theta_0\cos\theta', z-\tau\cos\theta_0)\cdot \\ \cdot \psi(\tau\sin\theta_0\cos\phi, \tau\sin\theta_0\sin\phi, \tau\cos\theta_0)\sin\theta'\,d\theta'\,d\tau \tag{38}$$

4. Particle number rate

4.1. Particle number rate for θ_0 angle initial pulse

Generally [3], the probabilistic interpretation of the distribution function f in the phase space gives the number of particles in a small volume $\Delta x\Delta y\Delta z$ as

$$\int_0^{2\pi}\int_{\pi-\theta_0}^{\pi}\int_x^{x+\Delta x}\int_y^{y+\Delta y}\int_z^{z+\Delta z} f\,dx\,dy\,dz\sin\theta\,d\theta\,d\phi \tag{39}$$

For a point receiver at x,y,z it is found as a limit

$$I(t,x,y,z)=\lim_{\Delta x\to 0,\Delta y\to 0,\Delta z\to 0}\int_0^{2\pi}\int_{\pi-\theta_0}^{\pi}\int_x^{x+\Delta x}\int_y^{y+\Delta y}\int_z^{z+\Delta z} f\,dx\,dy\,dz\sin\theta\,d\theta\,d\phi \tag{40}$$

here an aperture angle θ_0, that restricts possible velocities of particle directions is introduced.

Whereas in the LIDAR problem the receiver is placed at the origin [3], in our problem it is placed at a certain distance after the scatterer layer. We will place the receiver at the position $(x,y,z)=(0,0,z_0)$ and the layer at $z\in[\frac{z_0}{2}-\Delta,\frac{z_0}{2}+\Delta]$, being 2Δ of the layer's thickness. Our aim is the evaluation of the number of particles which enter the round area of radius ρ_0 laying in the plane $z=z_0$ (receiver) with the center in the origin and having the velocity vectors inclined to z-axis within the angle interval $\theta\in[0,\alpha]$. The angle α relates the aperture angle of a receiver. In its direct sense, the number is proportional to the number of particles (photons) per unit time and the volume is given by the general relation

$$I(t)=\lim_{\Delta t\to 0}\frac{1}{\Delta t}\int_0^{\alpha}\int_0^{2\pi}\big(f(t,0,0,z_0,\theta,\phi),\psi(x,y,z,\theta,\phi)\big)\sin\theta\,d\phi\,d\theta. \tag{41}$$

The choice of function ψ can be realized by concrete physical reasons. In the exemplary case we take here, the receiver has cylindrical symmetry and the function does not depend on θ, ϕ for the initial direction along z, so the value chosen is zero outside the receiver, and $\psi(x,y,z)=1$ for internal points of the domain $x^2+y^2\leq\rho_0^2,\qquad z_0\leq z\leq z_0+\Delta t|\cos\theta|$ and zero outside, being z_0 the coordinate and $|z_0|$ of the distance between the source of the pulse and the receiver. Therefore, we get for (10)

$$\begin{aligned}I_1(t,0,0,z_0)=&-\lim_{\Delta t\to 0}\lim_{\rho_0\to 0}\int_{z_0}^{z_0+\cos\theta_0\Delta t}\int_0^{2\pi}\int_0^{\rho_0}\int_0^{\alpha}\int_0^{t}E(\tau,z_0,\theta)\cdot\\&\cdot\int\sigma_{\mathrm{scat}}(\cos\theta\cos\theta',z-\tau\cos\theta)\cdot\\&\cdot f_0(t-\tau,x-\tau\sin\theta\cos\phi,y-\tau\sin\theta\sin\phi,z-\tau\cos\theta,\theta)\sin\theta'\,d\theta'\,d\tau\,d\theta\,d\rho\,d\phi\,dz\end{aligned} \tag{42}$$

We make the evaluation of single scattering by (38) for a point receiver as the limit:

$$I_1(t) = -\lim_{\Delta t\to 0}\lim_{\rho_0\to 0}\frac{1}{\Delta t}\int_0^{\rho_0}\int_0^{\alpha}\int_0^{t}\int_{z_0}^{z_0+\cos\theta_0\Delta t} E(\tau,z,\theta_0)E(t-\tau,z-\tau\cos\theta_0,\theta_0)\cdot \\ \cdot\int\sigma_{\mathrm{scat}}(\cos\theta_0\cos\theta',z-\tau\cos\theta_0)\cdot \\ \cdot\psi(\tau\sin\theta_0\cos\phi,\tau\sin\theta_0\sin\phi,\tau\cos\theta_0)\sin\theta'\,d\theta'\,d\tau\,d\phi\,d\rho\,dz \tag{43}$$

The nonzero I_1 values are obtained under conditions that are explained Figure 1. The area of integration lies between the horizontal lines $z = z_0, z_0+\Delta z$ and the inclined lines $z = \cos\theta_0 + a$ and $z = \cos\theta_0 + b$, where a, b are the boundaries of a "cloud" or metal plate. The vertical line marks the pulse arrival time $z = t$.

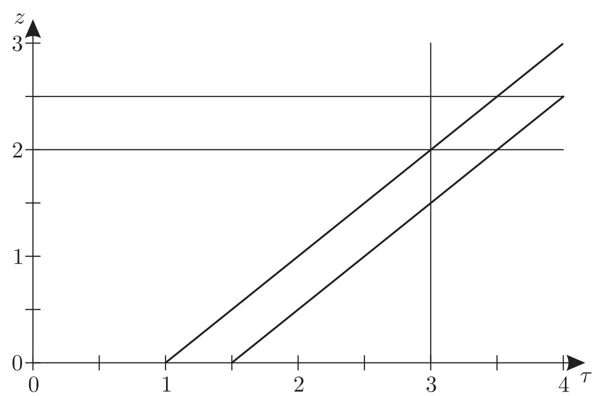

Figure 1. The figure explains conditions of nonzero contribution into intensity

In the case of fixed angle θ_0, $z' = \tau(\cos\theta_0 - 1) + t$, $\tau = (\cos\theta_0 - 1)^{-1}(z' - t)$, hence the argument of the δ-function is $z_0 + t - \tau - z' = z_0 + t - (\cos\theta_0 - 1)^{-1}(z' - t) - z' = z_0 - bt + az' = a(z' - \frac{b}{a})t + z_0/a$, where $a = -1 - (\cos\theta_0 - 1)^{-1} = \frac{\cos\theta_0}{1-\cos\theta_0}$, $b = 1 + (\cos\theta_0 - 1)^{-1}$. The second argument of the scattering amplitude σ_s is therefore $z_0 - \tau\cos\theta_0 = z_0 - (\cos\theta_0 - 1)^{-1}(z' - t)\cos\theta_0$.

The result for the zero angle for the point receiver is almost trivial from the geometrical point of view, the arriving pulse is infinitely short. The expression for intensity contains natural spherical divergence, exponential decay due to absorption and forward scattering at a level inside the layer. Some details may be found in the ArXive paper [19].

4.2. Modeling σ_{scat} and σ_{tot} from experimental data

Let us consider now the scattering in a homogeneous layer of a given material. It is possible to understand the situation better by looking at the picture (Figure 2).

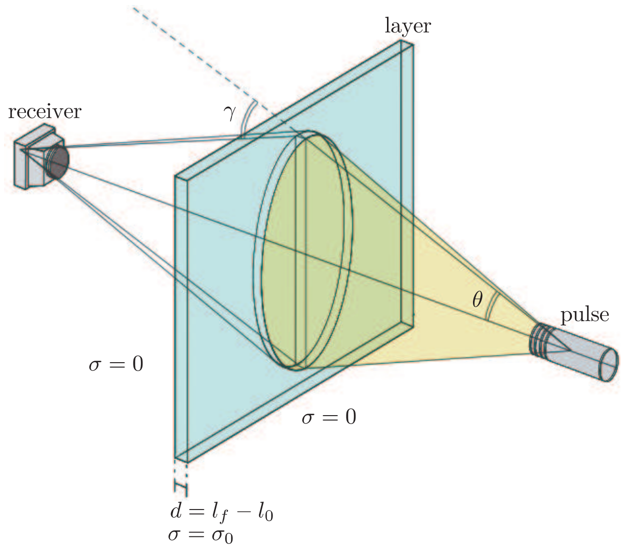

Figure 2. Modeled situation $\sigma = \sigma(1,z)$

Depending on the X-ray energy and the material of the layer, we will have different functions for σ_{scat}. First, let us consider a simple case (Figure 3). For $\cos\gamma = 1$

$$\sigma_{\text{scat}}(\cos\gamma, z) = \begin{cases} 0 & z \le \frac{z_0}{2} - \Delta \\ \sigma_0 & \frac{z_0}{2} - \Delta < z < \frac{z_0}{2} + \Delta \\ 0 & z \ge \frac{z_0}{2} + \Delta \end{cases} \tag{44}$$

$$\sigma_{\text{tot}}(z) = \begin{cases} 0 & z \le \frac{z_0}{2} - \Delta \\ \sigma_1 & \frac{z_0}{2} - \Delta < z < \frac{z_0}{2} + \Delta \\ 0 & z \ge \frac{z_0}{2} + \Delta \end{cases} \tag{45}$$

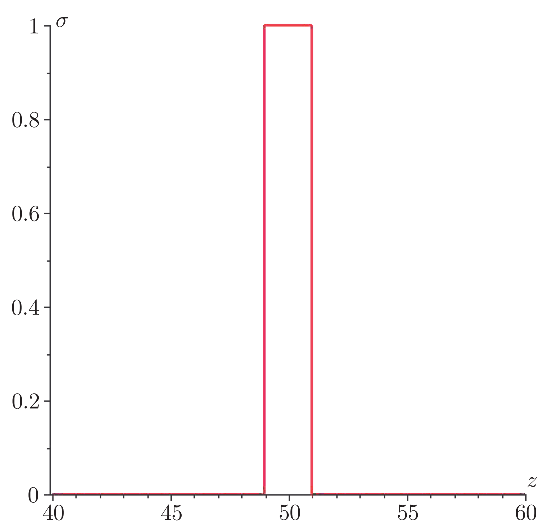

Figure 3. Proposed $\sigma_{\text{scat}}(1,z)$

The total attenuation cross section σ_{tot} can be divided into two terms: the scattering total cross section $\int_0^\pi \sigma_{\text{scat}}$ and the absorption total cross section σ_{abs}. To model $\sigma_{\text{tot}} = \int_0^\pi \sigma_{\text{scat}}(\cos\gamma, z)d\gamma + \sigma_{\text{abs}}$, let us first consider some theory. The attenuation Lambert-Beer law states:

$$I = I_0 e^{-\mu z} \tag{46}$$

where μ is the attenuation coefficient. In the next Figure 4 we can see how the intensity of the X-ray beam decreases as it penetrates a layer of beryllium.

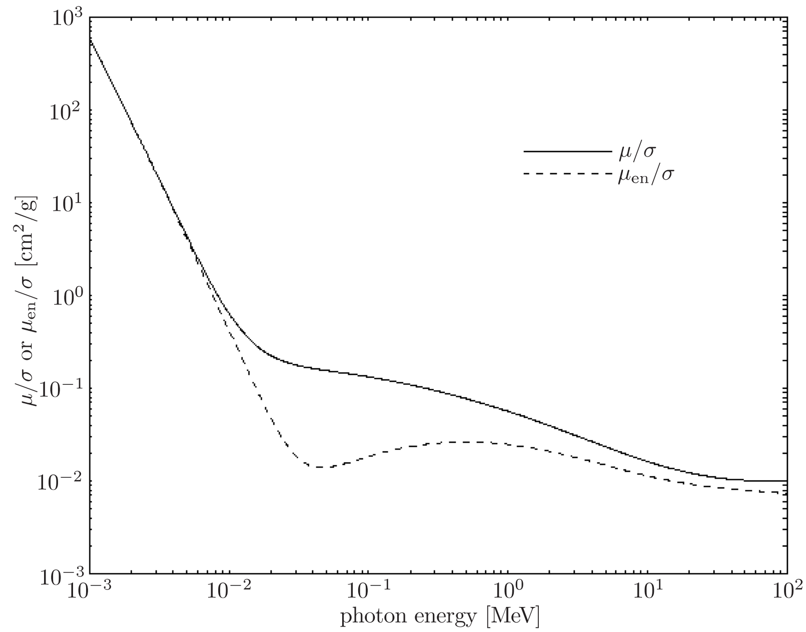

Figure 4. Beryllium intensity attenuation

Now, μ is defined as

$$\mu = \rho_a \sigma_{\text{tot}} = \rho \frac{N_0}{A} \sigma_{\text{tot}} \tag{47}$$

where $\rho_{atom} = \rho \frac{N_0}{A}$ is the atomic density, N_0 is Avogadro's number, A is the atomic mass number and ρ is the density (g/m^3).

$$\sigma_{\text{tot}} = \frac{A\mu}{\rho N_0} \tag{48}$$

On the other hand, the Rayleigh scattering cross section σ_{scat} expression taken from [20] is

$$\sigma_{\text{scat}} = \pi r_e^2 \int_{-1}^{1} (1 + \cos^2\gamma) f^2(q, Z) d(\cos\gamma) \tag{49}$$

where r_e is the electron radius, γ is the scattering angle, $2\pi d(\cos\gamma)$ is the solid angle between cones with angles γ and $\gamma + d\gamma$, $f(q, Z)$ is the atomic scattering factor, q is $\frac{\sin\gamma/2}{\lambda}$, the momentum transfer parameter, and λ is the wavelength expressed in Å.

Next you can see the plots of the experimental data for the atomic scattering factor $f(q,Z)$ for beryllium. We will consider the values for the total photon interaction cross section for beryllium from the tables of [20]. We are interested in beryllium due to its properties and feasible applications. The values in the table refer also the Compton scattering, i.e., $\sigma_{\mathrm{tot}} = \sigma_{\mathrm{Rayleigh}} + \sigma_{\mathrm{Compton}} + \sigma_a$. However, we will not talk about the Compton scattering as it is sometimes neglected due to its low influence in the X-ray scattering.

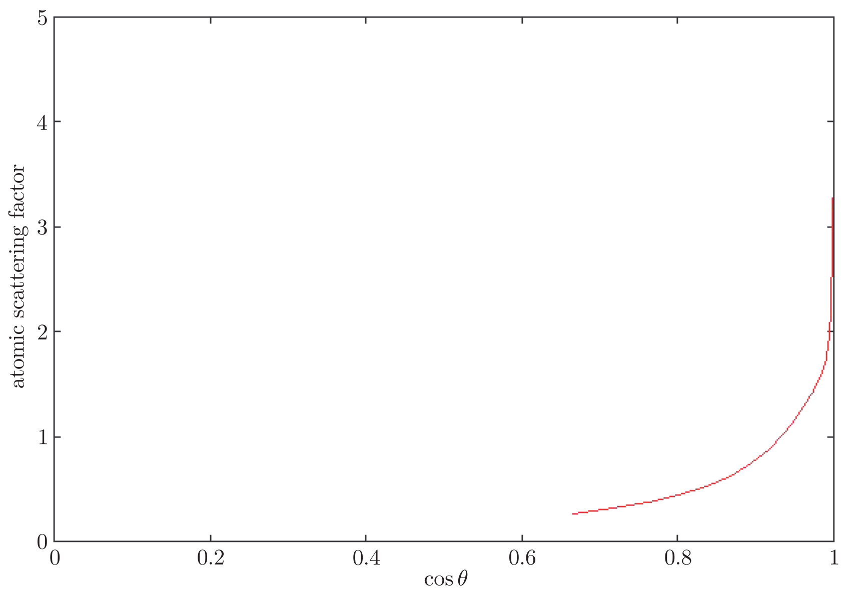

Figure 5. Atomic scattering factor for beryllium

Table 1. Scattering for Be

Radiation	Energy [KeV]	$\sigma_{\mathrm{atom}}\ \left[\frac{\mathrm{barns}}{\mathrm{atom}}\right]$
Ag $K\beta_1$	24.94	2.97
Zn K_α^-	8.63	13.8
Mn K_α^-	5.895	39.9

As can be seen in the table the total cross section is given in barns/atom units. We should normalize it per unit volume, *i.e.* cm^{-1}.

$$\sigma_{\mathrm{tot}} = N\sigma_{\mathrm{atom}} \quad \text{where} \quad N = \frac{\rho N_0}{A}$$
$$\left[\mathrm{cm}^{-1}\right] = \sigma_{\mathrm{tot}} = \frac{\rho N_0 \sigma_{\mathrm{atom}} 10^{-22}}{A} = \left[\frac{\frac{\mathrm{atom}}{\mathrm{mol}}\frac{\mathrm{g}}{\mathrm{cm}^3}\frac{\mathrm{cm}^2}{\mathrm{atom}}}{\frac{\mathrm{g}}{\mathrm{mol}}}\right] = \left[\mathrm{cm}^{-1}\right] \tag{50}$$

For beryllium $\rho = 1.85\frac{\mathrm{g}}{\mathrm{cm}^3}$, $A = 9.01$ and $\sigma_{\mathrm{atom}} = 2.97$ for energy radiation of 24.94 KeV.

4.3. Intensity plots

The following plots will be made taking in account a layer of beryllium of thickness 2Δ in the half way from the source to the receiver, i.e, at the range $\frac{z_0}{2}-\Delta \le z \le \frac{z_0}{2}+\Delta$. We will plot the results of the single scattering approach with the θ_0 angle initial pulse. The intensity plot comes from formula (42). The total cross-section dependence on z we model as

$$\sigma_{\text{tot}}(z)=\begin{cases}0 & z\le \frac{z_0}{2}-\Delta\\ \frac{\rho N_0}{A}\sigma_{\text{atom}} & \frac{z_0}{2}-\Delta<z<\frac{z_0}{2}+\Delta\\ 0 & z\ge \frac{z_0}{2}+\Delta\end{cases} \tag{51}$$

$\rho=1.85\frac{g}{cm^3}$, the density of beryllium, $A=9.01$ the beryllium atomic mass number, $\sigma_{\text{atom}}=2.97$ and N_0, Avogadro's number. For the scattering cross section we used the function fitted to the atomic scattering factor of beryllium from Figure 5. We can see both the data and fitted function in the next figure

$$\sigma_{\text{scat}}(\cos\gamma,z)=\begin{cases}e^{1.2238(\cos\gamma)^8}-1 & z\in(\frac{z_0}{2}-\Delta,\frac{z_0}{2}+\Delta)\\ 0 & z\notin(\frac{z_0}{2}-\Delta,\frac{z_0}{2}+\Delta)\end{cases} \tag{52}$$

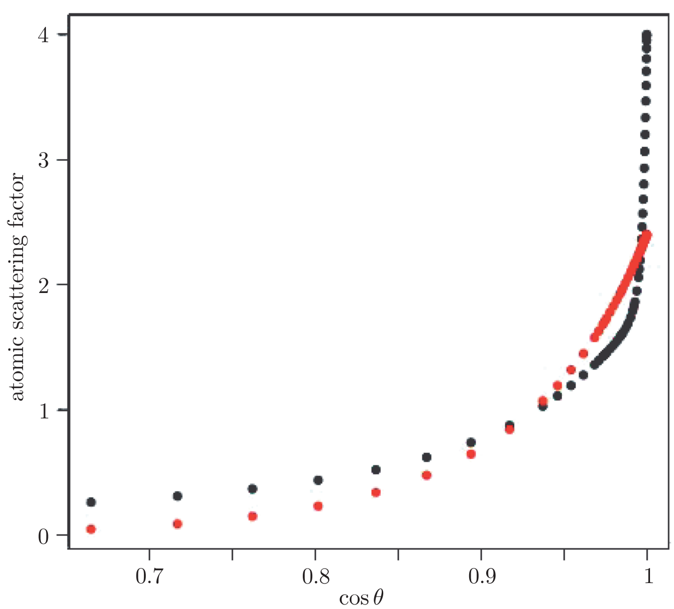

Figure 6. The data function is shown in black; the fitted function – in red

To plot the intensities we will consider the thickness of the beryllium layer 2Δ. The resulting formula for the point receiver intensity has direct geometrical interpretation (see Figure 7) As it is marked in the plot, the total time for the photon arrival is $t=t_1+t_2=\frac{z}{\cos\vartheta_0}+\frac{z_0-z}{\cos\beta}$.

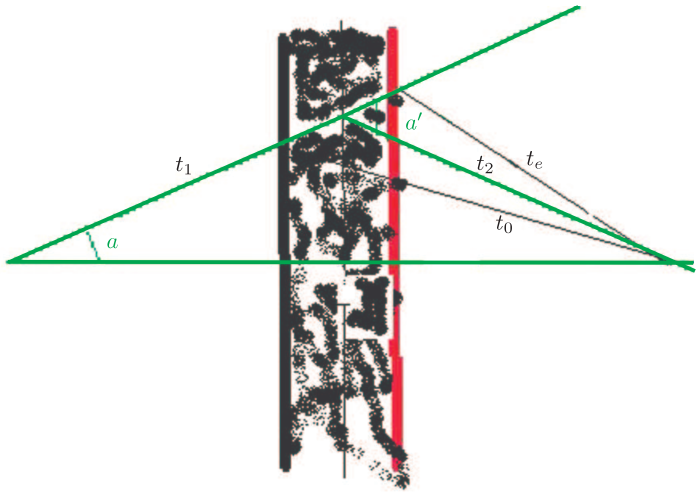

Figure 7. Trajectories of scattered photons from minimal to maximum scattering angles

The angle is evaluated via

$$\tan\beta = \frac{z\tan\vartheta_0}{z_0 - z} \tag{53}$$

and

$$\cos\beta = \sqrt{\frac{1}{1+\tan^2\beta}} = \sqrt{\frac{1}{1+(\frac{z\tan\vartheta_0}{z_0-z})^2}} = \sqrt{\frac{(z-z_0)^2}{z^2\tan^2\vartheta_0 + z^2 - 2zz_0 + z_0^2}} \tag{54}$$

Let us define

$$t = \frac{z}{\cos\vartheta_0} + \frac{z_0 - z}{\sqrt{\frac{(z-z_0)^2}{z^2\tan^2\vartheta_0+z^2-2zz_0+z_0^2}}} \tag{55}$$

Thus the expression of the scattering point height via time t is

$$\begin{aligned} z &= \frac{1}{2t\cos\vartheta_0 - 2z_0\cos^2\vartheta_0}\left(t^2\cos^2\vartheta_0 - z_0^2\cos^2\vartheta_0\right) \\ &= \frac{1}{2}(\cos\vartheta_0)(t-z_0)\frac{t+z_0}{t-z_0\cos\vartheta_0} \end{aligned} \tag{56}$$

with the correspondent $\cos\beta$ and $\sin\beta$ expressions. Recall that

$$\cos\gamma = \cos\beta\cos\vartheta_0 - \sin\beta\sin\vartheta_0 \tag{57}$$

The relative intensity formula also corresponds to its geometrical sense with spherical divergence

$$\frac{I}{I_0} \sim \frac{1}{(t_2)^2}\exp[-\sigma_t(t_3+t_4)]\sigma(\cos\gamma, z) \tag{58}$$

where

$$t_3 = \frac{z - \frac{z_0}{2} + \Delta}{\cos\vartheta_0} \quad \text{and} \quad t_4 = \frac{-z + \frac{z_0}{2} + \Delta}{\cos\beta} \tag{59}$$

the arrival time

$$t_0 = \left[\frac{z}{\cos\vartheta_0} + \frac{z_0 - z}{\sqrt{\frac{(z-z_0)^2}{z^2 \tan^2\vartheta_0 + z^2 - 2zz_0 + z_0^2}}} \right]_{z=\frac{z_0}{2}-\Delta} \tag{60}$$

and the end of the pulse is evaluated as

$$t_e = \left[\frac{z}{\cos\vartheta_0} + \frac{z_0 - z}{\sqrt{\frac{(z-z_0)^2}{z^2 \tan^2\vartheta_0 + z^2 - 2zz_0 + z_0^2}}} \right]_{z=\frac{z_0}{2}+\Delta} \tag{61}$$

The choice of plotting parameters, convenient for illustration, $\vartheta_0 = 0.1$, $z_0 = 0.01$, $\Delta = 0.001$ give $t_0 = 1.0033 \cdot 10^{-2}$, $t_e = 1.0075 \cdot 10^{-2}$. Note that the values are not related to real matter and geometry parameters. The plot has been made with SWP and is of a corresponding form.

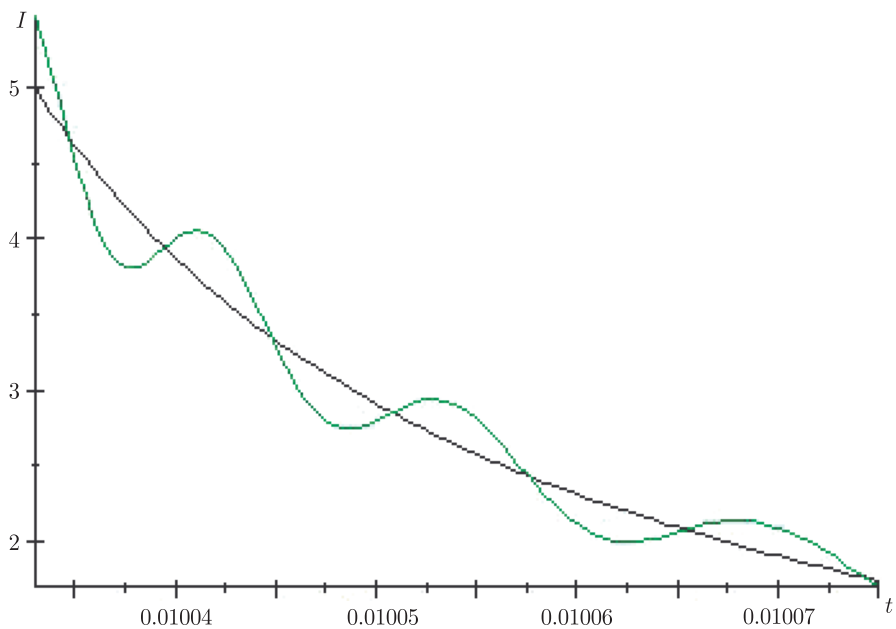

Figure 8. Intensity for single scattering approximation, inclined beam; the green line results from a superposition of the constant density with a periodic one

The beam has traveled from the source through air, where we do not account for scattering or absorption. It has penetrated the beryllium layer where the scattering and absorption phenomena have occurred. It has traveled through air again and finally has arrived to the receiver. We can see that the receiver will detect a delayed and spread pulse with peaks and it will rapidly decrease as the scattered photons arrive.

5. Conclusions

We have obtained a solution of the Kolomogorov [4] forward equation [21, 16] for single scattering for an initial pulse of angle $\theta = \theta_0$. We modeled the equations for the total scattering cross section σ_{tot} and the differential cross section σ_{scat} for beryllium. Once we had had this, an expression for the intensity rate was derived from the initial pulse arriving at a small receiver situated after the beryllium layer at position $z = z_0$. the results were obtained particularly with a point receiver. After plotting the result of this intensity it was shown that the pulse arrived at the receiver with a certain delay and spread. With this formulas, considering other materials and modeling the scattering cross section of them, we were able to predict the delay and intensity of the initial pulse. There is space for continuation of this work [22]. Multiple scattering approximation is in our interest. The next step is to calculate it using the recurrent relation (6). When f is calculated in the limit, we can count the stream for it. The properties of layers can be obtained by studying the plots from the receiver. There are many situations that could be studied in the future. It is a matter of changing the initial condition. To be more realistic, the initial pulse should be taken continuous in time. An initial continuous pulse distributed in a solid angle, $\theta \in [\theta_0, \theta_1]$, $\phi \in [\phi_0, \phi_1]$ can be studied. Different layer materials could be used as well as the position and thickness of the layer. A very interesting approach would be to consider heterogeneities inside layer materials, see Figure 3. In this case The distribution of heterogeneities in the media should be introduced. This would be more realistic, as materials present non-homogeneities in their structures.

Acknowledgements

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