3D Compton scattering imaging: study of the spectrum and contour reconstruction

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August 2019

Abstract. 3D Compton scattering imaging is an upcoming concept focusing on exploiting the photons scattered, following on from the so-called Compton effect, by the atomic structure of an object under study. This phenomenon rules the collision of particles with electrons and describes their energy loss after scattering. Consequently, a monochromatic source leads to a polychromatic response on the camera. Assuming the camera to collect continuously the photons in terms of energy, we model the measured spectrum for first- and second-order scattering. The second-order scattered radiation reveals itself to be structurally smoother than the radiation of first-order. Therefore, the contours of the electron density are essentially encoded within the first-order scattering radiation and can be recovered from the full spectrum using a filtered backprojection kind inversion technique. Our main results, modeling and reconstruction scheme, are successfully implemented on synthetic and Monte-Carlo data.

1. Introduction

Since the advent of Computerized Tomography (CT), many imaging concepts have emerged and the need in imaging has grown. One can mention Single Photon Emission CT, Positron Emission Tomography or Cone-Beam CT for the standard system based on an ionising source. In these configurations, the energy has a very limited use but the idea of exploiting it in order to enhance the image quality, optimize the acquisition process or to compensate some limitations (such as limited angle issues) has led to various works [20, 2, 23, 11, 34, 24, 15, 14].

Computerized Tomography (CT) is a well-established and widely used technique which images an object by exploiting the properties of penetration of the x-rays. Due to the interactions of the photons with the atomic structure, the matter will resist to the propagation of the photon beam, denoted by its intensity $I(x, \theta)$ at position $x$ and in direction $\theta$, following the stationary transport equation

$$\theta \cdot \nabla x I(x, \theta) + \mu_E(x) I(x, \theta) = 0, \quad x \in \Omega \subset \mathbb{R}^3$$

with $E$ the energy of the beam. The resistance of the matter is symbolized by the lineic attenuation coefficient $\mu_E(x)$. Solving this ordinary equation leads to the well-known Beer-Lambert law

$$I(y) = I(x)e^{-\int_{x \rightarrow y} \mu_E},$$
with $x \to y$ denotes the straight line $\{x + t(y - x), \ t \in [0,1]\}$. It describes the loss of intensities along the path $x$ to $y$. In two dimensions, it is then standard to interpret the measurement of the intensity in a CT-scan using the Radon transform, which maps the attenuation map $\mu_E(x)$ into its line integrals, i.e.

$$\ln \frac{I(s, \theta)}{I(d, \theta)} = R_\mu E(p, \theta) = \int_{\Omega} \mu_E(x) \delta(p - x \cdot \theta) dx$$

with $(p, \theta) \in \mathbb{R} \times S^1$ and where $s$ and $d$ stand for the position of the source and of a camera. The task to recover $\mu_E$ from the data $g(p, \theta)$ can be achieved by various techniques such as the filtered back-projection (FBP) which regularizes the inversion formula of the Radon transform, i.e.

$$\mu_E(x) = \frac{1}{4\pi} R^*(I^{-1} g)(x)$$

with $R^*$ the $L_2$-adjoint (back-projection) operator of $R$ and $I^{-1}$ the Riesz potential of order $-1$. When one focuses on the physics between the matter and the photons, four types of interactions come out: Thomson-Rayleigh scattering, photoelectric absorption, Compton scattering and pair production. In the classic range of applications of the x-rays or $\gamma$-rays, $[50, 500]$ keV, the photoelectric absorption and the Compton scattering are the dominant phenomena which leads to a model for the lineic attenuation factor due to Stonestrom et al. [33] which writes

$$\mu_E(x) = E^{-3} \lambda_{PE}(x) + \sigma(E)n_e(x)$$

where $\lambda_{PE}$ is a factor depending on the materials and symbolizing the photoelectric absorption, $\sigma(E)$ the total-cross section of the Compton effect at energy $E$ and $n_e$ the electron density at $x$. The Compton effect stands for the collision of a photon with an electron. The photon transfers a part of its energy $E_0$ to the electron. The electron suffers then a recoil and the photon is then scattered of an (scattering) angle $\omega$ with the axis of propagation, see Fig. 1. The energy of the photon after scattering is expressed by the Compton formula [9],

$$E_\omega = \frac{E_0}{1 + \frac{E_0}{mc^2}(1 - \cos \omega)}$$

where $mc^2 = 511$ keV represents the energy of an electron at rest.

The recent development of camera able to measure accurately the energy of incoming photons opens the way to an innovative 3D imaging concept, Compton
scattering imaging (abbreviated here by CSI). Although the technology of such detectors has not yet reached the same level of maturity as the one used in conventional imaging (CT, SPECT, PET), scientists have proposed and studied in the last decades different bi-dimensional systems, called Compton scattering tomography (CST), see e.g. [22, 27, 1, 3, 5, 6, 8, 12, 16, 19, 25, 4, 17, 30]. It is also possible to consider interior sources, for instance via the insertion of radiotracers like in SPECT. Then considering collimated detectors, it is possible to model the scattered flux through conical Radon transforms, see for instance [26, 28]. However, in this work, we consider only systems with external sources.

In this paper we assume that the source is monochromatic, i.e. it emits photons with same energy \( E_0 \). For sufficiently large \( E_0 \), larger than 80keV in medical applications, the Compton effect represents a substantial part of the radiation as more of 70% of the emitted radiation is scattered within the whole body. Therefore, the variation in terms of energy due to the Compton scattering, eq. (4), will produce a polychromatic response to the monochromatic impulse due to the source. We decompose the spectrum \( \operatorname{Spec}(d, E) \) measured at a detector \( d \) with energy \( E \) as follows

\[
\operatorname{Spec}(d, E) = \sum_{i=0}^{\infty} g_i(d, E).
\]

In this equation, \( g_0 \) represents the primary radiation which crossed the object without being subject to the Compton effect. It corresponds to the signal measured in CT, eq. (1). The functions \( g_i(D, E) \) corresponds to the photons that were measured at \( D \) with incoming energy \( E \) after \( i \) scattering events.

The purpose of this paper is to propose a strategy to extract features of the electron density \( n_e \) from the spectrum in eq. (4). The main idea arises from the smoothness properties of the operators modeling the scattered radiations at various orders. It appears that the first scattering encodes the richest information about the contours while the scattering of higher orders lead to much smoother data. To make our point but also for the sake of implementation, we focus on the first and second scattering only, which means \( g_1 \) and \( g_2 \). \( g_0 \) is also discarded as it brings no information related to the energy although the primary radiation could be used as rich supplementary information in the future.

The manuscript is organized as follows: we first recall the results from [31] which provides the modeling of the first scattering, \( g_1 \), and a reconstruction strategy based on contour extraction. Then we develop an analytic modeling for the second-order scattered radiation. The study of these two parts of the spectrum under Fourier integral operators shows that \( g_2 \) is substantially smoother than \( g_1 \) on the Sobolev scale. It follows that the contour based strategy proposed in [31] can be straightforwardly applied to the more general case of the full spectrum. The various modelings as well as the reconstruction technique are validated using Monte-Carlo simulations.

2. First-order scattering and toric Radon transforms

In this section, the first order scattering is characterized by a toric Radon transform. Let consider an "emission" point \( m \) and a "receiver" point \( n \). The photon beam emitted by \( m \) travels in the direction \( n - m \) within a solid angle \( d\Omega_c \), see Figure 1. The nature of the photon emission leads its intensity to reduce proportionally to the square of the travelled distance, the photometric dispersion, and exponentially due to the resistance of the matter to the propagation of light, the attenuation factor or
Beer-Lambert law. To represent these two physical factors, we define the following mapping of the attenuation map \( \mu_E \)

\[
A_E(m, n) := \|n - m\|^{-2} \exp \left( -\|n - m\| \int_0^1 \mu_E \left( m + t \frac{(n - m)}{\|n - m\|} \right) dt \right).
\]

Using this notation and considering an ionising source \( s \) with energy \( E_0 \) and photon beam intensity \( I_0 \), the variation of the number of photons \( N_c \) scattered at \( x \) and detected at \( d \) with energy \( E_\omega \), see \([10]\), can be expressed as

\[
dN_c = \frac{I_0 r_e^2}{4} P(\omega) A_{E_0}(s, x) A_{E_\omega}(x, d) n_e(x) \, dx,
\]

where \( P(\omega) \) stands for the Klein-Nishina probability \([21]\), \( r_e \) is the classical radius of an electron. This formula describes the evolution of the first scattered radiation which is detected at a given energy and at a given detector position.

Due to the Compton formula eq. (3), the scattered energy \( E_\omega \) corresponds to only one scattering angle \( \omega \) and thus delivers a specific geometry when focusing on the first scattering. Indeed, all scattering points \( M(x) \) responsible for a detected scattered photon at energy \( E_\omega \) belongs to

\[
\mathcal{T}(\omega, s, d) = \{ \angle(x - s, d - x) = \pi - \omega \}
\]

with \( \angle(\cdot, \cdot) \) the angle between two vectors. As depicted by Figure 2 this set corresponds to a part of a spindle torus. More precisely, \( \mathcal{T}(\omega, s, d) \) denotes the lemon part of the spindle torus for \( \omega \in [0, \frac{\pi}{2}] \) and to its apple part for \( \omega \in [\frac{\pi}{2}, \pi] \), see Figure 3. Assuming now \( d \) to be a point detector and integrating over \( \Omega := \text{dom}(n_e) \) the equation (5), one obtains an integral representation of the detected first scattered radiation, i.e.

\[
g_1(s, d, E_\omega) = N_c(s, d, E_\omega) \propto \int_{x \in \mathcal{T}(\omega, s, d)} A_{E_0}(s, x) A_{E_\omega}(x, d) n_e(x) \, dx.
\]
As proven into [31], the quantities $N_c(s, d, E_\omega)$ can be interpreted as a weighted toric Radon transform,

$$N_c(s, d, E_\omega) = \mathcal{T}(n_e)(p, s, d) = \int_{\Omega} w_c(x; p, s, d) n_e(x) \delta(p - \phi(x, s, d)) \, dx$$

with $p = \cot \omega$, $w_c = A_{E_0} \cdot A_{E_\omega}$ and the phase given by

$$\phi(x, s, d) = \frac{(x - s) \cdot (d - s) - \|x - s\|^2}{\sqrt{\|d - s\|^2 \|x - s\|^2 - ((x - s) \cdot (d - s))^2}}.$$

To simplify the study but also for the sake of potential applications, we propose to fix the source $s$. The induced modalities will then have the advantage to avoid any rotation/displacement of the source and thus enable fast acquisition time. In this case, for $v = d - s$ and $y = x - s$, the phase simplifies to

$$\phi(y, v) = \frac{y \cdot v - \|y\|^2}{\sqrt{\|v\|^2 \|y\|^2 - (y \cdot v)^2}}$$

and the first scattering radiation can be modelled by

$$g_1(d, E_\omega) = \mathcal{T}(n_e)(s, v) = \int_{\Omega} w_c(y; p, v) n_e(y) \delta(p - \phi(y, v)) \, dy.$$

We define $\mathcal{V}$ as the domain of definition of $v$. We voluntarily kept the same notation between both cases $s$ fixed or not for the sake of simplicity. One can also consider the adjoint operator in a weighted $L_2$ space, also called here a weighted back-projection operator

$$\mathcal{T}^*_b g(x) = \int_{\Theta} b(x, \theta) g(\phi(x, v), v) d\sigma(v)$$

with $b(x, \theta)$ a positive weight function, $\Theta$ the space of the displacement of the detector w.r.t the source and $d\sigma(v)$ the associated measure.

The inverse problem to solve $g = \mathcal{T}(n_e)$ is very difficult problem since first of all, $\mathcal{T}$ is a non-linear operator w.r.t the electron density $n_e$. Indeed the weight $w_c$ is an operator of the lineic attenuation factor which is also a function of $n_e$, see eq. [2]. Non-linear iterative techniques such as the Landweber iteration or the Kaczmarz’s method could provide satisfactory reconstruction of $n_e$ but at the cost of a tremendous
Figure 4. Four potential configurations of modalities on 3D CSI: (a) the source and one detector rotates around the object along a sphere see [37]; (b)-(c)-(d) the source is fixed and a set of detectors are located on a sphere (a), on a cylinder (b) or on two planes (c). The position of the source is not important as long as it remains outside the object.

computation time. Deep learning techniques could be used but the lack of large dataset with real/ground truth measurement prevents any training step. A first strategy was proposed in [31] for extracting the contours of \( n_e \) from \( g = T(n_e) \) using the following filtered backprojection formula:

\[
K n_e := -\frac{1}{8\pi^2} T_b * \partial^2 p g = n_e + \mathcal{E} n_e
\]  

(6)

with \( \mathcal{E} \) a \( C^\infty \)-smooth operator and \( b(x, v) = h(x, v)(w_c(x, x, v))^{-1} \) in which

\[
h(x, v) = \det \begin{pmatrix}
\nabla_x \phi(x, v) \\
\partial_{v_1} \nabla_x \phi(x, v) \\
\partial_{v_2} \nabla_x \phi(x, v)
\end{pmatrix}
\]

is assumed \( \neq 0 \). The contours (or high variations) of \( n_e \) are finally recovered by applying any differential operator (gradient, laplacian, wavelets, etc). The advantage of this approach is to not require specific geometry for the displacement/position of the detectors since no structure or invariances are assumed. We can then apply the approach for various architectures of 3D CSI, see Figure [3]

Eq. (6) assumes the weight \( w_c \) to be \( C^\infty \)-smooth in order to ensure the smoothness of \( \mathcal{E} \). This is an issue for our problem since assuming \( n_e \) to be a \( L_2 \) function with contours (singularities) will lead to a non-smooth weight \( w_c \). However, as pointed out in [31], this can be circumvented in practice by decorrelating \( w_c \) and \( n_e \). One
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3. Modeling the second order scattered radiation

In this section we derive an integral representation of the part of second-order scattering in the measured spectrum. The higher orders are difficult to handle but we expect a similar approach for the higher-orders (larger than 2), this is why we will postulate the extension of the results for higher orders.

The derivation of the second scattering will use the modelling of the first scattering seen above. In this case, a measured photon is scattered twice instead of once before to be detected. We denote by $M(x)$ and $N(y)$ the first and second scattering points respectively and by $\omega_1$ and $\omega_2$ the first and second scattering angles respectively. The key idea is to consider each first scattering point as a new polychromatic source with respect to the second scattering points and detectors.

Let us consider a detector $d$ with a detected energy $E_d$. Due to the Compton formula, the scattering angles must satisfy

$$\cos \omega_1 + \cos \omega_2 = 2 - mc^2 \left( \frac{1}{E_d} - \frac{1}{E_0} \right) =: \lambda(E_d) \in (0, 2). \quad (7)$$

The boundaries 0 and 2 are here excluded since they correspond to the degenerated...
cases - primary ($\omega = 0$) and backscattered ($\omega = \pi$) radiation - of the torus. In consequence, the second scattering angle will be expressed as a function of the first one:

$$\omega_2(\omega_1) = \arccos \left( \lambda(E_d) - \cos \omega_1 \right).$$

The first angle $w_1$ means that a photon arriving at $M(x)$ with energy $E_0$ is scattered by an angle $\omega_1$ and has afterwards an energy $E_{\omega_1}$. Such photons belong then to the cone with aperture $\omega_1$, vertex $M(x)$ and direction $x-s$, i.e. to the cone

$$C(\omega_1, x) := \{ y \in \mathbb{R}^3 : \psi(y, x) = \cos \omega_1 \}$$

with phase

$$\psi(y, x) = \frac{y - x}{\| y - x \|} \cdot \frac{x - s}{\| x - s \|}.$$ 

This phase leads to a standard representation of the cone, i.e.

$$C(\omega_1, x) = \left\{ x + \frac{t}{\cos \omega_1} R_1 \begin{pmatrix} \sin \omega_1 \cos \varphi \\ \sin \omega_1 \sin \varphi \\ \cos \omega_1 \end{pmatrix} : t \in \mathbb{R}^+, \varphi \in [0, 2\pi] \right\}$$

with $R_1$ the rotation matrix which maps $\frac{d-x}{\|d-x\|}$ into $\frac{x-s}{\|x-s\|}$. Such a matrix can be computed using the Rodrigues formula.

The second angle $w_2$ means that a photon arriving at $N(y)$ with energy $E_{\omega_1}$ is scattered by an angle $\omega_2$ and is afterwards detected at $d$ with an energy $E_d$. As seen in the previous section, such photons belong to the torus with fixed points $x$ and $d$, $T(\omega_2, x, d)$, such that

$$\cot \omega_2(\omega_1) = \phi(y, x, d).$$

A parametric representation of the spindle torus is given in [31] and writes

$$T(\omega_2, x, d) = \left\{ x + \|d - x\| \frac{\sin(\omega_2 - \alpha)}{\sin \omega_2} R_2 \begin{pmatrix} \sin \alpha \cos \beta \\ \sin \alpha \sin \beta \\ \cos \alpha \end{pmatrix} : \alpha \in [0, \omega_2], \beta \in [0, 2\pi] \right\}$$

with $R_2$ the rotation matrix which maps $e_z = (0, 0, 1)^T$ into $\frac{d-x}{\|d-x\|}$. Shifting the torus around $x$, it can be expressed as a unit vector multiplied by the radius

$$r(\omega_2, \alpha) = \|d - x\| \left( \cos \alpha - \frac{\sqrt{1 - \cos^2 \alpha}}{\tan \omega_2} \right).$$

Since the new source $M(x)$ emits photons with various energy in the corresponding cone, the Compton formula and the relationship $\omega_2(\omega_1)$ implies that a photon detected at $d$ with energy $E_d$ and scattered at $M(x)$ with angle $\omega_1$ must belong to the intersection

$$y \in T(\omega_2(\omega_1), x, d) \cap C(\omega_1, x).$$

This intersection and the principle described above is depicted in Figure 5.

To simplify the analysis, we consider the torus to be oriented in the direction $e_z$, which is achieved by applying the reverse matrix $R_2^{-1}$. In this setting, $\cos \alpha$ corresponds to the third component of the normalized vector. Since we are interested in the intersection of the cone and of the torus, one gets

$$\cos \alpha = R_1(3, 1) \sin \omega_1 \cos \varphi + R_1(3, 2) \sin \omega_1 \sin \varphi + R_1(3, 3) \cos \omega_1 =: z_\omega.$$
with $R_1(3, \cdot)$ the third row of the rotation matrix $R_1$. Using the parametrisation of the cone, one gets for the intersection, the following radius

$$r_\cap := ||\mathbf{d} - \mathbf{x}|| \left( z_\cap - \frac{\sqrt{1 - z_\cap^2}}{\tan \omega_2} \right)$$

and thus

$$y_\cap = \mathbf{x} + r_\cap R_2 R_1 \begin{pmatrix} \sin \omega_1 \cos \varphi \\ \sin \omega_1 \sin \varphi \\ \cos \omega_1 \end{pmatrix} \quad \text{if } r_\cap > 0.$$  

Since the torus is oriented ($\mathbf{x}$ to $\mathbf{d}$), we discard the intersection between the cone and the opposite torus which corresponds to negative radii in order to fit the physics. Practically we can ignore them since they lead to detected energies outside the considered range. Also, the case $r_\cap = 0$ is discarded as it is physically impossible and would correspond to two successive scattering occurring at the exact same location.

We have now the tools to give the first result of this paper.

**Theorem 3.1.** Considering an electron density function $n_e(\mathbf{x})$ with compact support $\Omega$, a monochromatic source $\mathbf{s}$ with energy $E_0$ as well as a detector $\mathbf{d}$ both located outside $\Omega$. Then, the number of detected photons scattered twice arriving with an energy $E_d$ are given by

$$g_2(\mathbf{d}, E_d) = \int_{\Omega} \int_{0}^{2\pi} \int_{0}^{\pi} w_2(\mathbf{s}, \mathbf{x}, y_\cap, \omega_1, \varphi) n_e(\mathbf{x}) n_e(y_\cap) dS_\cap(\omega_1, \varphi) d\mathbf{x}$$

with the physical factors symbolized by

$$w_2(\mathbf{s}, \mathbf{x}, y_\cap, \mathbf{d}, \omega_1, \varphi) = A_{E_0}(\mathbf{s}, \mathbf{x}) A_{E_{\omega_1}}(\mathbf{x}, y_\cap) A_{E_{\omega_2}}(y_\cap, \mathbf{d})$$

and the differential form of the intersection given by

$$dS_\cap(\omega_1, \varphi) = r_\cap \sqrt{\sin^2 \omega_1 (r_\cap^2 + (\partial_\omega_1 r_\cap)^2 + (\partial_\varphi r_\cap)^2)} d\omega_1 d\varphi$$

in which $y_\cap$ and $r_\cap$ are described in eqs [8] and [3].

**Proof.** The structure follows on from the physics of Compton scattering. Akin to the first scattering, the variation of photon scattered twice can be expressed as

$$d^2 g_2 = I_0 \left( \frac{1}{2} r_\cap \right)^4 P(\omega_1) P(\omega_2) A_{E_0}(\mathbf{s}, \mathbf{x}) A_{E_{\omega_1}}(\mathbf{x}, \mathbf{y}) A_{E_{\omega_2}}(\mathbf{y}, \mathbf{d}) n_e(\mathbf{x}) n_e(\mathbf{y}) d\mathbf{x} d\mathbf{y}.$$

Therefore, ignoring some physical constants and based on our development above, one can integrate to get the theoretical number of photons detected at $\mathbf{d}$ with energy $E_d$ after two scattering events,

$$g_2(\mathbf{d}, E_d) = \int_{\Omega} \int_{\mathcal{F}(\omega_2, \mathbf{x}, \mathbf{d}) \cap \mathcal{C}(\omega_1, \mathbf{x})} A_{E_0}(\mathbf{s}, \mathbf{x}) A_{E_{\omega_1}}(\mathbf{x}, \mathbf{y}) A_{E_{\omega_2}}(\mathbf{y}, \mathbf{d}) n_e(\mathbf{x}) n_e(\mathbf{y}) d\mathbf{y} d\mathbf{x}.$$

This intersection is characterized by eqs. [7] and [8]. We still have to compute the differential form along the intersection and thus

$$||\partial_{\omega_1} y_\cap \wedge \partial_\varphi y_\cap||$$
for $x, d, s$ given. First, one can compute

$$\partial_x y = R_2 R_1 \left( \begin{array}{c} \sin \omega_1 \sin \varphi \\ \sin \omega_1 \cos \varphi \\ 0 \end{array} \right) + \partial_x r \left( \begin{array}{c} \sin \omega_1 \cos \varphi \\ \sin \omega_1 \sin \varphi \\ \cos \omega_1 \end{array} \right)$$

and

$$\partial_{\omega_1} y = R_2 R_1 \left( \begin{array}{c} \cos \omega_1 \cos \varphi \\ \cos \omega_1 \sin \varphi \\ -\sin \omega_1 \end{array} \right) + \partial_{\omega_1} r \left( \begin{array}{c} \sin \omega_1 \cos \varphi \\ \sin \omega_1 \sin \varphi \\ \cos \omega_1 \end{array} \right).$$

This leads to

$$\partial_x y \wedge \partial_{\omega_1} y = R_2 R_1 \left( \begin{array}{c} \sin^2 \omega_1 \cos \varphi \\ \sin^2 \omega_1 \sin \varphi \\ \cos \omega_1 \sin \omega_1 \end{array} \right) + r \left( \begin{array}{c} \sin \varphi \\ -\cos \varphi \\ 0 \end{array} \right)$$

$$+ \partial_{\omega_1} r \left( \begin{array}{c} -\cos \omega_1 \sin \omega_1 \cos \varphi \\ -\cos \omega_1 \sin \omega_1 \sin \varphi \\ \sin^2 \omega_1 \end{array} \right).$$

Since the rotation matrices do not change the norm, they can be ignored in the computation of the norm. After some computations, one gets

$$\| \partial_{\omega_1} y \wedge \partial_x y \| = r \sqrt{\sin^2 \omega_1 (r^2 + (\partial_{\omega_1} r)^2) + (\partial_x r)^2}$$

where

$$\partial_{\omega_1} r = (z_{\omega_1}) \left( 1 + \cot \omega_1 \frac{z_{\omega_1}}{\sqrt{1 - z_{\omega_1}^2}} \right) - \frac{\sin \omega_1}{\sin^2 \omega_1} \sqrt{1 - z_{\omega_1}^2}$$

$$\partial_x r = (z_{\varphi}) \left( 1 + \cot \omega_1 \frac{z_{\omega_1}}{\sqrt{1 - z_{\omega_1}^2}} \right)$$

in which

$$(z_{\omega_1}) = R_1 (3, 1) \cos \omega_1 \cos \varphi + R_1 (3, 2) \cos \omega_1 \sin \varphi - R_1 (3, 3) \sin \omega_1$$

$$(z_{\varphi}) = R_1 (3, 2) \sin \omega_1 \cos \varphi - R_1 (3, 1) \sin \omega_1 \sin \varphi.$$
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$n_e$ must be considered in $C^\infty$. We, however, use a first result on the continuity of our operator $T$ in $L_2$.

**Theorem 4.1.** For $s$ and $d$ fixed, the spindle tori $\Xi(\omega, s, d)$ are one-to-one with $\mathbb{R}^3 \setminus \{s + t(d - s), t \in \mathbb{R}\}$.

**Proof.** First, we discard the degenerate case of the spindle torus which occurs when $\omega = 0$ (there is no scattering event, only primary radiation) and corresponds to the line $\{s + t(d - s), t \in \mathbb{R}\}$.

The parameter representation of the spindle torus is given by

$$\Xi(\omega, s, d) = \left\{ \textbf{x} = s + \|d - s\| \frac{\sin(\omega - \alpha)}{\sin \omega} R_2 \begin{pmatrix} \sin \alpha \cos \beta \\ \sin \alpha \sin \beta \\ \cos \alpha \end{pmatrix} : \alpha \in [0, \omega], \beta \in [0, 2\pi] \right\}$$

with $p = \cot \omega$ and $R_2$ the rotation matrix which maps $e_z = (0, 0, 1)^T$ into $\frac{d - s}{\|d - s\|}$. For $s$ and $d$ fixed, it is clear that $R_2 \begin{pmatrix} \sin \alpha \cos \beta \\ \sin \alpha \sin \beta \\ \cos \alpha \end{pmatrix}$ is one-to-one with the unit sphere. This is why each $\textbf{x} \in \mathbb{R}^3$ corresponds to only one pair $(\alpha, \beta)$. Now, since $\frac{\sin(\omega - \alpha)}{\sin \omega}$ is defined for $\omega > \alpha$, the norm of the vector $\textbf{x} - s$ is a bijective function on $\omega$.

Therefore, the spindle torus parametrized by $(\omega, \alpha, \beta)$ is one-to-one with $\mathbb{R}^3 \setminus \{s + t(d - s), t \in \mathbb{R}\}$. \qed

**Theorem 4.2.** Denoting by $T_d$, the restriction of $T$ to one detector $d$ and a given source $s$, then

$$T_d : L_2(\Omega) \rightarrow L_2(\mathbb{R}).$$

is continuous.

**Proof.** From [31], we know that

$$T n_e(p, v) = \int_0^{2\pi} \int_0^\omega w_e(y(p, \alpha, \beta); p, v)n_e(y(p, \alpha, \beta))J(p, \alpha, \beta)d\alpha d\beta$$

with $p = \cot \omega$, $v = d - s$ and $J$ the appropriate Jacobian given in [31]. Using the Cauchy-Schwarz inequality, one gets

$$|T n_e(p, v)|^2 \leq \int_0^{2\pi} \int_0^\omega (w_e(y(p, \alpha, \beta); p, v))^2 \chi_\Omega(\alpha, \beta)J(p, \alpha, \beta)d\alpha d\beta \cdot \int_0^{2\pi} \int_0^\omega (n_e(y(p, \alpha, \beta)))^2 J(p, \alpha, \beta)d\alpha d\beta$$

in which $\chi_\Omega$ stands for a smooth cut-off. Taking now the $L_2$ norm yields

$$\|T n_e\|_{L_2} \leq c \int_\mathbb{R} \int_0^{2\pi} \int_0^\omega (n_e(y(p, \alpha, \beta)))^2 J(p, \alpha, \beta)d\alpha d\beta dp$$

with

$$c = \int_\mathbb{R} \int_0^{2\pi} \int_0^\omega (w_e(y(p, \alpha, \beta); p, v))^2 \chi_\Omega(\alpha, \beta)J(p, \alpha, \beta)d\alpha d\beta dp$$
which is well-defined as the integrand is a compactly supported smooth function. Due to Theorem 4.1 and since the discarded line passing through \( s \) and \( d \) is negligible regarding the Lebesgue measure, one can finally apply the mapping \((p, \alpha, \beta) \mapsto x\) and gets
\[
\|T_{n_e}\|_{L^2}^2 \leq c \int_{\Omega} (n_e(x))^2 \, dx = c \|n_e\|_{L^2}^2.
\]

For our approach, the operator \( T \) has two main drawbacks: (i) it is non-linear in \( n_e \) as the physical factors, \( w_c \), depends on \( n_e \); (ii) the properties of Fourier integral operators cannot apply if the weight function and thus \( n_e \) are not \( C^\infty \) smooth. To circumvent these difficulties, we propose for this study to decorrelate the dependence of the weight \( w_c \) \( \text{w.r.t.} \) \( n_e \) with the integrand itself. At this purpose, we assume that \( n_e \) is \( C^\infty \) smooth and that there exists a function \( f \in L^2(\Omega) \) such that
\[
\|f - n_e\|_{L^2(\Omega)} \leq \epsilon \ll 1.
\]

Thanks to the continuity of the operator shown in Theorem 4.2, the spectral data \( g_1 \) can thus be seen as an approximation of
\[
T(f, n_e)(p, v) = \int_{\Omega} W_{n_e}(x, p, v) f(x) \delta(p - \phi(x, v)) \, dx
\]
with \( W \) the operator acting on the electron density and standing for the physical factors. For our study, the edges (high-variations) of the electron density \( n_e \) will be carried by the function \( f \) and we will consider the operator \( T(\cdot, n_e) \) instead of \( T \). Now we have the operator in a correct shape and we can recall some results from the theory on Fourier integral operators, see [35, 22].

**Definition 4.3** ([22]). Let \( Y \subset \mathbb{R}^m \) and \( X \subset \mathbb{R}^n \) be open subsets. A real valued function \( \phi \in C^\infty(Y \times X \times \mathbb{R}^N \setminus \{0\}) \) is called a phase function if
- \( \phi \) is positive homogeneous of degree 1 in \( \xi \), i.e. \( \phi(y, x, r\xi) = r\phi(y, x, \xi) \) for all \( r > 0 \).
- \( (\partial_y \phi, \partial_x \phi) \) and \( (\partial_x \phi, \partial_\xi \phi) \) do not vanish for all \( (y, x, \xi) \in Y \times X \times \mathbb{R}^N \setminus \{0\} \).

A Fourier integral operator \( \mathcal{P} \) is then defined as
\[
\mathcal{P}u(y) = \int e^{i\phi(y,x,\xi)} a(y,x,\xi) u(x) dx d\xi
\]
where the symbol/amplitude \( a(\cdot) \in C^\infty(Y \times X \times \mathbb{R}^N) \) and it satisfies:
For every compact set \( K \subset Y \times X \) and for every multi-index \( \alpha, \beta, \gamma \), there is a constant \( C \) such that
\[
|\partial^\alpha_y \partial^\beta_x \partial^\gamma_\xi a(y, x, \xi)| \leq C(1 + \|\xi\|)^{m-|\alpha|} \quad \forall \ x, y \in K \text{ and } \forall \ \xi \in \mathbb{R}^N.
\]

We write then that \( a \in S^m(Y \times X \times \mathbb{R}^N) \).

**Theorem 4.4** ([35]). Given a FIO \( \mathcal{P} \) with symbol \( a(\cdot) \in S^m(Y \times X \times \mathbb{R}^N) \)
then \( \mathcal{P} \) is a FIO of order \( m \) and maps continuously the Sobolev spaces \( H^s(X) \) into \( H^{s-m}_{loc}(Y) \) for every \( s \in \mathbb{R} \).
Corollary 4.5. Let \( n_e \in C^\infty(\Omega) \) given with \( \Omega \) an open subset of \( \mathbb{R}^3 \). Then the operator \( T(\cdot, n_e) : H^s(\Omega) \to H^{s+1}_{\text{loc}}(\mathbb{R} \times \mathbb{V}) \) is a continuous Fourier integral operator of order \(-1\).

Proof. The proof here is inspired from [18]. Using the Fourier representation of the Dirac distribution, one gets

\[
T(f, n_e)(p, \nu) = \frac{1}{\sqrt{2\pi}} \int_{\Omega} \int_{\mathbb{R}} \mathcal{W} n_e(x, p, \nu) f(x) e^{-i\sigma(p - \phi(x, \nu))} \, d\sigma dx.
\]

Defining the phase

\[ \Phi(p, \nu, x, \sigma) = \sigma(p - \phi(x, \nu)), \]

one needs to prove that \((\partial_{p, \nu} \Phi, \partial_{\sigma} \Phi)\) and \((\partial_x \Phi, \partial_{\nu} \Phi)\) do not vanish for all \((p, \nu, x, \sigma) \in \mathbb{R} \times \mathbb{V} \times \Omega \times \mathbb{R} \setminus \{0\}\). It is clear that

\[ \partial_{\sigma} \Phi = (p - \phi(x, \nu))d\sigma \quad \text{and} \quad \partial_{p, \nu} \Phi = \sigma(dp - \partial_{\nu} \phi(x, \nu)d\nu). \]

The second term is never zero, so \((\partial_{p, \nu} \Phi, \partial_{\sigma} \Phi)\) does not vanish. Also, setting \( y = x - s \) and \( \nu = r_c \theta_c \), one can prove that

\[
\nabla_y \phi(y, \nu) = \frac{\kappa(y)}{(1 - \lambda^2(y))^{3/2}} \left( \kappa(y) - \frac{\|y\|}{r_c} \right) \nabla_y \kappa(y) + \frac{\left( \nabla_y \kappa(y) - \frac{y}{\|y\| r_c} \right)}{\sqrt{1 - \lambda^2(y)}} \nabla_x \kappa(y)
\]

with

\[ \kappa(y) = \frac{y \cdot \theta_c}{\|y\|} \quad \text{and} \quad \nabla_x \kappa(y) = \|y\|^{-1} \left( \theta_v - \frac{\kappa(y) y}{\|y\|} \right). \]

The gradient of the phase is thus the sum of two vectors each one collinear with \( y \) and \( \theta_v \) respectively. Important cases here show up, first \( y \) must be different from \( 0 \), which means \( x \neq s \). This is naturally excluded by taking the source outside \( \Omega \). Then, comes the case \( \kappa(y) = 1 \), which means \( y \) and \( \theta_v \) are collinear. It corresponds to the spindle torus degenerating into the straight line \( s \) to \( d \) (no scattering only primary radiation). This case is also excluded since \( \omega > 0 \) strictly or equivalently \( p \neq \infty \). Since \( y \) and \( \theta_v \) cannot be collinear, the gradient \( \nabla_y \phi(y, \nu) \) is never zero and therefore, \( T(\cdot, n_e) \) is a FIO.

Due to the smoothness properties of the electron density, \( \mathcal{W} n_e \in C^\infty \) and is thus a symbol of order 0. Given Theorem 4.4 and that \((\partial_{p, \nu} \Phi, \partial_{\sigma} \Phi)\) and \((\partial_x \phi, \partial_{\nu} \phi)\) do not vanish, \( T(\cdot, n_e) \) is thus a FIO of order

\[ m = \frac{1}{2} - \frac{3 + 3}{4} = -1 \]

and therefore maps continuously \( H^s(\Omega) \) into \( H^{s+1}_{\text{loc}}(\mathbb{R} \times \mathbb{V}) \) where \( \mathbb{V} \) denotes the domain of definition of \( d - s \).

Corollary 4.6. Let \( n_e \in C^\infty(\Omega) \) given with \( \Omega \) an open subset of \( \mathbb{R}^3 \). Then, the scattered radiation of order 2 can be understood as a continuous mapping between \( H^s(\Omega) \) and \( H^{s+7/4}_{\text{loc}}(\mathbb{R}^+ \times \mathbb{V}) \) if the phase function

\[ \Psi(y, x, d) := \psi(y, x) + \cos(\cot^{-1} \phi(y, x, d)) \]

satisfies \((\nabla_x \Psi, \nabla_y \Psi) \neq 0\).
Proof. In order to write the second scattering data $g_2$ as a FIO, one needs to find the corresponding phase function of the intersection between the cone and the spindle torus. The phase is delivered by our condition on the scattering angles and the energy derived from the Compton formula eq. [7]. It yields

$$\psi(y, x) + \cos \left( \cot^{-1} \phi(y, x, v) \right) = \lambda(E_d) = \psi(y, x, v) \in \mathbb{R}^+. $$

$\Psi$ inherits essentially the properties of phase of $\psi$ and of $\phi$ as $\lambda$ is monotone w.r.t the energy. Although it can be empirically checked, it is unclear when $(\nabla_x \Psi, \nabla_y \Psi) \neq 0$ analytically, this is why this is assumed here. With this symbolism, $g_2$ can be understood as an approximation of the operator

$$S(f, n_c)(\lambda, v) = \int_{\Omega_1} \int_{\Omega_2} w_2(s, x, y, v)f(x)f(y)\delta(\lambda - \Psi(y, x, v))dydx.$$ 

The case $x = y$ is discarded as it corresponds for the torus to a singularity that shows up in the definition of the phase $\phi$ (it was the case $s = x$ for the first scattering). Physically, this case cannot occur as it would imply that the same local point is responsible for two successive scattering events which is impossible. To interpret this as a FIO, we embed the variable $(y, x)$ into $z \in \Omega_2 := \{(y, x) \in \Omega \setminus \mathcal{N}(x) \times \Omega\}$, with $\mathcal{N}(x)$ denoting a small neighborhood around $x$. Taking $\bar{f}(z) = f(x)f(y)$, it yields

$$S_2(\bar{f}, n_c)(\lambda, v) = \int_{\Omega_2} \tilde{w}_2(s, z, v)\bar{f}(z)\delta(\lambda - \bar{\Psi}(z, v))dz$$

$$= \int_{\Omega_2} \int_{\mathbb{R}} \tilde{w}_2(s, z, v)\bar{f}(z)e^{-i\sigma(\lambda - \bar{\Psi}(z, v))}d\sigma dz$$

with $\tilde{w}_2$ and $\bar{\Psi}$ the appropriate embedded version of $w_2$ and $\Psi$. Given Theorem 4.4 and assuming the properties of phase of $\bar{\Psi}$, $S_2$ is a FIO of order

$$m = \frac{1}{2} - \frac{6 + 3}{4} = \frac{-7}{4}$$

which ends the proof. \qed

Remark 4.7. The assumption that $(\nabla_x \Psi, \nabla_y \Psi) \neq 0$ is in fact almost always satisfied. Indeed, the computation of $\nabla_y \Psi$ is a linear combination of three vectors $x - s$, $y - x$ and $d - x$. Since the degenerated cases for the cone, $x - s$ and $y - x$ collinear, and for the spindle torus, $y - x$ and $d - x$ collinear, are excluded, there are two possibilities: either these three vectors are linearly independent, then $\Psi$ inherits the property of phase of $\phi$ ($(\nabla_x \Psi, \nabla_y \Psi) \neq 0$), or they belong to the same plane. In the latter case, the analysis is unclear. The desired property can however be checked empirically.

By analogy, the scattering of order $k$ ($k > 2$) will rely on the relation

$$\sum_{i=1}^{k} \cos \omega_i = k - mc^2 \left( \frac{1}{E_d} - \frac{1}{E_0} \right)$$

with $\omega_i$ the $i^{th}$ scattering angle. Unfortunately, the geometry of the scattering events becomes harder to model or even to implement. However, we expect the principle we developed for the second scattering to extend to higher orders since each additional scattering will add a new layer of intermediary sources. This extension is expressed in the following statement.
**Hypothesis 4.8.** When focusing on the Compton scattering, the measured spectrum can be decomposed into the different scattered radiation of $i^{th}$ order,

$$\text{Spec}(d, E) = \sum_{i=1}^{\infty} g_i(d, E)$$

with $g_i$ approximating the operator $T_i(\cdot, n_e)$ which maps continuously

$$H^s(\Omega) \mapsto H^{s+(3i+1)/4}_{\text{loc}}(\text{dom}(E) \times \forall).$$

Intuitively, the more scattering events, the smoother the corresponding part within the spectrum is.

**Theorem 4.9.** Assuming the attenuation factors to be known and $f \in L_2(\Omega)$ to be a sharp version of the smooth electron density $n_e$, the reconstruction operator $T_b^* \delta_p$ with the backprojection operator

$$T_b^* g(x) = \int_{\forall} (Wn_e(x, \phi(x, v), v))^{-1} h(x, v) g(\phi(x, v), v) dv$$

maps the spectrum $\text{Spec}$ onto $f$ up to an error $\epsilon \in H_{\text{loc}}^{3/4}(\Omega)$.

**Proof.** The result follows on from the smoothness properties given above and from [31]. The reconstruction operator recovers $f$ up to a $C^\infty$-smooth function and acts as a FIO of order 1 on the second scattering data $g_2 \in H^{7/4}$ which is compactly supported when considering the energy $E$ as variable instead of $p$.

Since the error $\epsilon$ produced by the reconstruction technique is smoother than $f$, it is possible to extract accurately the contours (jumps) of $f$ by applying suited operators (gradient, laplacian, wavelets, etc).

**Remark 4.10.** Following from [31], the weight (and thus here the attenuation factors) needs to be known to recover $f$ and not a weighted version. In practice, a rough approximation of the weight is sufficient to recover the contours of $f$ but the analysis of the reconstruction operator with inexact weights will be performed in future research.

## 5. Simulation results

In this section, we provide simulation results for the configuration (b) in Figure 4. As explained in [31], this configuration has the advantage to minimize the acquisition time (in comparison with the configuration (a)) while delivering data without limited angle issues (in comparison with (c) and (d)). However, this latter point will depend on the resolution of the detector. For this paper, we assumed that the detector has a continuous energy resolution. In practice, a fixed energy resolution will alter the accuracy of our integral representation for the back-scattered photons ($\omega > \pi/2$) leading to inconsistent data and thus limited data artifacts. This aspect constitutes the next step of our future research.

A slice of the scanner is depicted in Figure 6. The monochromatic source, emitting at $E_0 = 140$ keV, is fixed and located under the object while the detectors are located on a sphere (the half-circle on the slice) of diameter equal to 40 cm. Each detector is a disk of 2mm of radius. The volume to reconstruct is represented by a
cube in the middle of 10x10x10cm$^3$. We consider that the source has emitted $10^{12}$ photons; a sufficient amount in order to limit the Poisson noise in the Monte-Carlo data.

The electron density map is scaled on the value of the water, $3.23 \cdot 10^{23}$ electrons per cm$^{-3}$, noted $n_w$.

5.1. Comparison with Monte-Carlo data

We first compare our model of the spectrum for first- and second-order scattering with ground truth data obtained by Monte-Carlo simulation. To view the response of the different operators, we consider the well-known point spread function. In order to validate, the modeling of the second scattering, two points (small spheres of radius 2mm) are considered. Figure 6 displays the different results for one arc of detectors (the complete dataset is obtained for detectors along the complete sphere). Analytic data (middle column) are compared with ground truth data (right column). The first row shows the part of the first-scattering within the spectrum, $g_1$, the second row the part of the second scattering $g_2$, and the third row the spectrum (neglecting higher-order scattering) $g_1 + g_2$. The analytic spectrum and the different parts match with the realistic spectrum. One can observe some variations in the intensities which arise from the discretization of the modeling. In particular, for the Monte-Carlo simulations, the detector is no more a point but a disk of size 4mm and the detection of the energy is made on a range of energy $E \pm \Delta E$ and not a single value $E$. Here $\Delta E$ is set 0.25 keV. Combined together, the modeling is altered since we do not integrate over spindle torus (or over the intersection with the cone for $g_2$) but over a strip around the spindle torus. However, the analytical modeling is revealed to appropriately model the spectrum as shown by the reconstructions in the next paragraph.

5.2. Contour Reconstruction

We now provide the reconstructions and contour extractions for a toy object following on from the reconstruction strategy developed before. The object is a composition of spheres with electron densities $\{0, 1, 1.5, 2, 3\} \times n_w$ compactly supported in a cube of dimension 10x10x10cm$^3$.

The spectrum and its decomposition are depicted in Figure 7. The reconstructions are displayed in Figure 8. As anticipated, the application of the filtered back-projection type algorithm does not provide a satisfactory reconstruction of the object. This is essentially due to the physical factors which alter substantially the integral kernel. They produce smooth artifacts, noted $\mathcal{E}f$ in the reconstruction scheme, quite strong. By analogy with the attenuated Radon transform [32], the ill-conditioning of the reconstruction problem should increase exponentially with the intensity of the electron density which is observed in practice. The values of the electron density considered here as well as the variation of the physical factors are thus substantially amplified by the reconstruction strategy.

However, the extraction of the contours, Figure 9, enables a better visualization of the features of the object. Here, we simply take the gradient of the reconstructions from Figure 8 but more sophisticated techniques could be applied. The second column displays the contours obtained from the analytical data for $g_1$. In this case, the contours are well-recovered. However, we can observe some artifacts arising from the variations of the physical factors. These artifacts turn out more prominent for
Monte-Carlo data in the third and fourth columns. These can be explained by the smoothing effect of the acquisition, giving that the modeling itself is in reality not the torus but a strip around the torus giving smoother behaviour of the measurement than for the analytical modeling. Thence, the contours are smoothed making the artifacts more visible. Furthermore, as developed in this paper, the contours are encoded and preserved by the first-order scattered radiation and can be recovered even when considering the second-order scattering (fourth column). The key point here is that the second scattering is smoother than the first scattering. Consequently, the second derivative $\partial^2 p$ in the reconstruction scheme, highlights the variations of $g_1$ over $g_2$ and leads to a reconstruction almost not hindered by the second scattering. We expect the same behaviour for higher-ordered scattered radiation in the spectrum.

Due to the computation time of the data and of the Monte-Carlo simulations,
Figure 7. Different parts of the spectrum from the electron density $n_e$ depicted in Figure 8: top left: implementation of the integral representation of $g_1$; top right: corresponding Monte-Carlo data $g_{MC}^1$; bottom left: $g_{MC}^2$ obtained by Monte-Carlo simulation; bottom right: $g_{MC}^1 + g_{MC}^2$.

we restricted the sampling of our toy object to 80x80x80 voxels which is small for recovering contours. We expect sharper reconstructions of the edges and less prominent artifacts for higher resolution of the data.

6. Conclusion

In conclusion, we proved and tested that the contours of the object of interest are encoded essentially in the first-scattering within the spectrum. Sufficiently smooth, the rest of the spectrum (here only the second scattering was considered) does not hinder the extraction of the contours by a filtered back-projection type reconstruction formula. Even though, the method is sensitive to the variation of the physical factors, it constitutes an interesting and fast to implement first step to reverse the spectrum and/or provide initial conditions to more complex and expensive algorithms. Such algorithms will be the focus of our future research.

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Figure 8. first column: original electron density; Columns 2 to 4: Reconstruction from $g_1$, $g_{\text{MC}}^1$ and $g_{\text{MC}}^1 + g_{\text{MC}}^2$ respectively.

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| Contours reconstruction from | Original $n_e$ | Synthetic data 1st scattering | Monte-Carlo 1st scattering | Monte-Carlo 1st+2nd scattering |
|-----------------------------|----------------|-----------------------------|---------------------------|-----------------------------|
| Slice yOz                   |                |                             |                           |                             |
| Slice xOz                   |                |                             |                           |                             |
| Slice xOy                   |                |                             |                           |                             |

Figure 9. Corresponding gradients to the reconstructions in Figure 8.

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