A Regularization Method for Unfolding the Measured Data of Different X-ray Spectrometers in Compton Scattering Tomography

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Radiation imaging techniques are important tools in many fields of basic and applied sciences, from medical analyses to industrial applications. In addition to the conventional photon transmission tomography, methods based on the Compton scattering and X-ray diffraction have been developed in the last ten years. In this paper, we discuss some inverse problems relevant to the image recovering of scattering and diffraction tomography. In particular, the problem of recovering the X-ray spectrum from measured data is discussed in detail and it is shown that the original signal from both NaI(Tl) and HP-Ge spectrometers characterized by very different energy resolution, can be uniquely reconstructed.

I. INTRODUCTION

Nondestructive testing and evaluation techniques play an increasing important role in many fields of scientific and technological activities, from diagnostics in medicine to detection of defects in composite materials or analysis of concrete structure components. The traditional radiation imaging relies on the use of transmitted photons, such as in radiography and computed tomography, but its application is limited in time and space. Mainly for extended systems the conventional transmission tomography is not well suited and the possibility of utilizing Compton scattering in imaging applications has been investigated by a number of authors ^{1,2,3}.

In Compton interaction tomography the reflected or backscattered radiation from the interior of an extended object is measured in order to achieve a three-dimensional image of it. Photon source and detector do not have to be placed at the opposite sides of the object or body to be examined. Moreover, the physical principles of Compton interaction between incident electromagnetic radiation and matter are well known and the Compton scattering process dominates in most materials in the range of X and γ radiation originating from radioisotopes, namely below a few hundreds of keV, thus allowing the imaging of a wide range of materials and biological structures using readily available radioisotopic sources.

The modern gamma-ray spectroscopy dates back to the early '50s with the introduction of thallium-activated sodium iodide as a scintillation material for detectors, thus providing both high efficiency and sufficiently good energy res-

olution. In more recent years, solid-state detectors like the *Intrinsic* germanium (also called HPGe for *High Purity Germanium*) are became largely used for γ -ray spectroscopy. At the present, germanium detectors offer the highest resolution for γ -ray energies from tens of keV up to a 10 MeV. For the spectrum from the ^{251}Am , used as a sample test in this report, the difference in resolution with respect to the NaI detector is quite dramatic: at 59.54 keV the Ge resolution is about 0.6% while for NaI this value is about 20%. However HPGe detectors must be operated at low temperature and the need for cooling (liquid Nitrogen temperature) represents the principal drawback for medical and industrial applications.

Progress in using these techniques has suffered, apart from the basic problem of accounting for the radiation attenuation in the sample, for the complication represented by the image smearing associated with the finite response of the detector. In this report we present the results of a regularization technique applied to simulated data and realistic response function for both types of the detectors in order to develop a suitable method to be applied to the reconstruction of photon spectrum in a Compton tomography technique to evaluate the density variation in large object. It is shown that the proposed algorithm, based on the Tikonov-Phillips approach, might reproduce the same results, within the computer numerical accuracy, by unfolding the spectra measured by the detectors of high (HP-Ge) and poor (NaI(Tl)) intrinsic resolution.

II. THE X-RAY SPECTRUM INVERSE PROBLEM

A scattered photon reaching the X-ray spectrometer (detector), produces a signal whose pulse height is approximately proportional to the energy lost by the photon in the detector itself. Let $K(E, h)dh$ be the probability that a photon of incident energy, E , generates a pulse with height ranging in the interval $(h, h + dh)$; $K(E, h)$ is then called the *response function* of the detector.

Fig.1 Response functions of two different x-ray spectrometers, HP-Ge (right side) and NaI(Tl) (left side), respectively. The detailed structure of the HP-Ge response function is shown in the insert.

Typical response functions for high-resolution (semiconductor) and poor-resolution (scintillation) detectors are shown in fig.1, left and right side respectively. Both functions have been obtained by means of a suitable calibration procedure for the same incident photon energy, $E = 59.54$ keV. In these figures, the pulse height is scaled in energy units and the relevant scale set to reproduce at the rightmost peak (photopeak) the full energy of the incident photon. By this way, the pulsed height is a blurred measure of the energy lost by an incident photon entering the detector. Accordingly, the abscissa is labeled as *energy loss*.

As evident from fig.1, both the X-ray spectrometer functions are highly structured and there is a prominent photopeak corresponding to the deposition of all the incident photon energy. For the high-resolution detector (HPGe) the photopeak area is confined to a very small energy interval with *Full Width Half Maximum*, $\text{FWHM} \equiv 350$ eV at $E = 59.54$ keV, while in the NaI(Tl) case it is smeared over half the considered energy range ($\text{FWHM} \equiv 12$ keV). These figures show that a variable fraction of the whole response-function strength lies in the continuum region at low energy and in the additional peak arising from the escape of the fluorescent photon of the material itself. For the HP-Ge detector, this fraction amounts to a few percent — about 3% — of the response function; then, it is customary to approximate the whole response function by the photopeak area. On the contrary for the low-resolution detector, the escape peak is more evident, more than 15% of the response-function and can not be ignored. The spreading width of the response function of the poor-resolution NaI(Tl) detector is evident and makes the interpretation of a measured X-ray spectrum difficult with respect to an analogous one performed with a HP-Ge detector. Furthermore, due to the low resolution, a NaI(Tl) measurement requires a substantially larger statistics of detected photons and, therefore, very longer exposition times which are often impossible in real conditions (in clinical diagnostics, for instance). Both kind of detectors are commonly used in practice, depending on the needed resolution. However, the NaI(Tl) detector is always the most frequently used in many technological and biomedical applications because of its low cost, easy-to-use feasibility and transportation out of the laboratory, since calibration, stability of operation, etc., are easily achieved.

For an incident photon spectrum, $f(E)$, when $f(E)dE$ is the number of photons with energies between $[E, E + dE]$, a suitable detector with response function $K(E, h)$ produces a number of observed (detected) events given by $w(h)dh$ where the pulse height ranges in the interval $[h, h+dh]$, according to the following relation:

$$w(h) = \int_0^{E_{max}} K(E, h) f(E) dE + \epsilon(h), \quad (1)$$

where $\epsilon(h)$ is a unknown function representing the uncertainty in the measurement of $w(h)$, due to the error in photon statistics, the noise or other unpredictable phenomena; this function can assume both positive and negative values. The observed function, $w(h)$, is an energy loss spectrum which represents a raw estimate of the incident energy photon spectrum, $f(E)$. Since a single-photon detection event is commonly referred to as a *count*, function $w(h)$ is usually defined as a *continuous count spectrum*. It is an energy-loss spectrum from which the incident photon energy spectra, $f(E)$, have to be unfolded in order to reconstruct the true signal.

The adequacy of this estimate clearly depends on the intrinsic resolution of the adopted detector. As already mentioned, fig.1 presents the count spectrum

resulting from the measurement of a perfectly monoenergetic source. Whereas the HP-Ge response function might be assumed as a quite good approximation of the original signal, $f(E)$, this is not more true for the scintillation detector and unfolding $f(E)$ from the count spectrum is not a trivial problem.

In fact, eq.(1) is an integral equation of Fredholm type, and solving it for $f(E)$ is a classical example of inverse problem which is well-known to be ill-posed in the sense that its solution lacks both uniqueness and stability^{4,5}. These difficulties arise because the smoothing action of the response function and the experimental uncertainties both smear the information about the detailed structure of the original spectrum. From this point of view, the inverse problems represented by the two different detectors belong to the classes of slight ill-posed and severe ill-posed integral equations, respectively.

As for data from real spectrometers, the problem of ill-posedness is complicated from several factors: Firstly, the measured function, $w(h)$, is not continuous but is binned into various ranges of pulse heights referred as channels. Therefore, X-ray spectral data consist of a finite number, N , of integer quantities, n_i ,

$$n_i = \int_{h_i}^{h_{i+1}} w(h)dh, \quad (i = 1, \dots, N) \quad (2)$$

where the $N + 1$ values, h_i , correspond to the boundaries of the pulse height bins that define the N channels. Using eq.(1), eq.(2) can be rewritten in the form:

$$n_i = \int_0^{E_{max}} K(E, h_i) f(E) dE + \epsilon_i, \quad (i = 1, 2, \dots, N) \quad (3)$$

The number of bins, N , depends on the adopted energy channel width and is strictly related to the choice of the particular detector and to the time of the measurement (total fluency). Indeed, low energy resolution measurements requires long times of exposition, namely a high radiation dose delivered to the sample, or — as alternative — a large energy channel width in order to reduce the statistical uncertainty in the ϵ_i factor, i.e. to increase the smoothness of n_i .

In eq.(3) ϵ_i represents the channel uncertainty on the further assumption that it results from a random process with zero mean. The detector response function has been explicitated in terms of the channel height, h_i , accordingly to the fact that — due to geometrical effects — the profile of $K(E, h_i)$ kernel might strongly vary for different incident-photon energies. However, for the purpose of the present work, eq.(3) can be still simplified in the spectral energy range of practical interest (30–60 keV). In this interval, the detector response function can be considered energy independent in the first approximation, usually made in all the theoretical analyses, so that eq.(3) can be rewritten as a Fredholm's first-kind integral equation of the convolution type:

$$n_i = \int_{E_{min}}^{E_{max}} K(h_i - E_j) f(E_j) dE_j + \epsilon_i, \quad (i = 1, 2, \dots, N) \quad (4)$$

where E_j is the mid-point energy of each channel subdivision (in other words, it corresponds to the chosen energy sampling). It is worth noticing that solving eq.(4) instead of eq.(3) does not imply a loss of generality in the given problem. In fact, the regularizing algorithm adopted in the following can act to control possible instabilities in the solution due to an ill-condition inside the kernel itself^{6,7,8}.

III. SPECTRUM RECONSTRUCTION METHOD

The so-defined spectral reconstruction problem belongs to the class of inverse problems where the uniqueness and stability of the solution is related to the uncertainties of the count spectrum, $n(h)$, and to the kernel shape, $K(h, E)$. In order to evaluate the accuracy of the algorithm for the unfolding procedure discussed in the following section, we have introduced as a preliminary step a forward problem for both the detectors introduced in the previous section.

Our aim is, therefore, to estimate the expected value of a known spectral shape, $f(y)$, from a *measured* one, $g(x)$, obtained by convolving $f(y)$ with the high and low-resolution detector response function sampled at 100 and 1000 eV/channel, respectively. The different energy channel width were chosen to approximately meet the properties — FWHM — of each detector and to study the effectiveness of the algorithm to unfolding functions with high degrees of smoothness.

The photon-spectrum profile has been obtained by means of a Monte Carlo code^{9,10} developed for the simulation of energy spectra of inelastically (Compton) scattered X- and γ -rays, implemented to emulate experimental conditions frequently used to monitor variations in material composition and density in biomedical fields¹¹⁻¹⁸.

We adopt a particular regularization procedure based on the general approach developed by Tikhonov, Phillips and coworkers^{6,7,19}, starting from the following Volterra integral equation of first kind,

$$g(x) = K(x, u) \equiv \int_x^R k(x, y) f(y) dy, \quad (0 \leq x \leq R), \quad (5)$$

where the piecewise continuous kernel, $k(x, y)$, and the square sommable function, $f(x)$, are known. When the lower limit of integration is fixed, generally equal to zero, eq.(5) reduces to a Fredholm integral equation. Even in this case the classical method of solution based on the reduction to a corresponding differential equation cannot be always exploited since the observed $g(x)$ function is not exactly known from experiments and given over all the domain.

Assuming that the unknown function, $f(y)$, is piecewise continuous, eq.(5) can be converted into a well-posed variational problem by imposing suitable constraints on the boundary conditions of the solution^{6,7} which is then stable. One has to minimize the following functional in the class of square sommable functions:

$$U_\alpha(f, g) \equiv \int_0^R [k(x, y) f(y) - g(x)]^2 dx + \alpha^2 \int_0^R \left| \sum_{i=0}^n a_i f^{(i)}(y) \right|^2 dy. \quad (6)$$

The second term in the r.h.s. of eq.(6) is a regularizing functional^{6,7,19} which contains a linear combination of $f(y)$ and their derivatives, where some of the a_i ($a_i \in \mathbb{R}^+$) may be chosen equal to zero (generally, only one a_i coefficient is assumed different from zero and thus one speaks of zero-, first- or second-order regularization, etc.). Moreover, α , $\alpha > 0$, is a numerical parameter.

It can be shown⁷ that for any positive α value and any square sommable function, $g(x)$, there is a unique solution, $f_\alpha(y)$, yielding a minimum of eq.(6). This solution

is stable against perturbations on $g(x)$ and converges uniformly to the searched solution, $f(y)$, of eq.(5) when $\alpha \rightarrow 0$ and simultaneously the data error vanishes.

Therefore, the problem of solving eq.(5) is reduced to the equivalent but well-posed problem of finding a minimum for the functional (6), a task that can be easily accomplished by solving the relevant Euler equation⁷, which — in the case of second-order regularizing functional, for instance — reads as:

$$\int_0^y [\int_x^R k(x,y) k(x,z) f(z) dz - k(x,y) \tilde{f}(x)] dx + \alpha^2 \int_0^y f^{(2)}(x) dx = 0, \quad (7)$$

with suitable boundary conditions once a discretization procedure has been applied. Here, $f^{(2)}(x)$ is the second derivative of $f(x)$ and $\tilde{f}(x)$ is an approximation of $f(x)$ in the sense that

$$\int_0^R |f(x) - \tilde{f}(x)|^2 dx \leq \int_0^R \delta^2(x) dx = \Delta^2. \quad (8)$$

because of the experimental uncertainties.

It is worth remarking that the best value of the regularization parameter, α , depends on both the regularizing functional (6) and the uncertainties on the measured data, $\tilde{f}(x)$. In practice, α is determined by a numerical iteration procedure.

IV. NUMERICAL RESULTS

Fig. 2 show the results of convoluting the Monte Carlo simulations previously discussed, introduced in order to give an evaluation of the 'true' signal, with the detector response functions, for NaI(Tl) and HP-Ge detectors, respectively. It is worth noticing that the convolution procedure, the *Riemann sum* implies an additional numerical *unstructured* noise affecting the original signal.

Fig.2 Monte Carlo simulation of a Compton spectrum for photon of $E=59.54$ keV incident on a water cylinder at a scattering angle of $\theta = \pi/2$.

Numerical results obtained with the regularization procedure summarized in the previous section, are presented in Table I for the severely ill-posed problem represented by the deconvolution of the response function of the NaI(Tl) detector. Zero-, first- and second-order functional, $u^{(n)}$, have been adopted giving similar results on the whole. Second- and higher-order regularizations imply stronger correlations between neighboring function values than in the case of zero- or first-order ones. The U_α values, sum of the residual and the L_2 norm of regularizing functional times α , are given in Table I together with: (i) the percent error between the simulated and reconstructed function at the peak ($\Delta p\%$) as a measure of a good shape reconstruction; (ii) an indicator physical significance, *Total Scattering Fraction* (TS_F).

Table I — Results of the unfolding procedure for the NaI(Tl) response function as a function of the regularization parameter, α .

α	$u^{(0)}$			$u^{(1)}$			$u^{(2)}$		
	$\Delta p\%$	U_α	TS_F	$\Delta p\%$	U_α	TS_F	$\Delta p\%$	U_α	TS_F
$3 \cdot 10^{-5}$	46.19	3.53	0.80	46.95	3.12	0.81	47.06	2.93	0.82
$3 \cdot 10^{-6}$	29.98	1.35	0.80	34.94	1.64	0.80	38.30	1.93	0.81
$3 \cdot 10^{-7}$	11.52	0.33	0.77	17.01	0.53	0.77	22.82	0.84	0.78
$3 \cdot 10^{-8}$	3.28	0.15	0.76	6.48	0.16	0.76	10.07	0.26	0.76
$3 \cdot 10^{-9}$	7.03	0.17	0.76	9.94	0.16	0.76	4.54	0.15	0.76

The TS_F factor is an integral measure representing the percentage of the whole spectra in the physical important region centered around the peak resonance over the whole energy region. Usually the energy interval (*soft collimation*) used to calculate the TS_F factor (51-56 keV), is chosen to reduce the fraction of multiple scattered photons (MS) lying under the photopeak. The TS_F value of the 'true' signal is 0.76.

Fig. 3 shows some numerical results for α coefficients given in Table I. When $\alpha = 3.10^{-8}$, the reconstruction of the original signal is satisfactory and the errors — shown in the figure inserted at the top — are within acceptable limits comparable with the introduced (experimental and numerical) uncertainties.

As a further check of the proposed algorithm, the deconvolution problem for the HP-Ge detector has been solved in analogous manner and the results shown in fig. 4 present again satisfactory agreement with the Monte Carlo simulation of the 'true' signal independently of the adopted order of regularization, as it may be expected because of the weak ill-posedness of the particular problem.

V. CONCLUDING REMARKS

In the medical and industrial diagnostics, γ - or X-ray energy ranges from about 30 keV to 150 keV and for materials with low to intermediate atomic numbers, Compton scattering is by far the dominant interaction mechanism in the matter. This fact has led many Authors¹¹⁻¹⁸ to explore the possibility of imaging directly the energy-dispersive properties of Compton-scattered radiation.

Considering that a Compton scattering imaging is very attractive because of the free choice of measurement geometry, back-scattering included, the possibility of improving the image resolution by using the regularization techniques discussed in the previous sections is very promising. The preliminary tests discussed in the previous sections indicate that a simple regularizing procedure can effectively deal with both slight and severe ill-posed integral equations of convolution type.

Figs.3-4 Deconvolution of the response function of the NaI(Tl) (left) and HP-Ge (right) detectors, respectively, in comparison with the Monte Carlo simulated spectrum, for the first order of regularization.

The original image can be thus reconstructed once the detector response function — the kernel function in eq.(5) — is known. Other realistic cases corresponding to effective Compton tomography measurements are under study²⁰ and preliminary attempts to evaluate the multiple scattering contamination on Compton electron-density measurements are in progress, based on the same regularization technique.

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