PHYSICAL REVIEW

LETTERS

VOLUME 61

11 JULY 1988

NUMBER 2

Contours of Constant Scattering Angle

A. L. Hanson, ⁽¹⁾ G. E. Gigante, ⁽²⁾ and M. Meron ⁽¹⁾ ⁽¹⁾Brookhaven National Laboratory, Upton, New York 11973 ⁽²⁾Physics Department, University of Rome, Rome, Italy (Received 6 November 1987)

Traditionally, radiation-scattering experiments are conceived in terms of cylindrical geometry where the symmetry axis is the line between the source and the target. When the target becomes extended, as is the case in many real-life measurements, the analysis or the prediction of spectra becomes difficult. By definition of the axis of symmetry as being between the source and the detector, the extended target can be described in toroidal geometry with the surface of each toroid being a contour of constant scattering angle. With the scattering cross section constant over each contour, the calculation of total scattering intensities is greatly simplified.

PACS numbers: 03.80.+r, 07.85.+n, 32.80.Cy

The choice of proper geometry is crucial for the analysis of radiation scattering, the scattering being angle dependent. Traditionally the geometry of choice, for either analysis of data or prediction of spectra, is cylindrical with the source-target line serving as the symmetry axis. While being the most appropriate geometry when we deal with point targets, it loses its usefulness when the target is extended since now the target lacks a well-defined symmetry. This is the most common case in real-life measurements.

It turns out that some of the problems arising from extended targets can be circumvented by definition of the line between the radiation source and the detector as the main axis of symmetry. The scattering geometry relative to this axis is then best defined in terms of contours of constant scattering angle. These contours are meaningful regardless of the shape and extent of the target. Use of them can greatly simplify the formidable geometrical problems traditionally encountered in the analysis of scattering by distributed targets. Moreover, since they offer a new, and in many cases more general view of the scattering geometry, these contours can be extremely helpful in the determination and optimization of appropriate experimental geometries. In this Letter the geometrical properties of these contours are derived and discussed in the context of electromagnetic radiation scattering. It should be borne in mind, however, that, being defined by the scattering geometry alone, the contours of constant scattering angle can be applied equally well to any scattering process.

The coherent scattering of photons by bound electrons does not result in a change of either the phase or energy of the photon. The only angular dependence then is embedded in the scattering cross section. For kiloelectronvolt photons, the coherent scattering is strongly forward directed. In contrast, the incoherent scattering of photons by bound electrons results in a change of the phase and usually the energy of the photons. For the case of incoherent scattering, not only is the cross section angle dependent, but the magnitude of the change in energy is also angle dependent. This incoherent scattering is many times referred to as Compton or inelastic scattering.

Analysis of spectra resulting from the Compton scattering is compounded by an inherent width of the Compton-scattered x rays. This width results from a convolution of the "Compton profile" with geometrical effects. The Compton profile reflects the energy spread caused by the distribution of momenta of the bound electrons with respect to the initial photon. The geometry of the system can affect the width since the energy of the

© 1988 The American Physical Society

scattered photon depends on the scattering angle. For most experimental systems, acceptance of larger solid angles means acceptance of larger spreads in the energy of the incoherently scattered photons. To first order, the spread in energy, ΔE , about the mean Comptonscattering energy of E, resulting from the acceptance angle $\Delta \theta$ about θ , is

$$\frac{\Delta E}{E_0} = \frac{(e_0/m_0c^2)\sin\theta\Delta\theta}{[1 + (E_0/m_0c^2)(1 - \cos\theta)]^2}.$$
 (1)

Understanding of spectral peaks from coherently and incoherently scattered photons is important in many areas of physics. The measurement of the intensity of scattered radiation is being used as an analytical technique in materials sciences for characterization purposes¹ and in medical physics for bone-mineral and tissue-density determinations.^{2,3} Measurement of the width of the incoherently scattered radiation has become an important technique in materials science which is known as Compton profile measurements.⁴⁻⁷ Adequate modeling of the scattered radiation is essential to the understanding of the background in x-ray and γ -ray spectroscopy.

Figure 1 shows the proposed geometry. Both the source and the detector are assumed to be points. If we define coordinates so that the source and the detector are on the Z axis, we have cylindrical symmetry about the Z axis. For any given r, the value of θ will be constant as we rotate about the Z axis. If we normalize r and z to b, the angle θ can be related to r/b and z/b as

$$\tan\theta = \frac{r/b}{(z/b)(1-z/b) - (r/b)^2}.$$
 (2)

This can be written as the equation of a circle:

$$(r/b + 1/2\tan\theta)^2 + (z/b - \frac{1}{2})^2 = (1/2\sin\theta)^2.$$
 (3)

The circle is centered about $r/b = 1/2 \tan \theta$, $z/b = \frac{1}{2}$ with a radius of $1/2 \sin \theta$. For any angle θ we can now calculate contours, in r/b and z/b, of constant scattering angles. Figure 2 shows plots of the contours as functions of r/b and z/b. Since we have cylindrical symmetry about the Z axis the three-dimensional contours are toroidal. The contour for $\theta = 90^{\circ}$ is a sphere centered on the Z





axis at the midpoint between the source and the detector.

The intensity of the coherently scattered x rays from a distributed source, normalized to the total number of incident x rays can be determined from the integral

$$I_{E_0, \text{coh}} = \int_V \epsilon(E_0, E_0) g\left(\frac{r}{b}, \frac{z}{b}\right) \frac{d\sigma_{\text{coh}}}{d\Omega} dV, \qquad (4)$$

where $\epsilon(E_0, E_0)$, is the efficiency, g(r/b, z/b) is the geometry function, $d\sigma_{\rm coh}/d\Omega$ is the differential coherent scattering cross section for an x ray with an incident energy E_0 ,⁸ and V is the volume of the scatterer. In contrast to coherent scattering, incoherent scattering results in an energy distribution of the scattered x rays. The normalized intensity distribution (in energy) of the incoherently scattered x rays can be determined from the integral

$$J_{E_0,\text{incoh}}(E) = \int_{V} \epsilon(E_0, E) g\left(\frac{r}{b}, \frac{z}{b}\right) \frac{d^2 \sigma_{\text{incoh}}}{dE \, d \, \Omega} \, dV, \quad (5)$$

where $d^2 \sigma_{incoh}/dE d\Omega$ is the double-differential scattering cross section⁹ for incoherent scattering. The doubledifferential scattering cross section includes the probability of scattering of a photon of energy E_0 into E. Both the coherent and incoherent cross sections depend on the Z of the scatterer, the energy of the photon, and the angle of scatter. The volume, V, of the scatterer and the placement of it with respect to the contours of Fig. 2 determine how many contours lines are subtended. By our representing V in toroidal coordinates the integrals (4) and (5) are greatly simplified, since $d\sigma_{coh}/d\Omega$ and $d^2\sigma_{incoh}/dE d\Omega$ become constants over each contour.

The geometry function is the product of the solid an-



FIG. 2. Contours of constant scattering angle as a function of r/b and z/b. The label for each contour is in degrees.

gles subtended by the source and the detector (for nonpoint sources and detectors). If A_d is the area of the detector, A_s is the area of the source, d is the distance from the scatterer to either source or the detector, and ais the angle from the scatterer to the axis of respective aperture, then as long as $A \ll d^2$, g(r/b, z/b) can be approximated as

$$g\left(\frac{r}{b}, \frac{z}{b}\right) = \frac{A_d A_s}{16\pi^2} \frac{\cos\alpha_s \cos\alpha_d}{d_s^2 d_d^2}.$$
 (6)

Even though r/b and z/b are independent variables, if we select a constant scattering angle, then r/b and z/b will be related through Eq. (3).

The contours will be useful in the selection or in the attempt to understand a particular geometry not only for the analytical techniques previously mentioned, but also for measurements of scattering cross sections and for determination of geometrical effects. By our determining the dimensions of the sample with respect to r/b and z/b, Fig. 2 and Eq. (2) can be used to determine $\Delta\theta$ subtended by the sample. This aspect is important since $\Delta\theta$ is influenced not only by the width of the beam, but also by the thickness of the target being sampled. By writing the angle-dependent formula for the energy of the scattered photon or ion, we can now analytically determine the geometrical effects on the energy distribution of the scattered species $(d^2E/dr dz)$.

As far as Compton profile measurements are concerned, this work also tells us that by fabricating the sample properly, we can make physically large, curved samples while subtending small $\Delta \theta$'s. Fabrication of large samples is important in Compton profile measurements made with radioactive sources^{5,10} since counting statistics often limits Compton profile investigations. However, even for high-intensity sources, such as electron synchrotron storage rings, the counting statistics limits the investigations of the broad tails of the peaks, which result from the inner-shell electrons. Improvement of the statistics of the tails will not only help in the understanding of the changes of the inner-shell electrons, but also will help the unfolding of the data into contributions from each energy state.

While repeating of this analysis for other types of scattering problems is clearly beyond the scope of this Letter, the contours of constant scattering angle could be generally useful whenever extended targets are being used, regardless of the physical process being studied. In many cases their use may simplify the problem sufficiently to render the traditionally troublesome Monte Carlo techniques unnecessary. Finally, it is hard to avoid mentioning that by defining the axis of the geometry as the line from the source to the detector instead of the line from the source to the target, this approach offers a perception of scattering which is closer to the experimentalist view than the traditional one. While not necessarily offering practical benefits, this feature is nevertheless esthetically pleasing.

This research was supported in part by the Processes and Techniques Branch, Division of Chemical Sciences, Office of Basic Energy Sciences, U.S. Department of Energy, under Contract No. DE-AC02-76CH00016.

¹G. E. Gigante, L. J. Pedraza, and S. Sciuti, Nucl. Instrum. Methods B 12, 229 (1985).

²G. E. Gigante and S. Sciuti, Med. Phys. **12**, 321 (1985).

 3 G. Matscheko and R. Ribberfors, Nucl. Instrum. Methods A **255**, 326 (1987).

⁴M. J. Cooper, D. Laundy, D. A. Cardwell, D. N. Timms, R. S. Holt, and G. Clark, Phys. Rev. B **34**, 5984 (1986).

 ${}^{5}M$. V. Heller and J. R. Moreira, Phys. Rev. B **31**, 4146 (1985).

⁶W. A. Reed, P. Eisenberger, K. C. Pandey, and L. C. Synder, Phys. Rev. B 10, 1507 (1974).

 7 R. Tyk, J. Felsteiner, I. Gertner, and R. Moreh, Phys. Rev. B 32, 2625 (1985).

⁸A. L. Hanson, Nucl. Instrum. Methods A **264**, 471 (1988).

⁹G. A. Carlsson, C. A. Carlsson, K. F. Berggren, and R. Ribberfors, Med. Phys. 9, 868 (1982).

¹⁰D. R. Chipman and L. D. Jennings, Philos. Mag. B **49**, 127 (1984).