**X-ray Transmission in Cold Matter: Nonrelativistic
Correction^s for Compton Scattering**

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**X-RAY TRANSMISSION IN COLD MATTER:
NONRELATIVISTIC CORRECTIONS FOR COMPTON
SCATTERING**

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ABSTRACT

Obscuration by cold matter is frequently observed in a variety of X-ray sources. With the improved sensitivity and energy resolution of the new generation of X-ray detectors, such as those aboard *ASCA*, it may not always be possible to neglect electron scattering for column densities greater than $\sim 10^{23} \text{ cm}^{-2}$. We derive simple, approximate analytic expressions for a spherical geometry which enable the transmitted flux to be corrected for nonrelativistic Compton scattering. The method allows the use of arbitrary element abundances, photoelectric absorption cross-sections and input spectra and is computationally fast enough for use in a spectral fitting code. The approximations can be used for column densities up to $\sim 5 \times 10^{24} \text{ cm}^{-2}$. The maximum observed energy for which the approximations are valid depends on the column density and is $\sim 18.5 \text{ keV}$ for $N_H = 10^{23} \text{ cm}^{-2}$ and $\sim 10 \text{ keV}$ for $N_H = 5 \times 10^{24} \text{ cm}^{-2}$. The model provides a significantly improved description of the transmitted spectrum compared to the usual model in which only photons that have not interacted with the medium are included. An important consequence of neglecting electron scattering in absorbed sources is the observation of an apparent soft excess which could mistakenly be attributed to a different physical origin.

Subject headings: radiative transfer – scattering – galaxies: active – X-rays: general

treated more carefully. *ASCA* operates in the bandpass $\sim 0.5 - 10$ keV and has an energy resolution at 6 keV which is as high as $\sim 2\%$. We shall see that even for column densities of the order of $\sim 10^{23}$ cm $^{-2}$, approximating the X-ray transmission with only the uncollided flux (i.e. that which escapes without interacting with the medium) may be inadequate to model *ASCA* data with good signal-to-noise.

Now, the procedure of spectral fitting X-ray data with any model and deriving confidence regions of model parameters involves folding the model through the instrument response many hundreds of times. Numerical solution of the transfer equation or Monte Carlo simulations are not suitable for such a process. In principle one could generate grids of model solutions once and for all and interpolate on the model parameters. However, this is impractical for two reasons. Firstly, one frequently needs to allow the element abundances in the obscuring matter to be free parameters. Secondly, Compton scattering may be important for moderate to high energy resolution X-ray data. For example, photons at 7.1 keV the Fe-K edge threshold, could be down-shifted in only one Compton scattering from an energy as high as $7.1[1 + 7.1(2/511)] = 7.3$ keV. This shift is larger than the energy resolution of *ASCA* at these energies which is ~ 140 eV. For Thomson depths greater than unity, multiple scattering becomes important, smearing absorption edges even more. Thus the proper treatment of Compton scattering means that the transmitted continuum now depends on the shape of the input spectrum, making 'grid models' even more impractical.

In this paper we treat Compton scattering in the nonrelativistic limit using a discretized scattering probability approach, described in §2. Essentially, the probability distribution for photons to be scattered n times is replaced by a single, energy-weighted mean probability. The problem is then reduced to computing the escape functions which determine the fractions of photons escaping for each order of scattering. In §3 Monte Carlo simulations are used to find the nonrelativistic escape functions for a cold, spherical, uniform distribution

1. The Problem

X-ray absorption by cold material is a common phenomenon in low-luminosity Seyfert 1 galaxies (e.g. Turner & Pounds 1989; Warwick *et al.* 1993) and more so in Seyfert 2 galaxies (e.g. Awaki *et al.* 1991). An equivalent neutral Hydrogen column density (N_H) as large as $\sim 1 - 2 \times 10^{23} \text{ cm}^{-2}$ has been inferred in some Seyfert 1s (e.g. Warwick *et al.* 1993). Larger columns have been measured for Seyfert 2s, often pushing towards 10^{24} cm^{-2} (e.g. Awaki *et al.* 1991). X-ray absorption is also observed in X-ray binaries, in particular wind-fed X-ray pulsars which are found to have N_H in the range $\sim 10^{23} - 10^{24} \text{ cm}^{-2}$ (see White, Nagase and Parmar 1995, and references therein). Conventionally, X-ray data are compared with a very simple model of X-ray transmission in cold material. Usually, the effect of electron scattering in the medium is neglected and the ratio of transmitted to incident flux at an energy E is simply computed as $e^{-\sigma_{\text{abs}}(E)N_H}$. Here $\sigma_{\text{abs}}(E)$ is the photoelectric absorption cross-section as given, for example, in Morrison & McCammon (1983). Sometimes the transmission ratio is modified to $e^{-(\sigma_{\text{abs}}(E)+1.2\sigma_T)N_H}$ where σ_T is the Thomson cross-section. The idea here is that all photons which encounter electrons in the medium are scattered out of the line-of-sight and never observed. This effectively ignores all photons which escape after one or more scattering in the medium. In general, the scattered photons have a different spectrum to those which escape without scattering, *even if the scattering is elastic*, because the competition between absorption and scattering is energy-dependent. In the past these models have been adequate because proportional counters, with their limited sensitivity and energy resolution were incapable of distinguishing between models calculated with the transfer of radiation treated correctly (taking due account of the geometry of the obscuring medium) and models which ignore the escape of scattered radiation. However, with the advent of the superior sensitivity and spectral resolution of ASCA (see Tanka, Inoue and Holt 1994) and future X-astronomy missions, the radiation transfer needs to be

of matter illuminated by a central isotropic X-ray source. The escape functions are then fitted with simple analytic expressions. In §4 it is shown how the results can be used to calculate the transmitted spectra for arbitrary element abundances, photoelectric absorption cross-sections and input spectra.

2. The Escape Functions

The probability that a photon with initial energy E will escape the sphere without any interaction with the matter is

$$P_0 = e^{-\tau_0} \quad (1)$$

where τ_0 is sum of the scattering plus absorption cross-sections:

$$\tau_0 = \tau_s + \sigma_{\text{abs}}(E)N_H \quad (2)$$

and $\tau_s = 1.2\sigma_T N_H$. The fraction of photons, $1 - P_0$, which do not escape, interact with the medium and of these, a fraction λ_0 are scattered and $1 - \lambda_0$ are absorbed. Here λ_0 is the initial single-scattering albedo:

$$\lambda_0 = \tau_s / \tau_0 \quad (3)$$

A photon which is scattered will be down-shifted in energy so that its albedo continually decreases upon each scattering as it traverses the medium. The maximum energy shift per scattering is $\Delta E_{\text{max}} = E[1 + (m_e c^2 / 2E)]^{-1}$ and in terms of the dimensionless wavelength, $y \equiv m_e c^2 / E$, the maximum increase in wavelength is $\Delta y = 2$. In general, photons which

have been scattered n times will have some distribution in wavelength space, $F_n(y_{\text{obs}}, y)$, where we use the notation y_{obs} and E_{obs} to refer to observed quantities (i.e. after scattering). See for example, Burigana (1995) for expressions for the F_n . Here we give only the first (no relativistic) one:

$$F_1(y_{\text{obs}}, y) = \frac{3}{8}[1 + (y_{\text{obs}} - y - 1)^2]. \quad (4)$$

Note that the mean wavelength shift per scattering is unity and this corresponds to an energy shift $\Delta E_M = E[1 + (m_e c^2/E)]^{-1}$ which at 5, 10 and 20 keV is $\sim 0.05, 0.19$ and 0.75 keV respectively. The mean energy shift at 5 keV is already less than half the resolution of *ASCA* and becomes progressively smaller at smaller energies. Now, a group of photons which have been scattered n times will have a distribution in their albedo, $\lambda(E_{\text{obs}})$. But let's suppose that they can be well-represented by their weighted mean albedo, which can be computed from their initial energy, E :

$$\lambda_n(E) = \int_y^{y+2n} \lambda_0(m_e c^2/y') F_n(y', y) dy'. \quad (5)$$

Of the photons which are scattered once, a fraction, say G_1 , of them will escape from the medium. The fraction escaping after exactly one scattering is then $P_1 = \lambda_0[1 - P_0]G_1$. The fraction of photons remaining in the medium which have not escaped or been absorbed is $\lambda_0[1 - P_0](1 - G_1)$ and a fraction λ_2 of these are scattered a second time and of these a fraction, say G_2 , will escape. In this way the fraction of photons escaping after exactly n scatterings can be written in terms of the escape functions, G_n :

$$P_n = \left[\prod_{i=0}^{n-1} \lambda_i - \sum_{j=0}^{n-1} P_j \prod_{i=j}^{n-1} \lambda_i \right] G_n \quad (6)$$

The functions G_n depend on the spatial distribution of scattering centers after each

scattering and this depends on the total optical depth and geometry of the medium. Our approach will be to determine the G_n from Monte Carlo simulations and express them in terms of elementary functions. Then, supposing the initial X-ray spectrum is given by $N_i(E)$ photons $\text{cm}^{-2} \text{s}^{-1} \text{keV}^{-1}$, the transmitted spectrum consisting of photons which have undergone exactly n scatterings in the medium is

$$N_n(E_{\text{obs}}) = \frac{m_e^2 c^4}{E_{\text{obs}}^2} \int_{y_{\text{obs}} - 2r}^{y_{\text{obs}}} P_n(m_e c^2/y, \tau_s) F_n(y_{\text{obs}}, y) N_i(m_e c^2/y) y^{-2} dy. \quad (7)$$

Now the total spectrum can be computed, consisting of the uncollided flux and the flux from each order of scattering:

$$N(E_{\text{obs}}) = N_i(E_{\text{obs}}) e^{-\tau_0} + \sum_1^{n_{\text{max}}} N_n(E_{\text{obs}}). \quad (8)$$

Practical values of n_{max} are discussed in §4.

3. Analytic Forms For The Escape Functions

We perform Monte Carlo simulations to find the escape functions. Each run injects between 2×10^4 and 2.5×10^7 monoenergetic photons with initial energy E , at the center of a uniform sphere with radial column density N_H . In each case the statistical error on the fraction of photons escaping after only one scattering is always less than 15% and in most cases much better than 1%. Each photon is assigned an initial weight and a record is kept of the fraction of this weight which escapes after n scatterings until the weight in the medium drops below 10^{-7} of the initial value and the photon path is terminated. The cut-off weight determines the maximum number of scatterings which can be treated and is small enough to include more scatterings than are necessary for the level of accuracy we are

interested in. Higher order scatterings which have a statistical error on the escape fraction greater than 15% will not be used in the subsequent analysis. Standard photoelectric absorption cross-sections with cosmic abundances are assumed in these runs (Morrison and McCammon 1983) although the final results are expressed in such a way that arbitrary photoelectric absorption cross-sections can be used. The Thomson scattering cross-section is used and calculations are made for 30 initial energies between 1–20 keV (12 values between 7–8 keV in order to treat the Fe-K edge correctly) and 16 values of N_H in the range 10^{23} cm^{-2} to $5 \times 10^{24} \text{ cm}^{-2}$. At 20 keV relativistic effects are already setting in. The total Klein-Nishina cross-section is $\sim 93\%$ of the Thomson cross-section and the differential Klein-Nishina cross-section for back-scattering is $\sim 86\%$ of the nonrelativistic value. Below 1 keV the absorption optical depth becomes so large that in practice very few photons will be observed, or else a different, unabsorbed, X-ray emission component will already dominate the spectrum at low energies. Finally, for later use, an additional set of runs is made for 1 keV with all absorption opacities set to zero. For this case of pure scattering, $\lambda_0 = \lambda_n = 1$. Further details of the Monte Carlo method can be found in Pozdnyakov, Sobol and Sunyaev (1983).

We take the P_1 from the Monte Carlo simulations and form the functions G_1 given by equation 6. We find that the results can be well-fitted by

$$-\ln G_1 = a \ln \tau_s + b \tau_s^c \quad (9)$$

where the coefficients a , b , and c are given as follows,

$$a = \ln (2.4202 - 0.9685 \ln [-\ln \lambda_1]) \quad (10)$$

for $\lambda_1 \leq 0.0594$ and

$$a = 0.4849 \exp(-\lambda_1/0.1778) \quad (11)$$

for $0.0594 < \lambda_1 \leq 1.0$.

$$b = \exp[1.5247 - 0.09511 \ln \lambda_1 - 1.8356 \lambda_1^{0.6775}] \quad (12)$$

for $\lambda_1 \leq 0.576$ and

$$b = \exp[-0.1417 - 0.8261 \ln \lambda_1] \quad (13)$$

for $0.576 < \lambda_1 \leq 1.0$. Finally,

$$c^{-1} = 1.0873 - 0.09148 \lambda_1 + 2.4425 \exp(-\lambda_1/0.157) \quad (14)$$

for $0.0 \leq \lambda_1 \leq 1.0$. Now P_1 can be easily computed as

$$P_1 = \lambda_0 (1 + c^{-1}) \tau_s^{-n(\lambda_1)} \exp[-b(\lambda_1) \tau_s^{c(\lambda_1)}]. \quad (15)$$

Figure 1 illustrates how well equation 15 reproduces the Monte Carlo results. The agreement between the Monte Carlo results and analytic approximations is better than 5% in most cases and never more than 15% and 20% for $N_H \leq 10^{24} \text{ cm}^{-2}$ and $N_H \leq 5 \times 10^{24} \text{ cm}^{-2}$ respectively.

For the second and higher order scatterings we express the G_n in terms of G_1 as

$$G_n = G_1 (1 + \exp[f(\tau_n)]) \quad (16)$$

and find that, using the Monte Carlo results for all energies, good fits are obtained with

$$f(\tau'_n) = \alpha_n + \beta_n e^{-\tau'_n/\gamma_n} + [0.25 + 0.75 e^{-\tau'_n/\gamma_n}] \ln \tau'_n \quad (17)$$

where

$$\tau'_n = \frac{\tau_s \lambda_{n-1}}{\lambda_0 \lambda_{n-2}} \quad (18)$$

and the constants α_n , β_n and γ_n for $n = 2$ to 9 are given in Table 1. For $n > 9$ good results are obtained by setting $G_{n>9} = G_9$ because after many scatterings the spatial distribution of scattering centers does not change much after each scattering. The P_n can be calculated from the G_n using equation 6. It is important to bear in mind that the P_n are *not* explicitly normalized to unity. The accuracy with which the above prescription reproduces the Monte Carlo results is discussed in §4. Figure 2 compares the P_n calculated this way with the Monte Carlo results, at 20 keV (corresponding to $\lambda_0 \sim 0.83$ for cosmic abundances). Note that for initial values of the albedo, $\lambda_0 > 0.83$, and $\tau_s > 1$, the approximations begin to break down. For the extreme case of pure scattering ($\lambda_0 = 1$), and $\tau_s \leq 1$ the reproduction of the Monte Carlo results is better than 16%.

4. Spectra

First we consider the range of validity of the model for cosmic abundance matter. Since we have not allowed initial energies > 20 keV (§3), the maximum observed energy of data which can be modelled is $20/[1 + 40(n_{\max}/m_e c^2)]$ keV where $n_{\max}$ is the maximum number of scatterings considered. One needs to determine how accurately the spectrum needs to be computed for a given column density. This can be done by examining the fractional

increase in the number of transmitted photons due to the n th scattering, $\Delta_n \equiv P_n / \sum_0^{n-1} P_j$. Now Δ_n increases with N_H and with energy, as scattering becomes more important. For $N_H = 5 \times 10^{24} \text{ cm}^{-2}$ we find $n_{\text{max}} = 12$ in order that Δ_n is less than 1% for photons with an initial energy of 20 keV and this translates to an observed energy upper limit of ~ 10 keV. Typically, observed column densities are in the range $\sim 10^{23} - 10^{24} \text{ cm}^{-2}$ so in most cases one need only consider between 1 and 5 scatterings to achieve $\Delta_n \sim 1\%$. For $N_H = 10^{23} \text{ cm}^{-2}$ the approximations can be used up to ~ 18.5 keV. At low energies, below a few keV, depending on the data quality, one could neglect energy shifts in reconstructing the spectra from the P_n , further increasing computation speed. The effect of increasing element abundances is to decrease the albedo at a given energy so that multiple scattering becomes less and less important. The converse is true for decreasing element abundances.

We can estimate the accuracy of the calculated spectra with respect to the Monte Carlo results by examining the ratio of the quantity $\sum_0^{n_{\text{max}}} P_j$ obtained from the Monte Carlo runs and the analytic approximations. We find that the agreement is better than $\sim 3\%$ for $N_H < 10^{24} \text{ cm}^{-2}$ and $\lambda_0 > 0.18$ but never worse than 16% for λ_0 as small as 3.3×10^{-3} . In the wider regime corresponding to $3.3 \times 10^{-3} \leq \lambda_0 \leq 0.83$ and $N_H < 5 \times 10^{24} \text{ cm}^{-2}$, the agreement is never worse than 19%. Figure 3 (solid curves) shows the transmitted spectra for an input power-law spectrum, $N_i(E) = E^{-1.7}$ photons $\text{cm}^{-2} \text{ s}^{-1} \text{ keV}^{-1}$, using the method of equations 7 and 8, for $N_H = 10^{23} \text{ cm}^{-2}$, 10^{24} cm^{-2} and $5 \times 10^{24} \text{ cm}^{-2}$ with cosmic abundances. At each energy successive scatterings have been included until the change in flux is $< 1\%$. For comparison, the dashed curves show the uncollided spectra only and the dotted curves show the once-scattered spectra. It can be seen that using only the uncollided spectrum can result in an apparent soft excess even for $N_H = 10^{23} \text{ cm}^{-2}$. At 1 keV the observed flux is orders of magnitude above the uncollided flux. This is important because such a soft excess may mistakenly be interpreted as having a different physical origin or be spectrally confused with a genuine soft emission component if one exists. Finally, it should

be remembered that the P_n and the scattered spectra and therefore the apparent size of the soft excess are geometry-dependent. However, the same method given here can be applied to any geometry.

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TABLE 1
Parameters For The 2nd To 9th Compton Scatterings

n	α_n	β_n	γ_n
2	-0.50	-2.60	5.7
3	0.70	-3.50	5.9
4	1.15	-3.75	5.9
5	1.40	-4.00	5.9
6	1.65	-4.25	5.9
7	1.72	-4.32	5.9
8	1.80	-4.45	5.9
9	1.90	-4.55	5.9

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Figure Captions

Figure 1

(a) Monte Carlo calculations (crosses) of the fractions of photons escaping after only one scattering (P_1), having been injected isotropically at the center of a uniform, cosmic abundance sphere with radial column densities, N_H , of 10^{23} cm^{-2} and $5 \times 10^{23} \text{ cm}^{-2}$. The predicted fractions, P_1 , computed from equation 15 agree well with the Monte Carlo results (see text). The statistical errors for the Monte Carlo points are smaller than the symbols in most cases. (b) As (a) for $N_H = 10^{24} \text{ cm}^{-2}$ and $5 \times 10^{24} \text{ cm}^{-2}$.

Figure 2

A comparison of the escape probabilities, P_n , predicted by equations 6, 16, 17, and 18 (solid lines), with the Monte Carlo calculations (§3). From bottom to top, the filled circles correspond to $N_H = 10^{23} \text{ cm}^{-2}$, $5 \times 10^{23} \text{ cm}^{-2}$, and 10^{24} cm^{-2} . The crosses correspond to $N_H = 5 \times 10^{24} \text{ cm}^{-2}$. The initial energy of the photons is 20 keV (multiple scattering becomes less and less important for smaller energies). The statistical errors on the Monte Carlo points are smaller than the symbols.

Figure 3

The solid curves show transmitted spectra corrected for Compton scattering (using the method of equations 7 and 8) when the input spectrum is $E^{-1.7} \text{ photons cm}^{-2} \text{ s}^{-1} \text{ keV}^{-1}$, injected isotropically into a uniform, cosmic abundance sphere for three values of the radial column density. The spectra for $N_H = 10^{23} \text{ cm}^{-2}$, 10^{24} cm^{-2} and $5 \times 10^{24} \text{ cm}^{-2}$ include photons which have been scattered up to three, five and twelve times, respectively (see §4). Dashed curves show the transmitted spectra resulting from only uncollided photons (i.e. neglecting all escaping photons which have been scattered in the medium) and the dotted curves show the results of including only the first scattering.

Figure 1

Figure 2

Figure 3