A New Kinetic Equation for Compton Scattering

George B. Rybicki

Harvard-Smithsonian Center for Astrophysics

60 Garden Street, Cambridge, MA 02138 USA

ABSTRACT

A kinetic equation for Compton scattering is given that differs from the Kompaneets equation in several significant ways. By using an inverse differential operator this equation allows treatment of problems for which the radiation field varies rapidly on the scale of the width of the Compton kernel. This inverse operator method describes, among other effects, the thermal Doppler broadening of spectral lines and continuum edges, and automatically incorporates the process of Compton heating/cooling. It is well adapted for inclusion into a numerical iterative solution of radiative transfer problems. The equivalent kernel of the new method is shown to be a positive function and with reasonable accuracy near the initial frequency, unlike the Kompaneets kernel, which is singular and not wholly positive. It is shown that iterates of the inverse operator kernel can be easily calculated numerically, and a simple summation formula over these iterates is derived that can be efficiently used to compute Comptonized spectra. It is shown that the new method can be used for initial value and other problems with no more numerical effort than the Kompaneets equation, and that it more correctly describes the solution over times comparable to the mean scattering time.

Subject headings: atomic processes — radiation processes: general — radiative transfer

1. Introduction

The most fundamental approach to treating Compton scattering of photons from thermal electrons is to use a Boltzmann-like kinetic equation for the photon distribution function. The basic physics of the Compton process is incorporated into certain scattering functions, or kernel functions, that specify the probability of an initial photon scattering into various frequency and angular ranges. This Boltzmann equation gives highly accurate results, but
can also involve a heavy computational burden, especially when the number of scatterings is large.

The Boltzmann equation can be substantially simplified when certain conditions are met. Consider the case where the photons and electrons are both non-relativistic, so that \( h\nu/mc^2 \ll 1 \) and \( kT/mc^2 \ll 1 \). Here \( h \) is Planck’s constant, \( \nu \) is the photon frequency, \( m \) is the electron mass, \( c \) is the speed of light, \( k \) is Boltzmann’s constant, and \( T \) is the electron temperature. In this case the scattering kernel is relatively narrow in frequency. In fact the spreading is due to the thermal Doppler width is of order \( \Delta\nu \sim \nu \alpha^{1/2} \), where,

\[
\alpha = \frac{kT}{mc^2}.
\]  

When the width of the scattering kernel is small compared to the scale over which the radiation field changes substantially, it is possible to approximate the scattering terms in the Boltzmann equation by a second-order differential operator acting on frequency. Such approximate equations are generally called Fokker-Planck equations, but for Compton scattering the term Kompaneets equation is used, in honor of its originator (Kompaneets 1957). In its original form the Kompaneets equation applies strictly only to isotropic radiation fields, but since the Compton scattering process itself is not very anisotropic, the Kompaneets scattering term is often used with non-isotropic radiation fields, introducing some additional degree of approximation.

The Kompaneets equation has been a very useful tool for describing the process of Compton scattering from thermal electrons in astrophysics, when the conditions mentioned above are met. Second-order partial differential equations are much easier to handle numerically than full Boltzmann equations. Within its limitations the simple Kompaneets equation manages to incorporate a number of important physical properties and effects, namely,

2. Detailed balance (correct equilibrium solution).
3. The frequency spreading due to the thermal Doppler effect.
4. The frequency shift due to thermal Doppler effect (inverse Compton effect).
5. The frequency shift due to electron recoil (Compton effect).
The Kompaneets equation incorporates the first two properties exactly. The remaining effects are accurately represented only to lowest order in the parameters $h\nu/mc^2$ and $\alpha = kT/mc^2$.

For all its many positive features, however, the Kompaneets equation suffers from one major shortcoming: it is unable to treat cases where the radiation fields varies significantly on the scale of Compton frequency shifts, such as can occur in the neighborhood of spectral lines and continuum jumps. The usual approach in such cases has been to revert to the full Boltzmann equation, which contains the detailed scattering kernels, or to use a Monte Carlo method. The simplicity of the second order differential operator is thereby lost.

An entirely different approach to the treatment of Compton scattering was presented by RH, designed to apply to conditions typical in stellar atmospheres. Under these conditions the radiation fields change rapidly over the scale of the electron thermal frequency shift $\Delta \nu$ in the neighborhood of spectral lines and continuum edges. The method of RH handles such rapidly varying radiation fields in a numerically efficient way. An essential feature of the RH method is that it expresses the radiation field as a differential operator acting on the emissivity, not vice versa. This departure from the traditional Fokker-Planck type of operator leads us to call this an inverse operator method.

As originally formulated, the RH method incorporated only numbers 1 and 3 of the above physical effects, namely, photon conservation and the spreading due to the thermal Doppler effect. This was not a serious limitation when applied to normal stellar atmospheres, where these are the predominant effects. However, it seemed desirable for have a method that combined the advantages of the Kompaneets and RH equations, which then would be applicable to a much wider class of problems.

The purpose of this paper is to present such a new kinetic equation for Compton scattering, which (like the Kompaneets equation) incorporates all the physical effects 1–6 above, but which also (like the RH method) has the ability to treat rapidly varying radiation fields. While the idea for this new inverse operator method was motivated by the RH method, the derivation presented here is based on a simple alteration of the Kompaneets equation, which is considerably simpler than the approach used in RH. The new method is only accurate to first order in $h\nu/mc^2$ and $\alpha = kT/mc^2$, and it assumes that the scattering process can be well approximated by isotropic emission. However, since the Kompaneets equation itself has these same limitations, the new method cannot be judged inferior because of them.

From the standpoint of applications to stellar atmospheres, there are several advantages of the new kinetic equation. Like the Kompaneets equation, it now incorporates the processes of Comptonization of the radiation field and the Compton heating/cooling of the gas, which may be of importance in certain cases involving X-ray irradiation, for example. Another fea-
ture is that it satisfies detailed balance, and thus correctly describes the approach to thermal equilibrium. At the same time, like the RH method, it also can handle the distortion of the line profiles due to Doppler broadening due to scattering on the electrons. The numerical implementation of the method involves only a minor modification of the RH method, which essentially maintains the latter’s favorable timing requirements, namely proportional to the first power of the number of frequency points.

For problems other than stellar atmospheres, there are also advantages of the new method. For example, in studying Comptonization of X-rays, Lightman & Rybicki (1979a,b, 1980) wrote the solution to the transfer problem as a sum of products of probability of scattering $k$ times and the $k$-th iterated kernel function for Comptonization. As we shall see, the equivalent kernel function for the Kompaneets equation is not wholly positive and is highly singular, being a linear combination derivatives of delta functions up to order two. The “iterated” kernels would involve even higher derivatives, and any solution involving sums over such functions would be entirely unworkable. On the contrary, the kernel functions of the inverse operator method are quite normal functions, and their iterates can be found stably by numerical means, making the method of Lightman & Rybicki more practical.

In §2 the basic properties of the Kompaneets equation will be reviewed and the equations of the new inverse operator method will be derived. It is demonstrated that the inverse operator method, like the Kompaneets equation, satisfies all six of the properties listed above. A comparison with the RH method will be given. In §3 we discuss properties of a rather general Boltzmann equation and show how one may define the equivalent kernels of any approximate version of it. This is then done for the Kompaneets and inverse operator methods. Numerical results are presented for the inverse operator kernel, and its properties, including its accuracy, are discussed. In §4 iterates of the kernel function are defined and discussed, and numerical examples are given. In §5 a useful formula is derived that reduces certain summations occurring in the formalism of Lightman & Rybicki (1979a,b, 1980) to numerically tractable forms. In §6 it is shown how initial value problems can be treated using the inverse operator method. Numerical results show the advantages of the inverse operator method over the Kompaneets method for short times, of the order of the mean scattering time. In §7 a short review is given, and some possibilities for future work are discussed.
2. The Inverse Operator Method

For isotropic homogeneous radiation, the kinetic equation for Compton scattering can be written,

\[
\frac{1}{c} \frac{\partial n}{\partial t} = n_e \sigma_T (-n + e).
\]  

(2)

Here \( t \) is the time and the photon occupation number \( n = n(x, t) \) is a function of time and frequency, here given in terms of the scaled frequency \( x = h\nu/kT \). On the right hand side \( n_e \) is the electron density and \( \sigma_T \) is the Thomson cross section, which we assume is valid for the energies considered. Within the parenthesis the term \((-n)\) accounts for extinction and the term \(e = e(x, t)\) for the scattered emission.

The equation is completed by specifying a form for the scattering term \(e\). In the well-known Kompaneets equation (Kompaneets 1957; Rybicki & Lightman 1979, §7.6) this is given explicitly by,

\[
e = n + \alpha \frac{1}{x^2} \frac{\partial}{\partial x} \left[ x^4 \left( \frac{\partial n}{\partial x} + n + n^2 \right) \right].
\]  

(3)

This expression requires that the photon energy is small compared to the electron rest energy, \( h\nu/me^2 \ll 1 \), and that the thermal electrons are nonrelativistic, \( \alpha \ll 1 \). In addition, the radiation field \(n(x, t)\) must vary slowly with frequency \(x\) over the typical width of the scattering kernel, \(\Delta x \sim x\alpha^{1/2}\).

The equations of the new method are found as a simple alteration of the Kompaneets equation. The reversion of the functional relationship (3) between \(n\) and \(e\) is easily done to first order in \(\alpha\). Since \(e = n\) to lowest order, this may be used to replace \(n\) in the term multiplied by \(\alpha\), giving

\[
n = e - \alpha \frac{1}{x^2} \frac{\partial}{\partial x} \left[ x^4 \left( \frac{\partial e}{\partial x} + e + e^2 \right) \right].
\]  

(4)

This implicit equation for \(e\), combined with equation (2), represents our new formulation of Compton scattering.

The Kompaneets method and the new method differ significantly in how \(e\) is determined from \(n\). In the ordinary Kompaneets equation this is done by applying a differential operator to \(n\), as in equation (3). However, in the new method one solves a differential equation for \(e\), using equation (4). It might be characterized as applying to the radiation field the inverse of a certain operator related to the Kompaneets operator. For this reason we call this the inverse operator method.

The Kompaneets equation has the advantage that by substitution of equation (3) into equation (2) one obtains a single partial differential equation, which makes it much more
amenable to analytic treatment. In the inverse operator method one must deal with two separate equations, (2) and (4). However, we shall show below that for many problems this pair of equations is no more difficult to treat numerically than the Kompaneets equation.

The inverse operator method based on equation (4) has very different mathematical properties than the Kompaneets method. For example, if the radiation field \( n \) varies rapidly enough, application of the Kompaneets operator can lead to negative emission terms \( e \). This can be seen easily from the above equations. When the radiation field varies significantly on the scale of the frequency shift \( \Delta x \sim x^{\alpha^{1/2}} \), the second derivative term in the Kompaneets operator become of order \( \alpha^{-1} n \), so that the second term in equation (3) is no longer of order \( \alpha \), but is of order unity. The derivative terms, which can take either sign, are able to dominate the first, strictly positive, term. As we shall see below, the inverse operator method does not lead to such negative values of \( e \).

The manner of derivation of equation (4) automatically guarantees that it has the same order of accuracy in \( \alpha \) as the Kompaneets equation, and thus satisfies all the properties 3–6 above to order \( \alpha \). It can easily be shown that it \textit{exactly} satisfies the first two properties, namely, photon conservation and detailed balance.

To prove photon conservation, we multiply equation (4) by \( x^2 \) and integrate over all \( x \). The integrated derivative term vanishes at the endpoints, which gives,

\[
\int_0^\infty x^2 n \, dx = \int_0^\infty x^2 e \, dx. \tag{5}
\]

The photon density is proportional to

\[
\mathcal{N} = \int_0^\infty x^2 n \, dx. \tag{6}
\]

Multiplying equation (2) by \( x^2 \) and integrating over all \( x \), and using equation (5), then yields the photon conservation result, \( d\mathcal{N}/dt = 0 \).

Property 2, having the exact equilibrium solution, can be proved as follows. In equilibrium, \( \partial n/\partial t = 0 \), so by equation (3) we have \( n(x) = e(x) \). Substituting this into equation (4) and integrating once, using the fact that \( e(x) \to 0 \) strongly as \( x \to \infty \), we find,

\[
\frac{\partial n}{\partial x} + n + n^2 = 0. \tag{7}
\]

The general solution to this is the general Bose-Einstein distribution,

\[
n(x) = \frac{1}{e^{\gamma + x} - 1}, \tag{8}
\]
where the constant $\gamma$ is related to the chemical potential. This is the correct photon distribution for thermal equilibrium.

Thus we have shown that the inverse operator equation (4) has the same general properties 1–6 as the Kompaneets equation. Since the two equations differ only at an order of approximation beyond the validity of the Kompaneets equation itself, the inverse operator equation cannot be regarded a priori as inferior to the Kompaneets equation. As we shall show, the inverse operator equation is superior in some important respects.

We conclude this section by making contact with RH. In that work the mean intensity $J(\nu)$ and emission integral $E(\nu)$ based on the usual specific intensity were used. These are related to the quantities $n$ and $e$ by,

$$J(\nu) = \frac{2h\nu^3}{c^2} n(x), \quad E(\nu) = \frac{2h\nu^3}{c^2} e(x). \tag{9}$$

In terms of these variables, (4) becomes,

$$-\alpha\nu \frac{\partial}{\partial \nu} \left[ \nu \frac{\partial E}{\partial \nu} + \left( \frac{h\nu}{kT} - 3 \right) E + \frac{c^2 E^2}{2kT\nu^2} \right] + E(\nu) = J(\nu). \tag{10}$$

It is instructive to compare this to equation (25) of RH for $N = 1$, which in the present notation is

$$-\alpha\nu \frac{\partial}{\partial \nu} \left[ \nu \frac{\partial E}{\partial \nu} \right] + E(\nu) = J(\nu). \tag{11}$$

The new inverse operator method of equation (10) is seen to be a generalization of the RH method for $N = 1$ that includes extra terms involving first order derivatives of the radiation field. These extra terms will merely involve redefinitions of the coefficients of the second-order difference equations, so, from the numerical point of view, the new method is easily incorporated into the iterative solution scheme given in RH.

However, now, in addition to the treatment of Doppler broadening by scattering off thermal electrons, all the above Compton processes 1–6, including Compton heating/cooling, will be properly taken into account. The new method will now be applicable to a wider range of stellar atmosphere problems, including Comptonization of X-rays. In cases where the radiation should approach thermal equilibrium, this will occur correctly.

3. Associated Kernel Functions

Some understanding of the relationship between the Kompaneets method and the inverse operator method can be gained by comparison of the equivalent kernel functions associated
with each method. In this section we shall define these kernel functions and give some of their general properties. Then we shall derive explicit forms for them corresponding to the two methods.

The scattering process can be conveniently characterized by means of its kernel function, also called scattering function or redistribution function. This function determines the probability that an initial photon of given frequency and direction is scattered into a final photon of some other frequency and direction. For the simplest case of a homogeneous, isotropic radiation field (the case treated in this paper), the kinetic equation can be written,

$$\frac{1}{n_e \sigma T_c} \frac{\partial n}{\partial t} = \int \{ [1 + n(x)] K(x, x') n(x') - [1 + n(x')] \frac{x'^2}{x^2} K(x', x)n(x) \} dx'. \tag{12}$$

The kernel function is denoted by $K(x, x')$. The ratio $x'^2/x^2$, which ensures the conservation law for photons, has its origin in certain phase space factors in the derivation (see, e.g., Rybicki & Lightman 1978). Stimulated scattering is taken into account by the factors $1 + n$, which give rise to quadratic, as well as linear, terms in the radiation field.

The integral on the right side of equation (12) must vanish when the radiation field is in thermal equilibrium with the electrons, that is, when it is a Bose-Einstein distribution of the same temperature. The principle of detailed balance makes the stronger statement that, in thermal equilibrium, not only must the integral vanish, but the integrand itself must vanish frequency by frequency. That is,

$$[1 + n(x)] K(x, x') n(x') = [1 + n(x')] \frac{x'^2}{x^2} K(x', x)n(x), \tag{13}$$

for all $x$ and $x'$. Substituting the Bose-Einstein form (10) into this equation leads to the condition for detailed balance,

$$x^2 e^x K(x, x') = x'^2 e^{x'} K(x', x). \tag{14}$$

The kernel function does not depend on the radiation field $n$, so many of its general properties can be derived by considering radiation fields that are restricted in certain ways. In particular, it is very interesting to consider cases where $n \ll 1$, so that the quadratic terms in the equation can be ignored. The kinetic equation then becomes,

$$\frac{1}{n_e \sigma T_c} \frac{\partial n}{\partial t} = \int \left[ K(x, x') n(x') - \frac{x'^2}{x^2} K(x', x)n(x) \right] dx', \tag{15}$$

which is linear in the radiation field. Comparing this to equation (2) we have the general normalization property,

$$1 = \int \frac{x'^2}{x^2} K(x', x) dx'. \tag{16}$$
and the identification,
\[ e(x) = \int K(x, x')n(x') \, dx'. \] (17)

The kinetic equation can also be written,
\[ \frac{1}{n_e \sigma T_c} \frac{\partial n}{\partial t} = -n + \int K(x, x')n(x') \, dx'. \] (18)

The most significant distinction between the Kompaneets method and the new method presented here is found in the kernel functions associated with each. The kernel functions associated with each method are not immediately obvious, but there is a simple trick for determining them based on equation (17). After first changing the dummy variable of integration to \( x'' \) (say), we note that by substituting the special radiation field \( n(x) = \delta(x - x') \) into the integral, we obtain the kernel function \( e(x) = K(x, x') \), where \( x' \) is considered as a fixed parameter.

We shall now discuss these kernel functions, first for the Kompaneets equation, then for the new method.

3.1. The Kompaneets kernel

The Kompaneets equation is an approximation to the exact kinetic equation, which suggests the question, what is the equivalent kernel associated with the Kompaneets equation? This can be answered by comparing equation (18) to the Kompaneets equation without stimulated emission,
\[ \frac{1}{n_e \sigma T_c} \frac{\partial n}{\partial t} = \frac{\alpha}{x^2} \frac{\partial}{\partial x} \left[ x^4 \left( \frac{\partial n}{\partial x} + n \right) \right]. \] (19)

Using the trick given at the end of the previous section, The kernel function \( K_K(x, x') \) corresponding to this Kompaneets equation can be found by substituting \( n(x) = \delta(x - x') \) into equation (3), which gives,
\[ K_K(x, x') = \delta(x - x') + \frac{\alpha}{x^2} \frac{\partial}{\partial x} \left[ x^4 \{ \delta'(x - x') + \delta(x - x') \} \right]. \] (20)

Performing the differentiation, we can also write the Kompaneets kernel in the form,
\[ K_K(x, x') = (1 + 4\alpha x)\delta(x - x') + \alpha(x^2 + 4x)\delta'(x - x') + \alpha x^2\delta''(x - x'). \] (21)

This shows that the Kompaneets kernel is a linear combination of generalized functions, namely delta functions and derivatives of delta functions up to order 2, which keep it concentrated near the point \( x = x' \). In terms of a limiting process used to define the delta
function, such derivatives of delta functions take both positive and negative signs, and so in a real practical sense the Kompaneets kernel is not a completely positive function. This can also be verified by evaluating equation (17) for the Kompaneets kernel with a positive, but rapidly varying, function $n$, say a sufficiently narrow Gaussian, which will produce a result $e$ that can take negative values.

An important property of the kernel is its set of frequency moments, which characterize the frequency of the scattered photon relative to the frequency $x$ of the incident photon. These are defined as,

$$
\langle (x - x')^s \rangle = \int (x - x')^s \frac{x^2}{x'^2} K(x, x') \, dx,
$$

where $s = 0, 1, 2, \ldots$. The factor $x^2/x'^2$ is included to convert the kernel $K$ into the appropriate kernel for describing photon numbers, rather than occupation number. Substitution of the Kompaneets form for the kernel (20) and integration by parts, one obtains the general result,

$$
\langle (x - x')^s \rangle = \delta_{s0} + \alpha (4x' - x'^2) \delta_{s1} + 2\alpha x'^2 \delta_{s2}.
$$

In particular, we have,

$$
\begin{align*}
\langle (x - x')^0 \rangle &= 1, \\
\langle (x - x')^1 \rangle &= \alpha (4x' - x'^2), \\
\langle (x - x')^2 \rangle &= 2\alpha x'^2, \\
\langle (x - x')^s \rangle &= 0, \quad \text{for } s \geq 3.
\end{align*}
$$

The first of these is a simple restatement of the photon conservation law for scattering. The second and third give the results for the mean shift and variance of the emitted frequency relative to the incident frequency, respectively. These values for the moments are, of course, well known, and were used in the derivation of the Kompaneets equation. The above derivation simply verifies that the Kompaneets kernel we have obtained is consistent with these values.

The final result (27) states that all moments of order 3 or greater vanish. This is a consequence of the derivation of the Kompaneets equation, in which a Taylor series in the emitted frequency is only carried out up to second order, implicitly assuming that higher order moments would vanish.

### 3.2. The Kernel for the Inverse Operator Method

We have seen that the Kompaneets equation has an equivalent kernel that is a generalized function, containing up to second derivatives of delta functions. We now want to find...
the equivalent kernel for the inverse operator method for treating Comptonization. First of all the equation for the method will be written without the stimulated scattering terms, since, as we have seen, the kernel function can more easily be found for this purely linear equation. Dropping the $e^2$ term in equation (4) gives,

$$n = e - \alpha \frac{1}{x^2} \frac{\partial}{\partial x} \left[ x^4 \left( \frac{\partial e}{\partial x} + e \right) \right].$$

(28)

The kernel function determined by this equation will be denoted by $\tilde{K}(x, x')$. Applying the same trick as before, we set $n(x) = \delta(x - x')$ and $e(x) = \tilde{K}(x, x')$ in equation (28), which yields,

$$\delta(x - x') = \tilde{K} - \alpha \frac{1}{x^2} \frac{\partial}{\partial x} \left[ x^4 \left( \frac{\partial \tilde{K}}{\partial x} + \tilde{K} \right) \right].$$

(29)

That is, $\tilde{K} = \tilde{K}(x, x')$ is the Green’s function of the differential operator on the right hand side of equation (28).

It is actually possible to solve this equation analytically in terms of Bessel functions, but we omit details of this derivation. We only quote one analytic result for very small values of $\alpha$. Defining,

$$\mu = \left( \frac{9}{4} + \frac{1}{\alpha} \right)^{1/2},$$

(30)

the kernel is asymptotically,

$$\tilde{K}(x, x') \sim \frac{1}{2\alpha \mu} \left( \frac{x'}{x^3} \right)^{1/2} \exp\left( \frac{x'}{2x^2} \right) \left( \frac{x<}{x>} \right)^\mu.$$  

(31)

Here $x_>$ and $x_<$ denote the larger and smaller of $x$ and $x'$, respectively. Because $\mu \sim \alpha^{-1/2} \gg 1$, the last factor dominates the behavior of the kernel, making it very sharply concentrated about $x = x'$. By virtue of the slowly varying factors $(x'/x^3)^{1/2} \exp[(x' - x)/2]$, this approximate form of the kernel still obeys the detailed balance relation (14).

When the kernel is sufficiently sharp, one may set $x = x'$ in the slowly varying factors. Taking into account the differing notations, the kernel (30) then reduces to the form of the kernel given in equation (17) of RH for $N = 1$, showing again the relation of the inverse operator method to RH.

It is of great practical interest here, as it was in RH, that the scattering function $e$, or the kernel function $\tilde{K}$, is the solution of a second-order differential equation, (28) or (29), respectively, since these are easily solved numerically. The numerical solution begins with
the introduction of a frequency grid of $N_x$ points. Using an obvious matrix notation over the frequency space, the Kompaneets relation (3) becomes,

$$e = (1 + \alpha T)n,$$

(32)

where $1$ is the unit matrix and $T$ is a tridiagonal matrix formed from coefficients of the discretization of the second-order differential operator.

Similarly, the inverse operator relation (4) becomes,

$$n = (1 - \alpha T)e,$$

(33)

which can be solved for $e$ in terms of $n$,

$$e = (1 - \alpha T)^{-1}n.$$

(34)

Comparison of equations (32) and (34) should again make clear why we call this an “inverse operator” method. The numerical inversion of a tridiagonal system of equations is quite rapid, with timing of order $N_x$. This is the same order as the multiplication of a tridiagonal matrix times a vector, so that the numerical burden associated with the new operator for many applications is of the same order as that of the Kompaneets operator.

The inverse operator kernel is similarly found by discretization of equation (29), giving,

$$D = (1 - \alpha T)\tilde{K}.$$

(35)

Here $D$ is a discrete matrix version of the delta function $\delta(x - x_0)$; most simply it is a diagonal matrix with diagonal elements equal to the inverse of the local frequency differences. Equation (35) can be solved column by column in order $N_x^2$ operations to give the complete inverse,

$$\tilde{K} = (1 - \alpha T)^{-1}D.$$

(36)

If the kernel is only wanted for a few values of $x_0$, the number of operations is correspondingly smaller.

In figure 1 results for the inverse operator kernel function $\tilde{K}(x, x_0)$, obtained numerically in the above way, are plotted as the solid curves for $\alpha = 10^{-3}$ and for values of $x_0 = 0.1, 1,$ and 10. The normalizing factor $(x^3/x_0^2)$ is chosen to give equal areas under all the curves. Results for the asymptotic results (30) are also plotted as solid curves, but these are so close as to be indistinguishable. As expected, the kernel is skewed towards larger (smaller) values of $x$ for $x_0 \ll 1 (x_0 \gg 1)$, expressing the tendency for the radiation to approach thermal equilibrium. This can be seen most clearly for the $x_0 = 10$, less so for $x_0 = 0.1$. 
In order to get some idea of the absolute accuracy of the inverse operator results, we compare them to an expansion of the true kernel to third order in $\alpha$ given by equation (19) of Sazonov & Sunyaev (2000). These results are plotted as dashed curves in figure 1. These show that the relative errors in the inverse operator are less than 20% in a central region of the kernel about $x_0$, which extends out to values of frequency $x$ where the kernel itself falls to a few percent of the central value. Beyond this central region the relative errors increase rapidly, since the true kernel decays faster than any power law. However, we remark that the absolute errors outside the central region are actually quite small. More extensive comparisons show that the above errors are characteristic of all the cases for which $\alpha \leq 10^{-3}$ and $x/x_0 \leq 10$.

One can imagine cases where the large relative errors outside the central region could be a problem, for instance, for accurately describing the wings of a Compton-broadened line far away from line center. However, it is not common for the kernel to appear in such pure form, and more typically the small absolute errors in the kernel will cause lesser problems when integrations over frequency are done; recall that the kernel does have the proper frequency moments up to second order.

The errors in the inverse operator kernel are larger when $\alpha > 10^{-3}$, where additional relativistic corrections, omitted in the Kompaneets equation, begin to be important. The errors are also larger when $x_0 \gtrsim \alpha^{-1/2}$, since the dispersion associated with Compton recoil is not treated adequately by the Kompaneets equation, as first discussed by Ross et al. (1978). However, the Kompaneets equation suffers from the same problems in these regimes.

The inverse operator kernel shares some important properties with the exact kernel: It is positive and has roughly the right shape in the central regions, including the characteristic discontinuity of slope for $x = x_0$. Given that no physics beyond the Kompaneets equation has been assumed, even the modest accuracy of the inverse operator kernels seems most fortuitous, especially as the Kompaneets kernel itself is singular and not wholly positive.

4. Iterated kernels

A concept that often proves useful in practice is that of iterated kernels. The physical interpretation of equation (17) is that the kernel function $K(x, x')$ describes how photons of initial frequency $x'$ are redistributed to other frequencies $x$ after one scattering. The distribution after two scatterings is described by a function $K_2(x, x')$, clearly given by,

$$K_2(x, x') = \int K(x, x'')K(x'', x') dx'' , \quad (37)$$
and, more generally, after \( k > 2 \) scatterings, the distribution is described by a function \( K_k(x, x') \), which is defined by the recurrence,

\[
K_k(x, x') = \int K(x, x'') K_{k-1}(x'', x') \, dx''.
\] (38)

For convenience, the definition of iterated kernels may be extended to \( k = 1 \) and \( k = 0 \) by the formulas,

\[
K_1(x, x') = K(x, x'), \quad K_0(x, x') = \delta(x - x').
\] (39)

It follows that for any nonnegative \( k \) and \( l \),

\[
K_{k+l}(x, x') = \int K_k(x, x'') K_l(x'', x') \, dx''.
\] (40)

These formulas may, in principle, be applied to the Kompaneets kernel (21). However, without working out the details, it is obvious that the \( k \)-th iterated kernel is highly singular, involving derivatives up to order \( 2k \) of delta functions, and is not wholly positive. Consequently, even for moderate values of \( k \) and relatively smooth functions, finding iterated Kompaneets kernels by the above recurrence relations will be impractical numerically.

For the inverse operator method, the iterated kernels, like the kernel itself, will be ordinary positive functions, which can be easily computed numerically. Using the discretization introduced above, we note that the iterated kernel for the inverse operator method can be expressed as the recurrence relation

\[
\tilde{K}_k = (1 - \alpha T)^{-1} \tilde{K}_{k-1}.
\] (41)

The application of the inverse of a tridiagonal matrix involves of order \( N_x \) operations, so the recurrence relation can be applied using of order \( N_x^2 \) operations. This is an order than the naive \( N_x^3 \) operations if full matrices were involved. If one only wants the \( k \)-th scattered emission,

\[
e_k(x) = \int \tilde{K}_k(x, x') n(x') \, dx',
\] (42)

then the iterative step,

\[
e_k(x) = \int \tilde{K}(x, x') e_{k-1}(x') \, dx',
\] (43)

can be formulated, in matrix language, as,

\[
e_k = \tilde{K} e_{k-1} = (1 - \alpha T)^{-1} e_{k-1},
\] (44)

which can be computed in order \( N_x \) operations.
The iterates of the kernels in figure 1 up to \( k = 5 \) have been computed in this fashion and are shown in figure 2. The discontinuity in slope of the kernel itself disappears after one iteration, and the higher iterates become broader and quite smooth. The bias towards approach to thermal equilibrium can be seen in the tendency for the higher iterates to move toward the central Wien frequency of \( x \sim 3 \).

Repeated application of equations (41) and (44) lead to the explicit forms,

\[
\tilde{K}_k = (1 - \alpha T)^{-k} D, \quad (45)
\]

and

\[
e_k = (1 - \alpha T)^{-k} e_0, \quad (46)
\]

in terms of powers of the matrix \((1 - \alpha T)^{-1}\).

5. A Summation Formula

Equation (46) is the basis of a formula we have found very useful for the computation of Comptonized spectra using the formalism of Lightman & Rybicki (1979a,b, 1980). Putting that formalism into the present notation, a spectrum \( s(x) \) is expressed as the sum,

\[
s(x) = \sum_{k=0}^{\infty} p_k e_k(x), \quad (47)
\]

where \( p_k \) is the probability of a photon in the spectrum having scattered \( k \) times before escaping. Again, in matrix form,

\[
s = \sum_{k=0}^{\infty} p_k e_k. \quad (48)
\]

It turns out that \( p_k \) can often be accurately expressed as the linear combinations of exponential terms of the form \( Az^{-k} \), where \( A \) and \( z > 1 \) are constants. We shall derive a formula for the spectrum associated with just one term, since the large-\( k \) behavior of \( p_k \) is often dominated by one term; examples of this can be found in Nishimura et al. (1986). In any case, by linear superposition, we can use the formula to find the spectrum due to a sum of such terms.

Thus we consider the exponential expression for \( p_k \),

\[
p_k = A z^{-k} = (1 - z^{-1}) z^{-k}, \quad (49)
\]
where for convenience we take \( A = (1 - z^{-1}) \) so that the \( p_k \) are normalized,

\[
\sum_{k=0}^{\infty} p_k = 1. \tag{50}
\]

The summation (48) for this choice of \( p_k \) and with equation (46) is,

\[
s = A \sum_{k=0}^{\infty} \left[ z^{-1}(1 - \alpha T)^{-1} \right]^k e_k = A \left[ 1 - z^{-1}(1 - \alpha T)^{-1} \right]^{-1} e_k, \tag{51}
\]

summing the geometric series. A slight rearrangement yields the desired formula,

\[
s = Ae_0 + Az^{-1}(1 - \alpha T - z^{-1})^{-1} e_0. \tag{52}
\]

The second term may be found as the solution of a tridiagonal system in order \( N_x \) operations, so the computation is very fast.

Examples of spectra computed using our summation formula are given in figure 3 for a source \( e_0(x) \) of soft photons, emitted in a Wien law of temperature \( T_0 = 10^4 \) K, which are Comptonized by scattering in a hot medium of temperature \( T = 10^7 \) K, making \( \alpha = 1.68 \times 10^{-3} \). The choice of normalizing factors here for \( s(x) \) makes the plot analogous to a \( \log \nu F_\nu \) vs. \( \log \nu \) plot, where \( F_\nu \) is the photon flux. The values of \( z \) are conveniently characterized by the parameter,

\[
y_{*} = \alpha / \ln z, \tag{53}
\]

which is a kind of overall “\( y \)-parameter” for the scattering process. To see this, we examine the limit where \( z \) is close to unity, so that \( \ln z \approx z - 1 \). But the mean number of scatterings is \( \langle N \rangle = \sum_k kp_k = (z - 1)^{-1} \) from equation (49), so that in the limit we have,

\[
y_{*} \sim \alpha \langle N \rangle, \tag{54}
\]

which is a typical definition for a \( y \)-parameter; see, e.g., Eq. 7.41a]RL. In figure 3, as the values of \( y_{*} \) range from 0.03 to 10, the spectrum changes from being nearly a Wien law at the initial \( 10^4 \) K temperature to being nearly a Wien law at the temperature \( 10^7 \) K of the Comptonizing medium. For values of frequency between these two Wien laws, one sees an approximate power law, which is originally steep, but which eventually becomes flat.

6. Initial value problems

In an initial value problem the radiation field is specified at an initial time, say \( t = 0 \), and the problem is to find its subsequent behavior as a function of frequency and time,
that is, given \( n(x,0) \), find \( n(x,t) \). In this section we shall describe the results of numerical solutions of initial value problems for the Kompaneets and the inverse operator methods for the spatially homogeneous case. This will help clarify some of the distinctions between the two methods.

For simplicity the stimulated scattering process will be neglected, so that the equations are linear. The prototypical initial value problem is to start with an initial radiation field concentrated at a single frequency \( x_0 \), so that \( n(x,0) = \delta(x - x_0) \). The discretized vector version of this initial function will be denoted \( \mathbf{n}_0 \). Any initial value problem can then be solved by linear superposition of such solutions.

It is convenient to replace \( t \) by the Compton y-parameter,
\[
y = \alpha \tau = \left( \frac{kT}{mc^2} \right) n_e \sigma_T c t,
\]
which measures time in units of the time for significant Comptonization to take place. Combining equations (2) and (3) and writing the result in matrix form, we then have,
\[
\frac{\partial \mathbf{n}}{\partial y} = \mathbf{Tn}.
\] (56)
This equation can be solved by the well-known Crank-Nicholson method. Introducing a discretization in \( y \) (time), indicated by a subscript \( j \), we write,
\[
\frac{\mathbf{n}_{j+1} - \mathbf{n}_j}{\Delta y} = \frac{1}{2} \mathbf{Tn}_j + \frac{1}{2} \mathbf{Tn}_{j+1}.
\] (57)
That is, we use a differencing scheme that is semi-implicit in time. This can be rearranged into the form,
\[
(1 - \Delta_0 \mathbf{T})\mathbf{n}_{j+1} = (1 + \Delta_0 \mathbf{T})\mathbf{n}_j,
\] (58)
where,
\[
\Delta_0 = \Delta y/2.
\] (59)

For the initial value problem we are given the radiation field \( \mathbf{n}_0 \) at \( y = 0 \), and we construct the \( \mathbf{n} \)'s at succeeding times by using (59) as a recurrence relation. Given the solution \( \mathbf{n}_j \) we evaluate the right hand side (this involves multiplying by a tridiagonal matrix) then solving the resulting equation for \( \mathbf{n}_{j+1} \) (this involves solving a linear system with tridiagonal matrix). Both operations involving tridiagonal matrices requires only \( N_x \) operations, so they are very rapid.

Now let us turn to the initial value problem using the inverse operator method. Using the same discretization, equations (2) and (4) become,
\[
\frac{\partial \mathbf{n}}{\partial y} = \alpha^{-1} [-\mathbf{n} + (1 - \alpha \mathbf{T})^{-1} \mathbf{n}] = (1 - \alpha \mathbf{T})^{-1} \mathbf{Tn}.
\] (60)
This can be differenced using the Crank-Nicholson method, as before, so that,

\[ \frac{n_{j+1} - n_j}{\Delta y} = \frac{1}{2} (1 - \alpha T)^{-1} T n_j + \frac{1}{2} (1 - \alpha T)^{-1} T n_{j+1}. \]  

(61)

After multiplication by \((1 - \alpha T)\), this can be rearranged into the form,

\[ (1 - \Delta_+ T) n_{j+1} = (1 + \Delta_- T) n_j, \]

(62)

where,

\[ \Delta_+ = \Delta y/2 + \alpha, \quad \Delta_- = \Delta y/2 - \alpha. \]

(63)

Equation (62) is a trivial modification of (58), the only change being the replacement of the two appearances of \(\Delta_0\) with \(\Delta_+\) and \(\Delta_-\) on the opposite sides of the equation. Thus the numerical method developed for the Kompaneets equation can be trivially adapted to solve the initial value for the inverse operator method, and it will be equally fast.

One distinction between the two methods is now apparent. For the Kompaneets equation, the time variable \(t\) and \(\alpha\) can be combined into a single variable, the \(y\)-parameter. This implies that all initial value problems starting from the same initial radiation field will have exactly the same evolution for different values of \(\alpha\), except for a simple rescaling of the time variable. For the inverse operator method, even using the \(y\)-parameter does not completely eliminate the dependence on \(\alpha\), as can be seen from equation (60), or from the fact that \(\alpha\) appears in the definitions of \(\Delta_+\) and \(\Delta_-\). This implies that the inverse operator method describes the solution not only on the time for significant Comptonization, but also on the typically much shorter mean free time for scattering.

An example of the numerical solution of initial value problems is shown in Figure 4. Here \(\alpha = 10^{-3}\), and the initial radiation field is a delta-function at the frequency \(x_0 = 10^{-2}\). The values of the \(y\)-parameter range from 0 to 4 in steps of 0.1. For the larger values of \(y\), the solution is seen to be converging to the Wien law, \((1/2)x^3 \exp(-x)\), shown as the dotted curve. Both the Kompaneets and the inverse operator results are plotted in figure 4, but for this set of \(y\) values the two solutions cannot be distinguished to plotting accuracy.

The discussion above suggests that the distinctions between the two methods will become manifest for times comparable to the mean free scattering time, \(t \lesssim (n_e \sigma_T c)^{-1}\), that is, when \(\tau \lesssim 1\) or \(y \lesssim \alpha\).

Figure 5 demonstrates that the behaviors of the two methods at relatively short times are indeed very different. The upper set of curves show the inverse operator results and the lower set the Kompaneets results. To avoid confusing overlapping curves, the times have been divided into two sets, \(\tau = 0.25\) to 1.5 in steps of 0.25 for the left panels (a), and \(\tau = 1.5\) to 15 in steps of 1.5 for the right panels (b). The initial radiation field \(n(x,0) = \delta(x - x_0)\)
with $x_0 = 10^{-2}$ has not been plotted here, but would have appeared as a vertical line in all plots.

For the inverse operator method, one component of the solution is clearly a remnant of the localized initial delta function. Immediately outside this, there is an extended component that increases with time until $\tau \sim 1.5$, then falls. The extended component originally has a noticeable discontinuity of slope at $x = x_0$, but eventually becomes smoother as it broadens.

This behavior of the inverse operator results is easily understood analytically. One shows by direct substitution that the solution to the time dependent equation (18) with $n(x,0) = \delta(x - x_0)$ can be written in terms of iterated kernels,

$$n(x,\tau) = \sum_{k=0}^{\infty} \frac{\tau^k e^{-\tau}}{k!} K_k(x, x_0).$$  \hfill (64)

For moderate times $\tau \lesssim 1$, we expect only a few terms of this series to contribute, so that

$$n(x,\tau) = e^{-\tau}\delta(x-x_0) + \tau e^{-\tau} K(x, x_0) + \ldots.$$  \hfill (65)

Thus, for the inverse operator method, we expect an early time behavior of a decaying delta function plus a rising contribution of the noniterated kernel, peaking at $\tau = 1$, then decaying away. The presence of the delta function expresses the fact that after a time $\tau$, some fraction (in fact, $e^{-\tau}$) of the photons have not yet scattered; in principle, this delta function never goes away, but in the numerical solution it eventually becomes negligible. The presence of the noniterated kernel can be recognized by the discontinuity in slope at $x_0$, but at later times this feature decays and disappears as further terms involving iterated kernels begin to dominate. This is precisely what is seen in the numerical solutions for the inverse operator method in the upper panels of figure 5.

Equation (64) is not a useful representation of the solution of the Kompaneets equation, due to the singular nature of the iterated kernels, so the preceding discussion is not applicable to it. The numerical solution of the Kompaneets shown in the lower panels of figure 5 never exhibits a trace of a delta function for $\tau > 0$, but rather shows quasi-Gaussian forms, which continually broaden and shift with time. For the largest time ($\tau = 15$) the results are virtually indistinguishable from those of the inverse operator method.

The coefficient of the iterated kernel in the representation (64), that is, $\tau^k e^{-\tau}/k!$, has the same form as the Poisson probability distribution, and for large $\tau$ (or large $k$) is sharply peaked about $k = \tau$. This suggests the large-$k$ asymptotic approximation to the iterated kernels,

$$K_k(x, x_0) \sim n(x, \tau = k),$$  \hfill (66)
where \( n(x, \tau) \) is the initial value problem with \( n(x, 0) = \delta(x - x_0) \). Indeed, this is essentially the basis of the method of Sunyaev & Titarchuk (1980), who used it to determine Compton spectra.

For small \( \tau \) the mixing of the different values of \( k \) in equation (64) is significant, and the approximation (66) is not so good. Nonetheless, Sazonov & Sunyaev (2000) suggested using equation (66) for \( k = 1 \) to define the approximate kernel,

\[
K_{SS}(x, x_0) = n(x, \tau = 1),
\]

which they call the “Kompaneets kernel.” This differs from our “Kompaneets kernel” \( K_K \), which is the true kernel of the Kompaneets equation, as given in equation (21). The kernel \( K_{SS}(x, x_0) \) does have the desired property that the \( k \)-th iterate of it is exactly equal to \( n(x, \tau = k) \), so it does give asymptotically accurate iterates through equation (66). However, we find that \( K_{SS} \) is not as accurate as the inverse operator kernel in the central regions, and it does not have the characteristic discontinuity of slope at \( x = x_0 \). In addition, \( K_{SS} \) is actually harder to compute than the inverse operator kernel, since it is defined by an integration of the time-dependent Kompaneets equation over a finite interval of time.

7. Summary and Discussion

We have demonstrated a simple modification of the Kompaneets method that maintains most of its desirable properties, but which has much better behavior at very short times, of order of the mean free scattering time. This inverse operator method has an equivalent kernel function that is positive and nonsingular, unlike that of the Kompaneets equation. The kernel function is roughly of the right shape in the central regions with an accuracy of about 20%. We have shown that for many applications the inverse operator method requires no more numerical effort than the Kompaneets equation.

We have shown how the iterated kernels of the inverse operator method can be efficiently computed numerically. A summation formula involving iterated kernels is given that reduces the effort in computing Comptonized spectra using the method of Lightman & Rybicki (1979a,b, 1980). We have shown that initial value problems can be solved using the inverse operator method with no more effort than the Kompaneets equation, but with noticeable improvement in the solution at times comparable to the mean scattering time.

In this paper there has been no attempt to advance beyond the physics of the Kompaneets equation. The main goal has been simply to point out the special advantages that occur when one reverses the role of the second order differential operator that connects the radiation field with the emission coefficient. However, in future work it would be desirable
to overcome some of the limitations of the inverse operator method, as others have done for the Kompaneets equation. There does not seem to be any reason to expect any difficulties in extending the present theory to anisotropic scattering or polarization.

It would be desirable to find ways to increase the accuracy of the inverse operator method. Obvious improvements would come with using higher order expansions of the coefficients in the parameters $\alpha$ and $h\nu/mc^2$, but this will not solve all of the accuracy issues.

More improvement might be gained by expressing the emission coefficient as a sum of $N > 1$ terms, as in RH. Alternatively, and more in keeping with the present approach, one could include higher order moments and derivatives in a Kramers-Moyal expansion (?, see, e.g., )][Riskin of the Boltzmann equation, and then use this to form new, higher order, inverse operators.

The present work has concentrated on one particular Fokker-Planck equation, the Kompaneets equation. However, the idea of using inverse operators clearly could be generalized and applied to other Fokker-Planck equations. Since each physical situation has its own special properties, it is not possible to predict whether an inverse operator approach would provide significant advantages in any particular case, but it might be worth investigating. An intriguing possibility is that higher order Kramers-Moyal expansions might have better properties when modified by the use of inverse operators, which perhaps might avoid some of the difficulties known to exist for the traditional expansions beyond the Fokker-Planck approximation (Pawula 1967).

The author wishes to thank Avi Loeb and Ramesh Narayan for useful discussions and comments on the paper.

REFERENCES


Nishimura, J., Mitsuda, K., & Itoh, M. 1986, PASJ, 38, 819


Fig. 1.— Kernel functions for $x_0 = 0.1$, 1, and 10, and for $\alpha = 10^{-3}$. The solid lines are the inverse operator kernels. The dashed curves are accurate approximations based on expansions of Sazonov & Sunyaev (2000).

Fig. 2.— Iterates $\tilde{K}_k(x, x_0)$ of the inverse operator kernels of figure 1 for $k = 1, \ldots, 5$. The narrowest curves are the noniterated kernels ($k = 1$). The iterates become broader as $k$ increases.
Fig. 3.— Comptonized spectra from a soft initial Wien source ($T_0 = 10^4$ K) scattering in a hot Comptonizing medium ($T = 10^7$ K) with simple model for the escape probability (see text). The solid curves, progressing from left to right, are for values of $y_\ast = 0.03, 0.1, 0.3, 1, 3,$ and 10. The Wien curves for $10^4$ K and $10^7$ K are shown as dotted on the left and right, respectively.
Fig. 4.— Solutions (solid) for the initial value problem with an initial delta-function at $x_0 = 10^{-2}$ (vertical line) and for $y = 0, 4(0.1)$. For large values of $y$ the solutions approach the Wien law (dotted). The Kompaneets and inverse operator solutions are virtually indistinguishable in this plot.
Fig. 5.— Short time behavior of the initial value problem with $\alpha = 10^{-3}$ and an initial delta-function at $x_0 = 10^{-2}$ for the inverse operator method (upper panels) and the Kompaneets equation (lower panels). Values of $\tau$ are (a): 0.25,1.5(0.25) for the left panels and (b): 1.5,15(1.5) for the right panels. Note the linear vertical scale here.